COMSOL
MULTIPHYSICS

CHEMICAL ENGINEERING
MODULE

MODEL LIBRARY

VERSION 3.4

COMSOL

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Chemical Engineering Module Model Library

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Introduction

The *Chemical Engineering Module Model Library* consists of a large number of models from various areas of chemical engineering. In particular, many of the examples come from the fields of unit operations, chemical reaction engineering, and transport phenomena.

Model Library Overview

The purpose of this Model Library is to assist you in learning, by example, how to model sophisticated chemical-engineering units, processes, and phenomena. Through them you can tap the expertise of top researchers in the field, examining how they approach some of the most difficult modeling problems you might encounter. You can thus get a feel for the power that COMSOL Multiphysics® offers as a modeling tool. In addition to serving as a reference, the models can also give you a head start if you are developing a model of a similar nature.

We have divided these models into nine chapters:

- Fluid Flow—Tutorials and Benchmarks
- Heat Transfer and Non-isothermal Flow—Tutorials and Benchmarks
- Multicomponent Transport—Tutorials and Benchmarks
- Mixers and Stirred Vessels
- Multiphase Flow
- Microfluidics
- Transport, Reactions, and Reaction Engineering
- Electrochemical Cells and Electrochemical Engineering
- Electrophoresis and chromatography

The first three chapters include tutorial and benchmark models that contain complete descriptions of the main phenomena captured by the Chemical Engineering Module—*transport phenomena*. The following chapters include examples from specific application areas and models that are made up of coupled systems of the three balances—*multiphysics*. In this Model Library you also find advanced models of, for example, multiphase flow and reaction-engineering applications, including coupling the Chemical Engineering Module to the COMSOL Reaction Engineering Lab®.

These models illustrate various chemical-engineering-specific application modes in the Chemical Engineering Module. These specialized application modes are not available in the base COMSOL Multiphysics package, and they come with their own user interfaces that make it quick and easy to access their power.

Note that the model descriptions in this book do not contain every detail on how to carry out every step in the modeling process. Before tackling these in-depth models, we urge you to first read another book in the Chemical Engineering Module documentation set. Titled the *Chemical Engineering Module User's Guide*, it introduces you to the basic functionality in the module, covers basic modeling techniques, and includes reference material of interest to those working in chemical engineering. The models that it presents are far simpler than those given in the Model Library and might be more appropriate for your first introduction to COMSOL Multiphysics.

Further information on how to work with the COMSOL Multiphysics graphical user interface can be gained from the *COMSOL Multiphysics User's Guide* or the *COMSOL Multiphysics Quick Start* manual. An explanation on how to model with a programming language is available in the *COMSOL Multiphysics Scripting Guide*.

This *Chemical Engineering Module Model Library* provides details about a large number of ready-to-run models that illustrate real-world uses of the module. Each entry comes with theoretical background as well as instructions that illustrate how to set it up. The models are written by our staff engineers, who have years of experience in chemical engineering. The terminology in the book should be familiar to you.

Finally, the software includes as loadable Model MPH-files (`.mph`) files all the examples in the *Chemical Engineering Module Model Library* as well as the *Chemical Engineering Module User's Guide*. Click the **Model Library** tab in the **Model Navigator** to find them under the chapter headings just listed. They are great to investigate if you are familiar enough with the COMSOL Multiphysics structure and user interface but still would like an idea on how to set up a certain model. You can even use them as a starting point for models that are similar.

Model Library Guide

The following table summarizes key information about the entries in the *Chemical Engineering Module Model Library* as well as the *Chemical Engineering Module User's Guide*. The solution time is the elapsed time measured on a machine running Windows Vista with a 2.6 GHz AMD Athlon X2 Dual Core 500 CPU and 2 GB of

RAM. For models with a sequential solution strategy, the Solution Time column shows the elapsed time for the longest solution step.

TABLE 1-1: CHEMICAL ENGINEERING MODULE MODEL LIBRARY

MODEL	**PAGE**	**APPLICATION MODES**	**SOLUTION TIME**	**1D**	**2D**	**3D**	**STATIONARY**	**TIME DEPENDENT**	**NONLINEAR**	**PARAMETRIC STUDY**
FLUID FLOW—TUTORIALS AND BENCHMARKS										
thermal decomposition	UG16	Navier-Stokes	35 s		√			√	√	
gravity tutorial	UG48	Weakly Compressible Navier-Stokes	3 s		√		√		√	
diverging duct	10	Navier-Stokes	5 s		√axi		√		√	
fuel cell stack*	18	Navier-Stokes	124 min			√	√		√	
non-newtonian flow	30	Non-Newt Flow	12 s		√axi				√	√
parallel plates	39	Navier-Stokes	3 s		√		√		√	
darcy 3d	46	Darcy’s Law	4 s			√	√		√	
porous free	57	Brinkman, Navier-Stokes	4 s		√		√		√	
bending pipe	65	k-ε Turbulence Model	7 min			√	√		√	
oscillating droplet	75	Navier-Stokes, Conv&Conduction	86 min		√axi			√	√	
turbulent backstep	87	k-ε Turbulence Model	5 min		√		√		√	
HEAT TRANSFER AND NON-ISOTHERMAL FLOW—TUTORIALS AND BENCHMARKS										
forced turbulent convection	98	Turbulent Fluid-Thermal	7 min		√		√		√	
slab	114	Conduction	1 s	√				√		
mems heat exchanger 3d	119	Conv&Conduction	9 s			√	√		√	
non-isothermal flow	129	Non-Isothermal Flow	16 s		√		√		√	
sinusoidal heat exchanger	142	Conv&Conduction, Navier-Stokes	2 min		√		√		√	
MULTICOMPONENT TRANSPORT—TUTORIALS AND BENCHMARKS										

TABLE 1-1: CHEMICAL ENGINEERING MODULE MODEL LIBRARY

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME DEPENDENT	NONLINEAR	PARAMETRIC STUDY
dialysis	152	Conv&Diffusion, Navier-Stokes, Diffusion	1 s		√		√		√	
stefan tube	164	Maxwell-Stefan	1 s	√			√		√	
maxwell stefan diffusion	173	Maxwell-Stefan	14 s		√		√		√	
MIXERS AND STIRRED VESSELS										
laminar static mixer	186	Conv&Diffusion, Navier-Stokes	28 min			√	√		√	
turbulent residence time 2d	197	k-ε Turbulence Model, Conv&Diffusion	49 s		√		√	√	√	
turbulent residence time 3d	197	k-ε Turbulence Model, Conv&Diffusion	34 min			√	√	√	√	
rotating disk	216	Swirl Flow	38 s		√axi				√	√
schematic pump	227	Rotating Navier-Stokes	10 min		√				√	
MULTIPHASE FLOW										
rigid body motion	236	Level Set	7 s		√			√	√	
rising bubble	243	Navier-Stokes, Conv&Diffusion	7 s		√			√	√	
boiling flow	255	Level Set Two-Phase Flow, Laminar, Conv&Conduction	36 min		√			√	√	
droplet breakup	270	Level Set Two-Phase Flow, Laminar	13 min		√			√	√	
bubble column	279	Bubbly Flow, Conv&Diffusion	3 min		√			√	√	
sedimentation	294	Mixture Model, k-ε Turbulence Model	6 min		√			√	√	
dense suspension	305	Mixture Model, Laminar PDE, General Form	7 min		√			√	√	

TABLE 1-1: CHEMICAL ENGINEERING MODULE MODEL LIBRARY

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME DEPENDENT	NONLINEAR	PARAMETRIC STUDY
MICROFLUIDICS										
biochip	320	Navier-Stokes, Conductive DC	4 s		√		√		√	
capillary filling	334	Level Set Two-Phase Flow, Laminar	149 min		√axi			√	√	
electrokinetic valve 2d	348	Electrokinetic Flow, Navier-Stokes, Conductive DC	6 s		√			√		
electrokinetic valve 3d	365	Electrokinetic Flow, Navier-Stokes, Conductive DC	9 min			√		√	√	
electroosmotic flow	389	Electrokinetic Flow, PDE General Form	10 s		√			√		
h cell	403	Navier-Stokes, Conv&Diffusion	58 s			√			√	√
TRANSPORT, REACTIONS, AND REACTION ENGINEERING										
fixed bed reactor	418	Conv&Conduction, Conv&Diffusion	8 s		√axi		√		√	√
falling film	433	Conv&Diffusion	2 min	√ps				√		
boat reactor	447	Navier-Stokes, Conv&Diffusion	5 s		√axi		√		√	√
monolithic reactor	461	Conv&Diffusion	2 s		√ps			√		
nox reduction	470	Navier-Stokes, Darcy's Law, Conv&Diffusion	7 s		√axi		√		√	
porous reactor	494	Navier-Stokes, Conv&Diffusion, Brinkman	45 s			√	√		√	
ELECTROCHEMICAL CELLS AND ELECTROCHEMICAL ENGINEERING										
chlor alkali	530	Conductive DC	1 s		√		√		√	

TABLE 1-1: CHEMICAL ENGINEERING MODULE MODEL LIBRARY

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME DEPENDENT	NONLINEAR	PARAMETRIC STUDY
mcfc	541	Conductive DC, Diffusion	3 s		√		√		√	
tumor	552	Nernst-Planck	14 s	√				√		
fc cathode	565	Conductive DC, Maxwell-Stefan, Darcy's Law	30 s			√	√		√	
pemfc	580	Conductive DC, Maxwell-Stefan, Darcy's Law	16 s		√		√		√	
serpentine	602	Navier-Stokes, Maxwell-Stefan	5 min			√	√		√	
ELECTROPHORESIS AND CHROMATOGRAPHY										
capillary electrophoresis 1	620	Electrokinetic Flow, PDE General Form	11 s	√				√		
capillary electrophoresis 2	620	Electrokinetic Flow, PDE General Form, Conv&Diffusion	2 min	√				√		
liquid chromatography 1	635	Conv&Diffusion	42 s	√				√		
liquid chromatography 2	635	Conv&Diffusion	4 min	√				√		
liquid chromatography 3	635	Conv&Diffusion	5 min		√			√		

*This model has been solved on a machine running Linux with an AMD64 processor and 12 GB of RAM.

Typographical Conventions

All COMSOL manuals use a set of consistent typographical conventions that should make it easy for you to follow the discussion, realize what you can expect to see on the screen, and know which data you must enter into various data-entry fields. In particular, you should be aware of these conventions:

- A **boldface** font of the shown size and style indicates that the given word(s) appear exactly that way on the COMSOL graphical user interface (for toolbar buttons in the corresponding tooltip). For instance, we often refer to the **Model Navigator**, which is the window that appears when you start a new modeling session in COMSOL; the corresponding window on the screen has the title **Model Navigator**. As another example, the instructions might say to click the **Multiphysics** button, and the boldface font indicates that you can expect to see a button with that exact label on the COMSOL user interface.

- The names of other items on the graphical user interface that do not have direct labels contain a leading uppercase letter. For instance, we often refer to the Draw toolbar; this vertical bar containing many icons appears on the left side of the user interface during geometry modeling. However, nowhere on the screen will you see the term “Draw” referring to this toolbar (if it were on the screen, we would print it in this manual as the **Draw** menu).
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** means: Open the **COMSOL Multiphysics** folder, open the **Heat Transfer** folder, and select **Conduction**.
- A `Code` (monospace) font indicates keyboard entries in the user interface. You might see an instruction such as “Type `1.25` in the **Current density** edit field.” The monospace font also indicates COMSOL Script codes.
- An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or in the Glossary. The names of books in the COMSOL documentation set also appear using an italic font.

2

Fluid Flow—Tutorials and Benchmarks

This chapter contains a selection of fluid flow models. Among the examples you find models of laminar and turbulent flow, non-newtonian flow and porous media flow. There is also a two-phase flow example that accounts for surface tension. All models within this chapter are simple and instructive, demonstrating how you can use the fluid flow application modes to model different kinds of isothermal fluid flow.

Pressure Recovery in a Diverging Duct

Introduction

When the diameter of a pipe suddenly increases, as shown in Figure 2-1, the area available for flow increases. A fluid with relatively high velocity decelerates into a relatively slow moving fluid. Depending on the Reynolds number, this can cause turbulence, and much of the excess kinetic energy converts into heat and is therefore wasted. If the change of the cross section is gradual, it is possible to recover the kinetic energy as pressure energy.

This example presents a qualitative study of the pressure-recovery phenomenon in a uniformly diverging duct. It also shows the implementation of the Navier-Stokes equations in cylindrical coordinates.

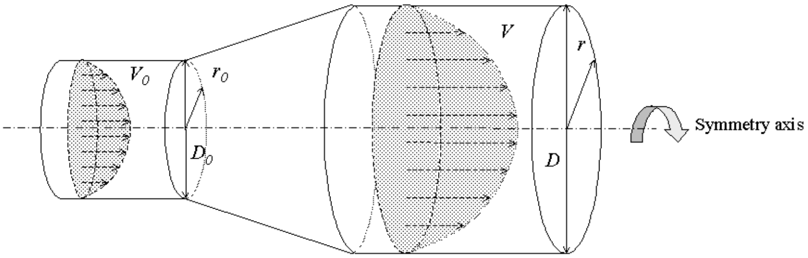


Figure 2-1: Geometrical representation of the modeling geometry.

Model Definition

The inlet condition is described by water flowing in a pipe with a diameter of 1 cm. The flow is laminar and has a fully developed laminar velocity profile, a so-called Hagen-Poiseuille profile. After 2 cm the water enters a uniformly diverging duct whose length is 5 cm and whose outlet diameter is 2 cm.

Because water is a Newtonian fluid and its density is constant at isothermal conditions, the Navier-Stokes equations combined with a continuity equation characterize the flow:

$$\begin{gathered}\eta\nabla^2\mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 \\ \nabla\cdot\mathbf{u} = 0\end{gathered} \tag{2-1}$$

Here η denotes the dynamic viscosity (Pa·s), **u** represents the velocity (m/s), ρ gives the fluid density (kg/m^3), and p denotes the pressure (Pa). The model becomes axisymmetrical and can be described in the r and z coordinates.

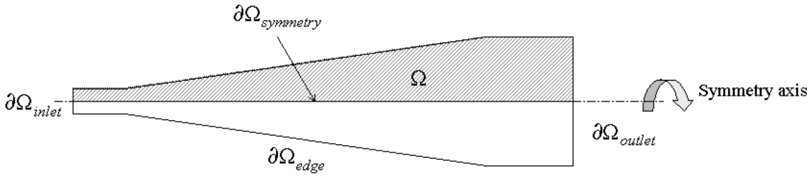


Figure 2-2: Simplification of the modeling geometry showing the symmetry axis and boundary labels.

The following equations describe the relevant boundary conditions at the symmetry axis, the outlet, the inlet, and the edge (wall) respectively:

$$\begin{aligned} \mathbf{n}\cdot\mathbf{u} &= 0 && \text{at } \partial\Omega_{\mathrm{symmetry}} \\ \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} &= \mathbf{0}, p = 0 && \text{at } \partial\Omega_{\mathrm{outlet}} \\ \mathbf{u} &= \left(0, v_{\mathrm{max}}\left(1 - \left(\frac{r}{R}\right)^2\right)\right) && \text{at } \partial\Omega_{\mathrm{inlet}} \\ \mathbf{u} &= (0, 0) && \text{at } \partial\Omega_{\mathrm{edge}} \end{aligned} \tag{2-2}$$

In these equations, for each boundary point **n** is the normal vector and **t** is any tangential vector, Furthermore, v_{max} is the maximum flow speed in the axial direction and R is the pipe radius at the inlet. The analytical expression above provides the velocity distribution at the inlet, a parabolic Hagen-Poiseuille profile.

Results

Figure 2-3 clearly shows that the velocity vector magnitude decreases as the cross-sectional area for the flow increases. You can additionally see the velocity vector itself by introducing arrows. The arrow plot also shows how a small radial velocity component is introduced due to the expansion. Note that the radial and axial scales differ in the plot.

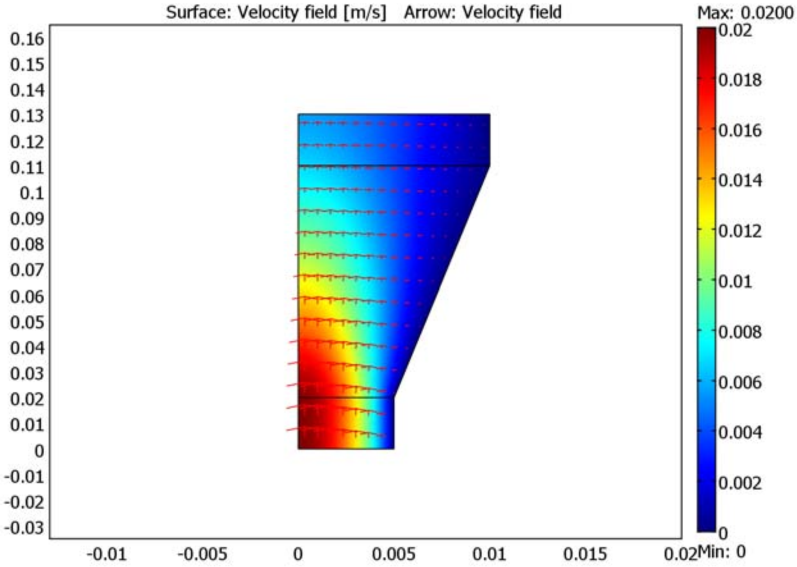


Figure 2-3: The velocity field.

Figure 2-4 shows that the pressure starts to recover when water enters the expansion zone after having dropped substantially in the narrow inlet zone. The pressure reaches a local maximum at the end of the expansion zone (at about z = 0.1 m), after which it starts to drop again due to frictional and viscous losses.

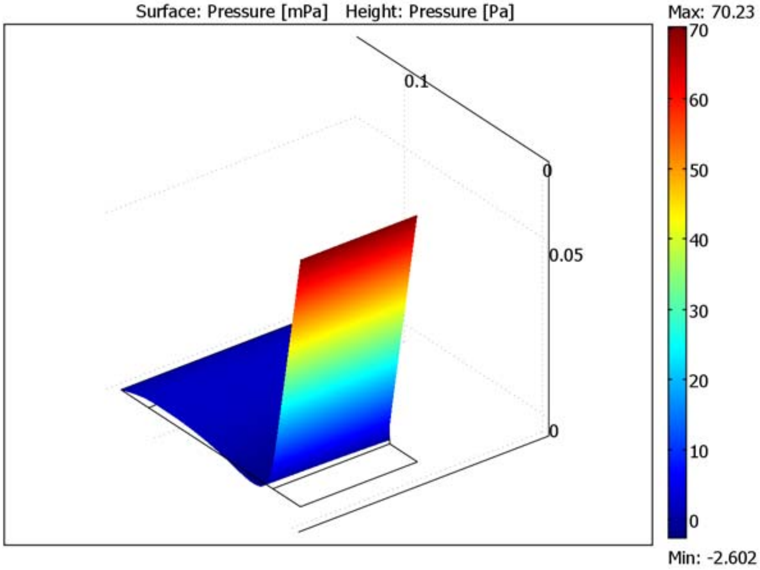


Figure 2-4: Relative pressure distribution throughout the duct. Pressure drops through the narrow part of the duct but increases to a maximum in the region of the expansion.

In order to quantify the pressure drop over the diverging duct, integrate the pressure over the inlet and the outlet of the expansion zone, and divide by the respective cross-sectional areas. Taking the difference gives the pressure drop over the expansion zone:

$$\Delta p = 5.95\text{ mPa} - 2.09\text{ mPa} = 3.9\text{ mPa} \qquad (2\text{-}3)$$

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/diverging_duct`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list.

3 Choose the application mode **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Axes/Grid Settings**. Specify axis and grid settings according to the following table:

AXIS		GRID	
r min	`-0.1`	r spacing	`0.005`
r max	`0.1`		
z min	`-0.005`	z spacing	`0.005`
z max	`0.135`		

2 Be sure to clear the **Auto** check box on the **Grid** tab, then click **OK**.

3 From the **Options** menu open the **Constants** dialog box. Define the following constants for later use; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`998[kg/m^3]`	`Density`
`eta`	`1.01e-3[Pa*s]`	`Viscosity`
`v_max`	`2[cm/s]`	`Maximum flow velocity at inlet`

GEOMETRY MODELING

1 Click the **Line** button on the Draw toolbar and draw a sequence of lines by using the left mouse button to click at points (0, 0), (0, 0.13), (0.01, 0.13), (0.01, 0.11), (0.005, 0.02), and (0.005, 0).

2 Click the right mouse button to close the curve and create a solid object CO1.

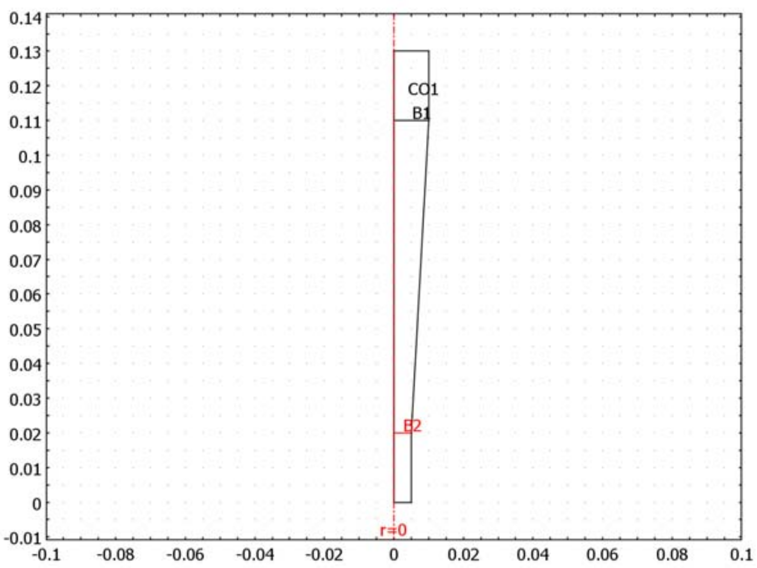
3 Click the **Line** button on the Draw toolbar and draw a line between (0, 0.11) and (0.01, 0.11).

4 Click the right mouse button to create an interior boundary B1.

5 Click the **Line** button again and draw a line between (0, 0.02) and (0.005, 0.02).

6 Click the right mouse button to create a second interior boundary B2.

This completes the geometry modeling stage. The geometry in the drawing area on your screen should look like that in the following figure.



PHYSICS SETTINGS

Subdomain Settings

From the **Physics** menu, select **Subdomain Settings**. Select all three subdomains, then enter material properties according to the following table; when done, click **OK**.

SETTINGS	SUBDOMAINS 1–3
ρ	`rho`
η	`eta`

Boundary Conditions

From the **Physics** menu, select **Boundary Settings**. Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARIES 1, 3, 5	BOUNDARY 7	BOUNDARIES 8–10
Boundary type	Inlet	Symmetry boundary	Outlet	Wall
Boundary condition	Velocity	Axial symmetry	Pressure, no viscous stress	No slip
u_0	0			

SETTINGS	BOUNDARY 2	BOUNDARIES 1, 3, 5	BOUNDARY 7	BOUNDARIES 8–10
v_0	`v_max*(1-s^2)`			
p_0			0	

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar.

2 Click the **Refine Mesh** button on the Main toolbar twice.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 2-3, follow these steps:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 On the **General** page, select the **Arrow** check box in the **Plot type** area. Click **OK**.

3 In the **Options>Axes/Grid Settings** dialog box click the **Axis** tab and clear the **Axis equal** check box. Specify **r min** as `-0.013` and **r max** as `0.02`, then click **OK**.

Generate Figure 2-4 with the following instructions:

1 In the **Plot Parameters** dialog box, clear the **Arrow** check box on the **General** page.

2 Click the **Surface** tab. Select **Incompressible Navier-Stokes (chns)>Pressure** from the **Predefined quantities** list on the **Surface Data** page.

3 In the **Unit** edit field, type `mPa` to obtain the result in millipascals.

4 Still on the **Surface** page, click the **Height Data** page. Select the **Height data** check box and choose **Incompressible Navier-Stokes (chns)>Pressure** from the **Predefined quantities** list on this page.

5 Click **OK**, then click the **Zoom Extents** button on the Main toolbar.

To compute the pressure drop, as discussed on page 13, do as follows:

1 From the **Postprocessing** menu, select **Boundary Integration**.

2 Select the **Compute surface integral (for axisymmetric modes)** check box.

3 Select Boundary 4 (the inlet). In the **Expression** edit field type `p/(pi*(5[mm])^2)`, that is the pressure divided by the cross-sectional area of the inlet. Integrating this expression over the inlet thus gives the average pressure at the inlet.

4 In the **Unit of integral** edit field, type `mPa` to obtain the result in millipascals.

5 Click **Apply**.

The average inlet pressure, roughly 5.95 mPa, appears in the message log below the drawing area.

6 Select Boundary 6 (the outlet), Modify the contents in the **Expression** edit field to `p/(pi*(10[mm])^2)`, then click **OK**.

The average outlet pressure, approximately 2.09 mPa, appears in the message log.

Flow in a Fuel Cell Stack

Introduction

A key optimization parameter in a fuel cell is the design of the reactant and product channels and inlets and outlets. Good designs require that the electrodes are well fed with a reactant and that products are removed as quickly as possible. A further desire for a good fuel-cell design is that fuel cells are as compact as possible. This saves on material costs and allows them to fit into smaller spaces (such as in a car).

One important parameter for deciding good design is the fluid-flow characteristics of the feed stream to a fuel cell stack. This example deals with the gas channels on the air side of three bipolar plates. The channels in these plates are interconnected through cylindrical headers for the air inlet and outlet. This model solves the Navier-Stokes equations.

Model Definition

GEOMETRY

Figure 2-5 shows a 3D view of the model domain.

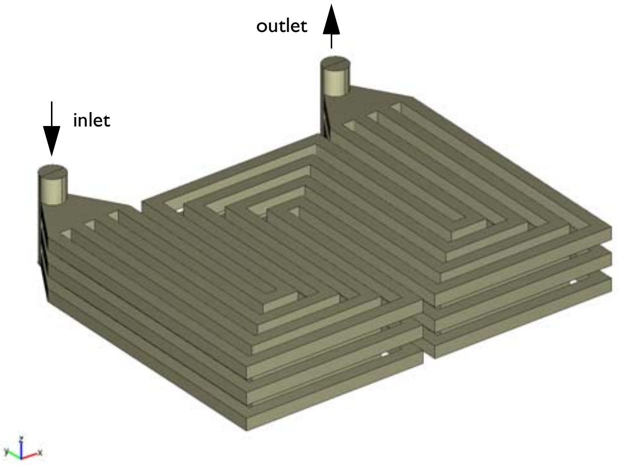


Figure 2-5: Diagram of the modeling geometry. The model shows the sixteen separate channels that are separated by the (not shown) electrodes and membrane in the z-dimension as well as the current collectors in the xy-plane.

Figure 2-6 shows the shape of each channel.

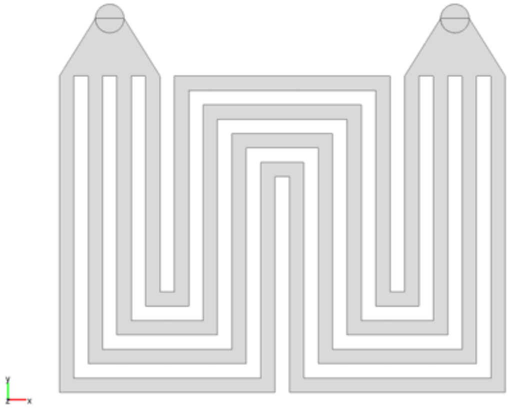


Figure 2-6: A view of the model geometry (Figure 2-5) from above. Flow occurs through the gray-shaded areas.

DOMAIN EQUATIONS

The fluid flow is described by the Navier-Stokes equations

$$\rho\frac{\partial\mathbf{u}}{\partial t}-\nabla\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p=0 \tag{2-4}$$
$$\nabla\cdot\mathbf{u}=0$$

where ρ denotes the density (kg/m^3), **u** represents the velocity (m/s), η is the viscosity (Pa·s), and p is the pressure (Pa). The modeled fluid is a gas with a viscosity of 10^{-5} Pa·s and a density of 1 kg/m^3.

BOUNDARY CONDITIONS

The model uses pressure boundary conditions for both the inlet and the outlet. The pressure boundary condition fixes the pressure and assumes that the viscous stress is zero at the boundary, that is

$$\mathbf{n}\cdot[\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]=0 \tag{2-5}$$

and

$$p=p_0. \tag{2-6}$$

The pressure, p_0, is set to zero at the outlet and to the total pressure drop, dp, over the stack at the inlet. All other boundaries have the *no slip* condition

$$\mathbf{u} = 0 . \tag{2-7}$$

SOLVER AND MESH

This model utilizes the the iterative FGMRES solver with a geometric multigrid preconditioner, which reduces memory requirements considerably. The solver uses several meshes: one base mesh and one or several coarser meshes. In this model one coarse level is sufficient. The solver is by default set to generate the coarser meshes automatically; however, in this model it is set manually.

For the base mesh it is appropriate to resolve the channel width with two to three elements when using 2nd-order basis functions for the velocities. This is because the channel dimensions are small and the velocities are comparably small. The base mesh used in the model consists of approximately 31,400 elements yielding approximately 220,000 degrees of freedom (DOF). The coarser mesh uses the same mesh but 1st-order elements. It results in 49,000 DOF. Figure 2-7 shows a picture of the mesh.

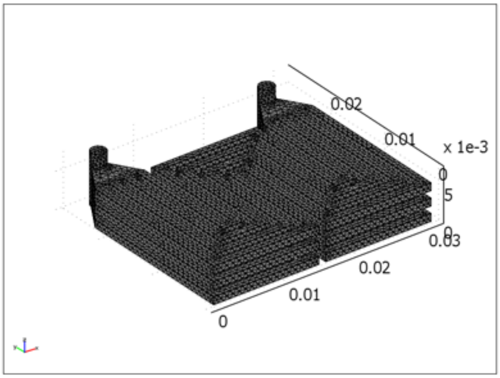


Figure 2-7: Computational mesh.

Results

The pressure distribution (see Figure 2-8) is a key result. As almost all fuel cells run on gas streams, so the local pressure can affect their volumetric properties.

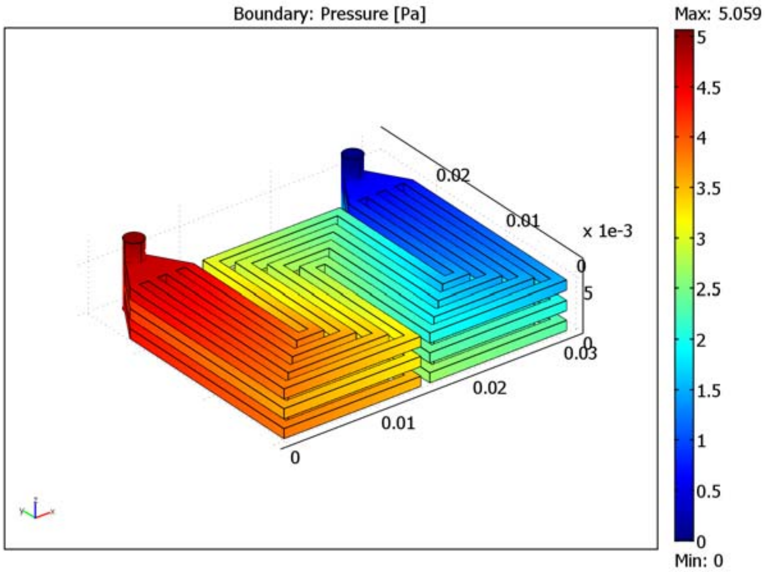


Figure 2-8: Pressure distribution in the feed channels of the fuel cell stack.

A more significant result is the velocity magnitude throughout the feed channels. Figure 2-9 shows the flow regime for all layers. For each layer, it is apparent that the velocity is greatest in the innermost channel, which has the shortest length.

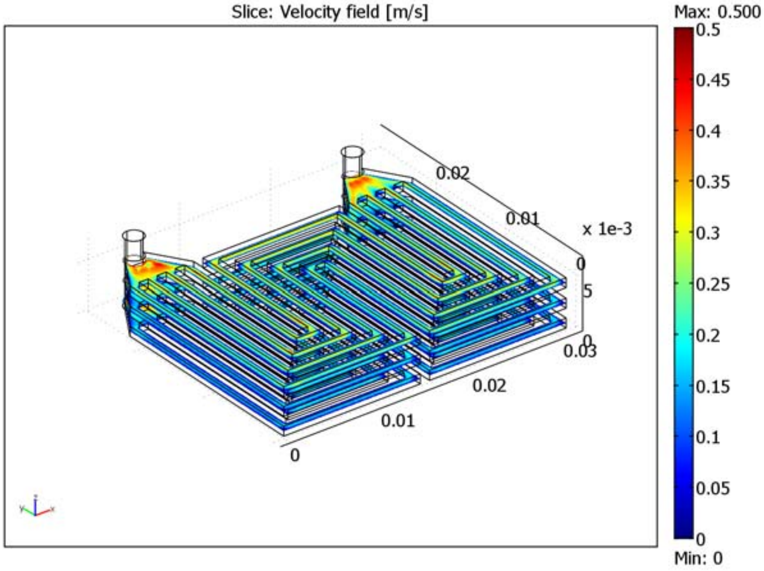


Figure 2-9: Velocity magnitude in the feed channels of the fuel cell stack.

Figure 2-10 shows a close-up of the feed channels. You can see that the velocity is greater in the upper layers than in the lower ones.

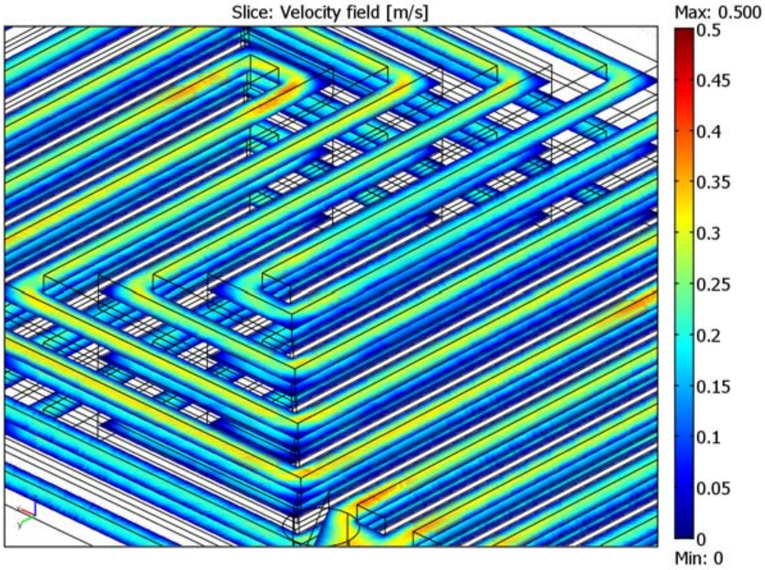


Figure 2-10: A close-up of the velocity magnitude.

A more uniform distribution in the channels is desired. Modifying the design by placing the outlet header toward the bottom of the stack would be preferable.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/fuel_cell_stack`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

2 In the **Model Navigator** set the **Space dimension** to **3D**.

3 In the list of application modes select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes>Steady-state analysis**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 Open the **Constants** dialog from the **Options** menu.

2 Enter the constants in the following table; when done, click **OK**.

NAME	EXPRESSION
`rho`	`1`
`eta`	`1e-5`
`p0`	`5`

GEOMETRY MODELING

Start to draw a cross section of the flow channels in a 2D cross section.

1 Select **Work-Plane Settings** from the **Draw** menu.

2 Leave the default values in the dialog box and click **OK**.

In the 2D work plane specify suitable axis and grid settings.

3 Select **Axes/Grid Settings** from the **Options** menu.

4 On the **Axis** page set **x-y limits** according to:

PROPERTY	EXPRESSION
x min	`-0.005`
x max	`0.035`
y min	`-0.005`
y max	`0.028`

5 Go to the **Grid** page and clear the **Auto** check box.

6 Specify **x-y grid** according to:

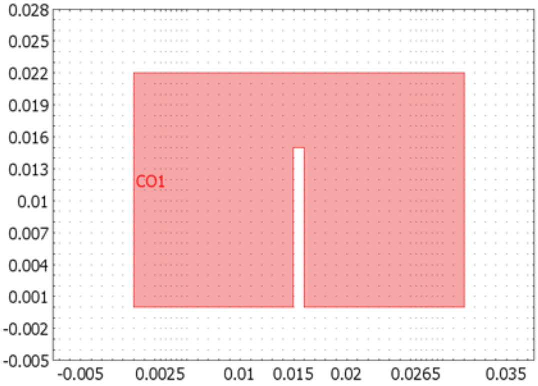
PROPERTY	EXPRESSION
x spacing	`1e-3`
Extra x	`linspace(2.5e-3,4.5e-3,3) linspace(26.5e-3,28.5e-3,3)`
y spacing	`1e-3`
Extra y	

7 Click **OK**.

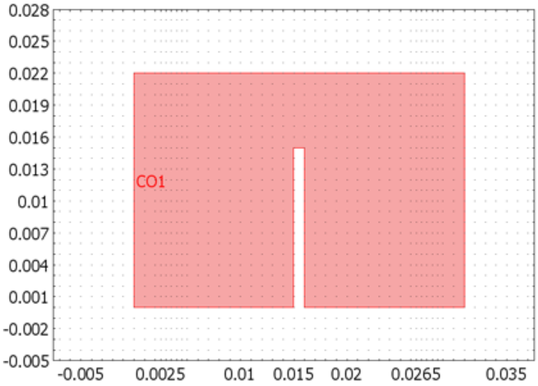
8 Click the **Line** button on the Draw toolbar.

9 Start by clicking at position (0, 0.022). Continue with points (0, 0), (0.015, 0), (0.015, 0.015), (0.016, 0.015), (0.016, 0), (0.031, 0), and (0.031, 0.022).

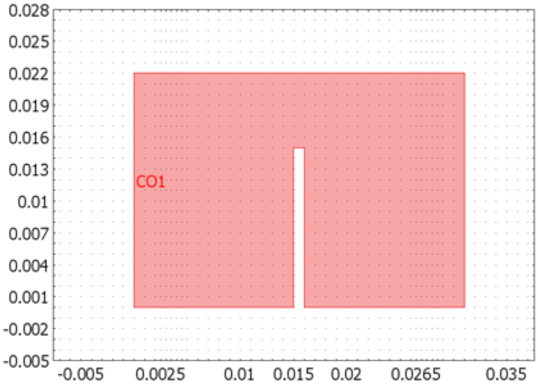
The outer shape of the channels is now finished.



10 Continue to finish the first channel by clicking the points (0.03, 0.022), (0.03, 0.001), (0.017, 0.001), (0.017, 0.016), (0.014, 0.016), (0.014, 0.001), (0.001, 0.001), and (0.001, 0.022).

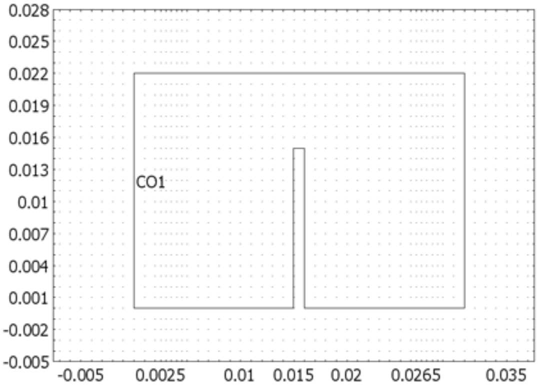


11 Continue in the same fashion to create the rest of the channel structure as shown in the next figure.



12 Click the points (0.0045, 0.026) and (0.0025, 0.026).

13 Close the geometry by right-clicking anywhere in the geometry.



Draw the top of the right portion of the channel system.

14 Click the **Line** tool on the Draw toolbar. Click the positions (0.024, 0.022), (0.0265, 0.026), (0.0285, 0.026), and (0.031, 0.022). Close the geometry by right-clicking anywhere.

15 Continue to draw a circle with radius 0.001 centered in the position (0.0035, 0.026) using the **Ellipse/Circle(Centered)** tool from the Draw toolbar.

16 Open the **Create Composite Objects** window from the **Draw** menu.

17 Enter the formula `CO1+CO2`, clear the **Keep interior boundaries** check box, and click **OK**.

18 Select **Extrude** from the **Draw** menu.

19 Select the channel geometry (CO3) from the **Objects to extrude** list.

20 Set the **Distance** to `1e-3` and click **OK**.

21 Click the **Array** button on the Draw toolbar.

22 Set the **z displacement** to `2e-3` and the **Array size: z** to `3`. Click **OK**.

23 Select all three object and click the **Union** button on the Draw toolbar.

24 Switch back to **Geom2**.

25 Open the **Extrude** window from the **Draw** menu.

26 Extrude the circle E1 by a distance of `7e-3`. Click **OK**.

27 Back in the 3D geometry, click the **Block** button on the Draw toolbar. Specify the block according to the following table:

PROPERTY	VALUE
X length	`3e-3`
Y length	`2e-3`
Z length	`5e-3`
x base point	`2e-3`
y base point	`24e-3`
z base point	`0`

28 Click the **Create Composite Objects** button on the Draw toolbar.

29 Type the **Set formula** `EXT1-BLK1` and click **OK**.

30 Click the **Array** button on the Draw toolbar. Set the **x displacement** to `24e-3` and the **Array size: x** to `2`. Click **OK**.

31 Select all the geometry objects by pressing Ctrl+A. Make a union by clicking the **Union** button on the Draw toolbar.

32 Click the **Delete Interior Boundaries** button on the Draw toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 Open the **Subdomain Settings** dialog box from the **Physics** menu.

2 Select Subdomain 1, type `rho` in the **Density** edit field, and type `eta` in the **Viscosity** edit field.

3 Click **OK**.

Boundary Conditions

1 Open the **Boundary Settings** dialog box from the **Physics** menu.

2 Select the inlet boundary (Boundary 36) from the **Domain selection** list.

3 Select the type **Inlet**, then select **Pressure, no viscous stress** from the **Boundary condition** list. Type `p0` in the **Pressure** edit field.

4 Select the outlet boundary (Boundary 194), and select **Outlet** from the **Boundary type** list. The default condition **Pressure, no viscous stress** is correct.

5 Click **OK**.

MESH GENERATION

1 Open the **Free Mesh Parameters** dialog box from the **Mesh** menu.

2 On the **Global** page, select **Normal** from the **Predefined mesh sizes** list.

3 Click the **Custom mesh size** button and set the **Resolution of narrow regions** to `1.5`.

4 Click **Remesh** and then click **OK**.

The model is solved with a geometric multigrid preconditioner. Instead of using the built-in automatic generation of the coarser mesh, this model uses a manual definition of the necessary mesh cases. In the next step you generate the second mesh case used by the solver:

5 Select **Mesh>Mesh Cases**.

6 Click the **New button** and select the **Use same mesh as mesh case** check box and select **0** from the corresponding list.

7 Click **OK**.

To complete the settings for the new mesh case, change the element type to use 1st-order elements for all velocities and the pressure:

8 Select the menu item **Physics>Subdomain Settings**, and select Subdomain 1.

9 On the **Element** page select **Lagrange-Linear** from the **Predefined elements** list.

10 Click **OK**.

You have now created two mesh cases: Case 0 with the default P2–P1 element, and Case 1 with a lower element order using the same mesh as Case 0.

COMPUTING THE SOLUTION

Set up the geometric multigrid preconditioner with the appropriate settings for this Navier-Stokes problem using the manually generated mesh hierarchy.

1. Select **Solve>Solver Parameters**.
2. Click the **Settings** button.
3. In the tree to the left in the dialog box, select **Preconditioner**.
4. Select **Manual** from the **Hierarchy generation method** list.
5. Click **OK** to close the **Linear System Solver Settings** dialog and click **OK** once more to close the **Solver Parameters** dialog box.
6. Click the **Solve** button on the Main toolbar. Note that computing the solution takes at least 30 minutes, depending on the performance of your computer.

POSTPROCESSING AND VISUALIZATION

To create Figure 2-8, perform the following steps.

1. Open the **Plot Parameters** dialog box from the **Postprocessing** menu.
2. On the **General** page clear the **Slice** check box and select the **Boundary** check box.
3. On the **Boundary** page select **Incompressible Navier-Stokes (chns)>Pressure** as **Boundary data**. Click **Apply**.

To create Figure 2-9, follow these steps:

1. On the **General** page clear the **Boundary** check box and select **Slice** as the plot type.
2. Clear the **Element refinement auto** check box and enter `4` in the corresponding edit field.
3. On the **Slice** page set **Slice data** to **Velocity field**. Set **x-slice levels** to `0`, leave **y-levels** at `0`.
4. Select the **Vector with coordinates** radio button for the **z-levels** and type `0.5e-3 2.5e-3 4.5e-3` in the corresponding edit field.
5. Click the **Range** button, clear the **Auto** check box and set **Max** to `0.5`. Click **OK** to close the **Color Range** dialog box. Click **OK**.

To create the view in Figure 2-9, rotate the geometry and zoom in a bit.

Non-Newtonian Flow

Introduction

This model shows the influence of shear rate dependent viscosity on the flow of a linear polystyrene solution. For this type of flow, you can use the Carreau viscosity model described by Equation 5-30 on page 134 of the *Chemical Engineering Module User's Guide*. Due to rotational symmetry, it is possible to reduce the model dimensions from 3D to axisymmetric 2D (see Figure 2-11).

Model Definition

For non-Newtonian flow, η denotes the viscosity (kg/(m·s)), $\mathbf{u}$ the velocity (m/s), ρ the density of the fluid (kg/m^3) and p the pressure (Pa). The equations to solve are the momentum and continuity equations.

$$\begin{aligned}\rho\frac{\partial\mathbf{u}}{\partial t}-\nabla\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+\rho\mathbf{u}\cdot\nabla\mathbf{u}+\nabla p &= 0\\ \nabla\cdot\mathbf{u} &= 0\end{aligned}\tag{2-8}$$

In the Carreau model, the viscosity depends on the shear rate, $\dot{\gamma}$, which for an axisymmetric model in cylindrical coordinates is defined according to Equation 2-9:

$$\dot{\gamma} = \sqrt{\frac{1}{2}\left((2u_r)^2+2(u_z+v_r)^2+(2v_z)^2+4\left(\frac{u}{r}\right)^2\right)}\tag{2-9}$$

The viscosity is given by Equation 2-10:

$$\eta = \eta_\infty+(\eta_0-\eta_\infty)[1+(\lambda\dot{\gamma})^2]^{\frac{(n-1)}{2}}\tag{2-10}$$

where η_∞ is the infinite shear rate viscosity, η_0 is the zero shear rate viscosity, λ is a parameter with units of time, and n is a dimensionless parameter. A solution of linear polystyrene in 1-chloronaphthalene has the properties listed in Table 2-1 (Ref. 1).

TABLE 2-1: PROPERTIES OF A SOLUTION OF LINEAR POLYSTYRENE IN 1-CHLORONAPHTALENE.

PARAMETER	VALUE
η_∞	0
η_0	166 Pa·s
λ	$1.73\cdot10^{-2}$ s

TABLE 2-1: PROPERTIES OF A SOLUTION OF LINEAR POLYSTYRENE IN 1-CHLORONAPHTALENE.

PARAMETER	**VALUE**
n	0.538
ρ	450 kg/m^3

The model domain is depicted in Figure 2-11.

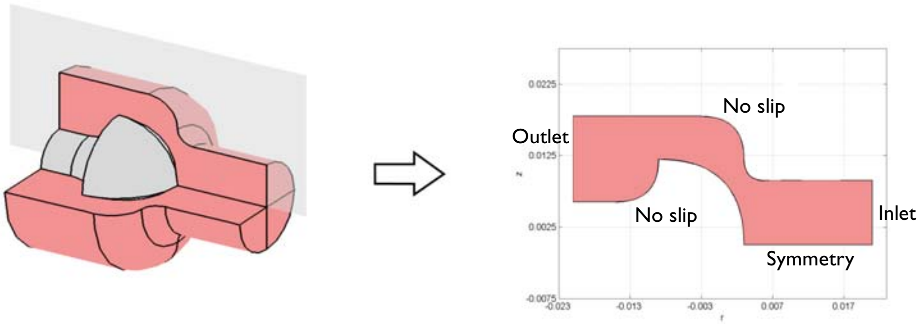


Figure 2-11: Model domain. The geometry can be simplified assuming axisymmetry.

The boundary conditions at the inlet and the outlet are set to fixed pressures and vanishing viscous stresses:

$$\begin{aligned} p &= p_{\mathrm{in}} \\ p &= 0 \end{aligned} \tag{2-11}$$

and

$$\mathbf{n}\cdot[\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)] = 0 \tag{2-12}$$

To study the effect on viscosity at different inlet pressures, the model makes use of the parametric solver to vary p_{in} from 10 kPa to 210 kPa. The axis of rotation requires the symmetry condition:

$$\mathbf{u}\cdot\mathbf{n} = 0 \tag{2-13}$$

while all other boundaries impose the no-slip condition:

$$\mathbf{u} = \mathbf{0} \tag{2-14}$$

Results

Figure 2-12 shows that the velocity distribution is more pronounced at the inlet compared to the outlet. This is because the cross-section is greater at the outlet. The figure also shows that the region of greatest velocity is in the contraction, which means that the shear rate will be largest there.

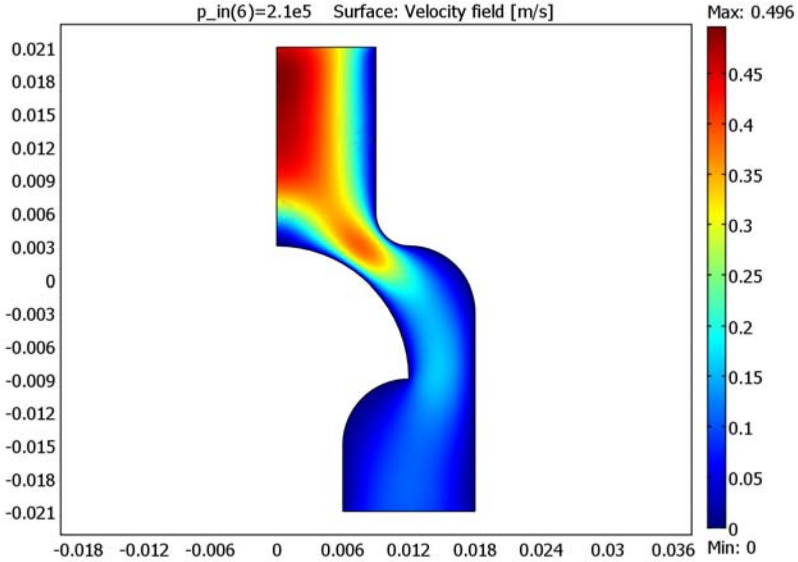


Figure 2-12: Velocity field throughout the modeling domain. The distribution is more pronounced at the inlet as opposed to the inlet.

Because the fluid is shear-thinning, the viscosity depends on the shear rate and is shown in Figure 2-13. It reaches its lowest value close to the wall in the contraction between the piston and the wall.

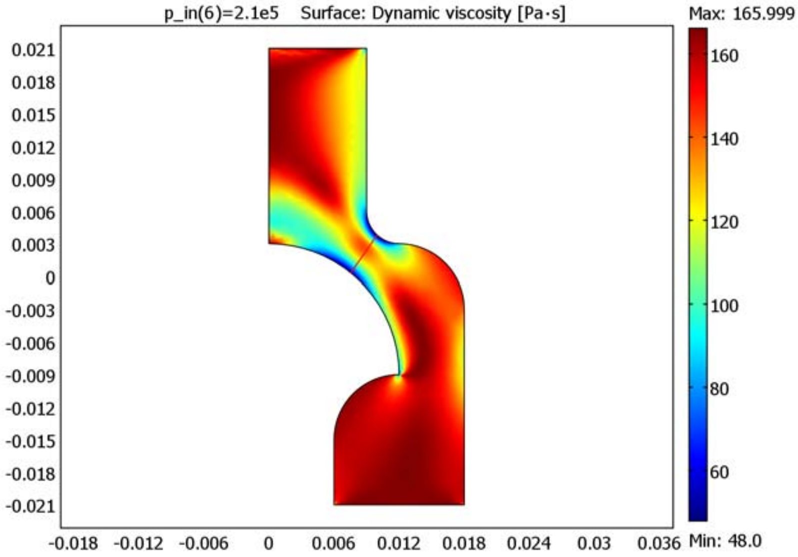


Figure 2-13: Viscosity distribution in the model domain. The lowest viscosity occurs at the wall in the contraction region.

Showing the result of a parametric study of the inlet pressure, Figure 2-14 contains a cross-sectional plot of the viscosity across the contraction (indicated by a red line in Figure 2-13). Sweeping through a range of inlet pressures imposes greater velocities on the non-Newtonian fluid. As the velocity increases, the shear rate also increases and the viscosity decreases. An optimal condition is to have as flat a viscosity profile as possible. This is hindered by also wanting to put through as high a flow rate as possible.

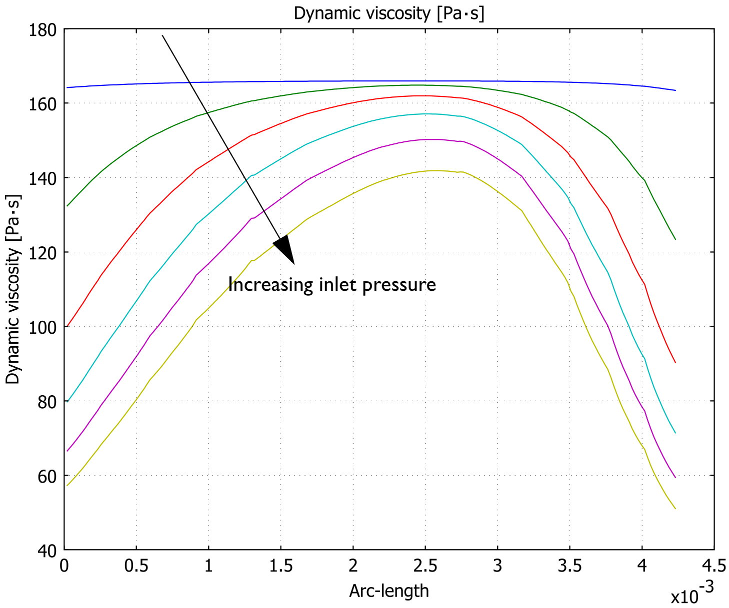


Figure 2-14: Parametric study of the process, sweeping the inlet pressure from 10 kPa to 210 kPa, while investigating a cross-sectional viscosity plot. The greater the inlet pressure (and pressure differential) the less the viscosity and more varied its distribution through the cross section.

Reference

1. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/non_newtonian_flow`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list.

3 From the list of application modes, select **Chemical Engineering Module>Momentum Transport>Laminar Flow> Non-Newtonian Flow**.

4 Click **OK**.

GEOMETRY MODELING

The first step in the modeling process is to draw the geometry which is explained below.

1 Press the Shift key and click the **Rectangle/Square** button.

2 Enter the rectangle dimensions according to the values below in the corresponding edit fields.

OBJECT DIMENSIONS	EXPRESSION
Width	`9e-3`
Height	`21e-3`
r-position	`0`
z-position	`0`

3 Click **OK**.

4 Repeat the procedure for another rectangle with the following dimensions.

OBJECT DIMENSIONS	EXPRESSION
Width	`12e-3`
Height	`27e-3`
r-position	`6e-3`
z-position	`-21e-3`

5 Click **OK**.

6 Click the **Zoom Extents** button in the Main toolbar.

7 Open **Axes/Grid Settings** in the **Options** menu.

8 Click the **Grid** tab.

9 Clear the **Auto** check box and set **r spacing** and **z spacing** to `3e-3`.

10 Click the **2nd Degree Bézier Curve** tool and click the coordinate sequence (0, 3e-3), (12e-3,3e-3), (12e-3, –9e-3), (6e-3, –9e-3), and (6e-3, –15e-3).

11 Select the **Line** tool and click the coordinate (0, –15e-3).

12 Create a solid object by clicking the right mouse button once.

13 Select the **2nd Degree Bézier Curve** tool and click the coordinate sequence (9e-3, 6e-3), (9e-3, 3e-3), (12e-3, 3e-3), (18e-3, 3e-3), and (18e-3, –3e-3).

14 Click the **Draw Line** tool and click the coordinate (18e-3, 6e-3).

15 Click the right mouse button to create a solid object.

16 Click the **Create Composite Object** button.

17 Type `R1+R2-CO1-CO2` in the **Set formula** edit field.

18 Clear the **Keep interior boundaries** check box, then click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 On the **Physics** tab select **Carreau model** from the **Viscosity model** list.

3 Type `450` in the **Density** edit field.

4 Click the **Carreau** tab. Select Subdomain 1, then specify settings according to the table below.

PROPERTY	VALUE
η_∞	`0`
η_0	`166`
λ	`1.73e-2`
n	`0.538`

5 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the boundary conditions according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 4	BOUNDARIES 3, 5–12
Boundary type	Symmetry boundary	Inlet	Outlet	Wall
Boundary condition	Axial Symmetry	Pressure, no viscous stress	Pressure, no viscous stress	No slip
p_0		`p_in`	`0`	

3 Click **OK**.

MESH GENERATION

1 Select the **Free Mesh Parameters** dialog box in the **Mesh** menu.

2 Click the **Point** tab.

3 From the **Point selection** list, select Points 2, 3, 8, 9, and 11.

4 Set the **Maximum element size** to `1e-4`.

5 Click the **Boundary** tab.

6 Select Boundary 2, then set the **Maximum element size** to `5e-4`.

7 Select Boundaries 9 and 11, then set the **Maximum element size** to `2e-4`.

8 Click **OK**.

9 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 Select **Parametric** from the **Solver** list.

3 Type `p_in` in the **Parameter name** edit field and `10000:40000:210000` in the **Parameter values** edit field.

4 Click **OK**.

5 Click the **Solve** button in the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default plot, displayed in Figure 2-12 on page 32, shows the magnitude of the velocity field.

To visualize the variations of the viscosity in a surface plot, as in Figure 2-13, follow these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Click the **Surface** tab.

3 From the **Predefined quantities** list on the **Surface Data** page, select **Non-Newtonian Flow (chns)>Dynamic viscosity**.

4 Click **OK**.

You can also visualize the value of the viscosity along a cross-section, perpendicular to the main flow, at the position of the contraction:

1 From the **Options** menu, select **Axes/Grid Settings**.

2 Click the **Grid** tab.

3. Select the **Auto** check box and click **OK**.
4. From the **Postprocessing** menu, open the **Cross-Section Plot Parameters** dialog box.
5. On the **General** page, select all parameter values in the **Solutions to use** list.
6. Click the **Line/Extrusion** tab.
7. From the **Predefined quantities** list, select **Non-Newtonian Flow (chns)>Dynamic viscosity**.
8. Enter the following cross-section line data:

r0	`7.55e-3`
r1	`9.97e-3`
z0	`0.32e-3`
z1	`3.79e-3`

9. Click **OK**.

The resulting plot reproduces that in Figure 2-14. It shows the viscosity along the cross section indicated by a straight red line in Figure 2-12 at different flow rates for the polymer solution.

Flow Between Two Parallel Plates

Introduction

This example models the developing flow between two parallel plates. The purpose is to study the inlet effects in laminar flow at moderate Reynolds numbers, in this case around 40.

Although the problem might seem academic in nature, the conditions and parameters described in the model are fairly common in catalytic reactors, heat exchangers, micro reactors, and other process units.

The domain is visualized in Figure 2-15. Neglecting end effects in the z direction, you can assume symmetry throughout this dimension and reduce the three-dimensional problem to two dimensions. This reduction means that you assume that the flow velocity's z-component is zero.

You model the flow just below and between two parallel plates. Fluid enters at the inlet, which is the lower horizontal boundary, while slip/symmetry conditions describe the lower vertical boundaries just below the position of the plates. The vertical plates, positioned 1 cm above the inlet, impose a no-slip condition on the vertical boundaries. Specify a pressure condition at the outlet.

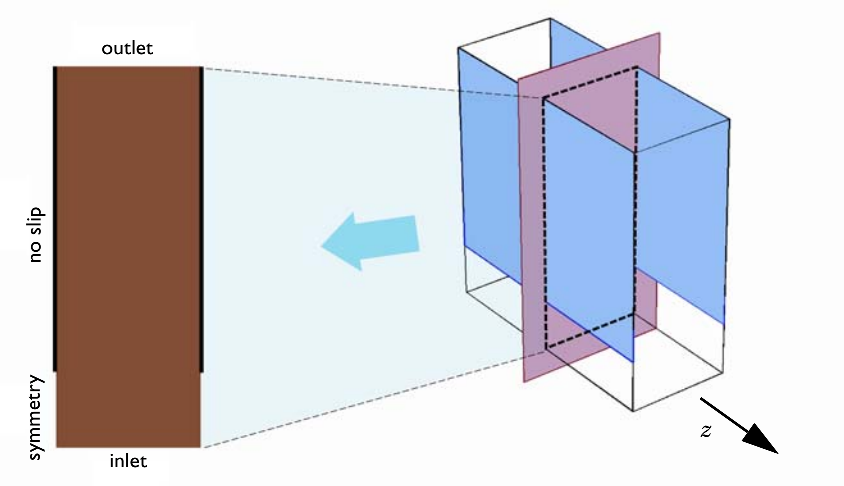


Figure 2-15: The model geometry. Assuming there is no flow in the z direction, the problem reduces to a 2D model.

Model Definition

This example uses the Navier-Stokes equations and the continuity equation with constant viscosity and density:

$$
\begin{aligned}
\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p &= 0 \\
\nabla\cdot\mathbf{u} &= 0
\end{aligned}
\qquad (2\text{-}15)
$$

Here η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ the velocity (m/s), ρ the fluid density (kg/m^3), and p the pressure (Pa).

The boundary conditions according to Figure 2-15 are:

$$
\begin{array}{rc}
\mathbf{u}\cdot\mathbf{n} = v_0 & \text{Inlet} \\
\mathbf{u}\cdot\mathbf{n} = 0 & \text{Symmetry} \\
\mathbf{t}\cdot(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}))\mathbf{n} = 0 & \text{Symmetry} \\
\mathbf{u} = \mathbf{0} & \text{No slip} \\
p = 0 & \text{Outlet}
\end{array}
\qquad (2\text{-}16)
$$

The pressure variable in this example is relative to the outlet pressure, which is set to zero. The model's input data are tabulated below.

NAME	EXPRESSION	DESCRIPTION
ρ	10^3 kg/m^3	Density
η	10^{-2} Pa·s	Viscosity
v_0	2 cm/s	Inlet velocity

Results

Figure 2-16 displays the modulus of the velocity vector. The development of the viscous layer as the fluid encounters the solid walls at the lateral boundaries appears clearly.

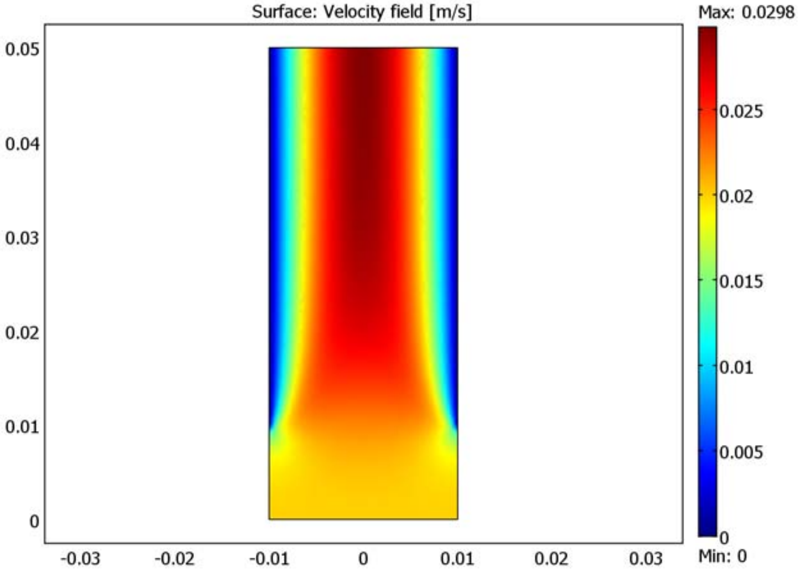


Figure 2-16: Flow-velocity magnitude. It is apparent that the flow develops along the length of the modeling domain, once it has encountered the no-slip condition at the parallel plate walls.

The development from a uniform velocity profile to the fully developed Poiseuille flow can be depicted by plotting the flow along a number of horizontal cross-sections along the length of the channel, as in Figure 2-17. Because the flow is incompressible, the areas below the curves are the equal. The presence of nearly overlapping profiles shows that the flow is almost fully developed at the outlet.

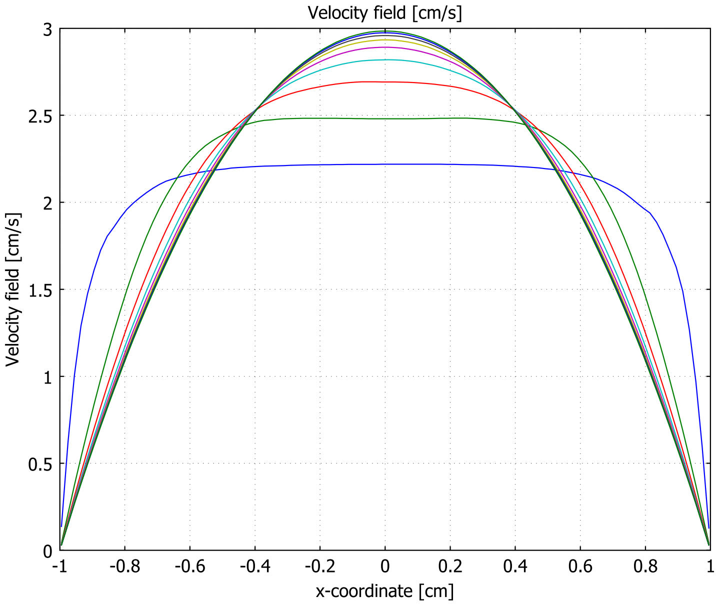


Figure 2-17: Velocity profiles at equidistant positions along the length of the modeling domain. The flat velocity profile at the inlet gradually develops into a Poiseuille or parabolic profile, which is almost fully developed at the outlet.

The section below describes in detail how to reproduce this model in COMSOL Multiphysics.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/parallel_plates`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click the **New** page

3. Select **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.
4. Click **OK**.

OPTIONS AND SETTINGS

The first step of the modeling process is to create a temporary data base for the input data. Define the following constants in the **Constants** dialog box in the **Option** menu.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1e3[kg/m^3]`	`Fluid density`
`eta`	`0.01[Pa*s]`	`Viscosity`
`v0`	`2[cm/s]`	`Inlet velocity`

GEOMETRY MODELING

1. Simultaneously press the Shift key and click the **Rectangle/Square** button.
2. Type the values below in the respective edit fields for the rectangle dimensions.

OBJECT DIMENSIONS	EXPRESSION
Width	`0.02`
Height	`0.05`
Base	Corner
x	`-0.01`
y	`0`

3. Click **OK**.
4. Click the **Zoom Extents** button on the Main toolbar.
5. Use the **Draw Point** button to place two points by clicking at (–0.01, 0.01) and (0.01, 0.01).

PHYSICS SETTINGS

Subdomain Settings

1. From the **Physics** menu, select **Subdomain Settings**.
2. Select Subdomain 1.

3 Define the physical properties of the fluid, in this case the viscosity and the density, according to the table below.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARIES 1, 5	BOUNDARY 4	BOUNDARIES 3, 6
Type	Inlet	Symmetry boundary	Outlet	Wall
Condition	Velocity	-	Pressure	No slip
u_0	0			
v_0	`v0`			
p_0			0	

MESH GENERATION

In this case you want to customize some settings for the initial mesh.

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 On the **Boundary** page, select Boundaries 3 and 6 from the **Boundary Selection** list.

3 In the **Maximum element size** edit field, type `1e-3`. This creates elements with a maximum edge length of 10^{-3} m for Edges 3 and 6.

4 Click the **Remesh** button.

5 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default plot, displayed in Figure 2-16 on page 41, is a surface plot of the velocity magnitude.

Execute the following instructions to generate the cross-section plots of the velocity along horizontal lines at different positions along the channel displayed in Figure 2-17.

1. From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
2. Click the **Line/Extrusion** tab.
3. In the **y-axis data** area, keep the default choice **Velocity field** in the **Predefined quantities** list. Type `cm/s` in the **Unit** edit field.
4. In the **x-axis data** area, click the lower option button, then click the **Expression** button to open the **X-Axis Data** dialog box.
5. From the **Predefined quantities** list, select **Geometry and Mesh>x-coordinate**. From the **Unit** list, select **cm**. Click **OK** to close the **X-Axis Data** dialog box.
6. Specify the **Cross-section line data** according to the table below.

PROPERTY	VALUE
x0	`-0.01`
x1	`0.01`
y0	`0`
y1	`0`

7. Select the **Multiple parallel lines** check box.
8. Click the **Vector with distances** option button then type `linspace(0.01,0.05,9)` in the associated edit field. This gives a vector with nine equidistant elements between 0.01 to 0.05, which specify the *y*-coordinates for the lines.
9. Click **OK**.

The resulting plot shows how the velocity profile develops along the main direction of the flow. At the outlet, the flow is almost a fully developed parabolic velocity profile.

Variations in Density in Porous Media Flow

Introduction

This example studies the steady flow of an ideal gas in a porous medium, taking variations in gas density into account. Darcy's law describes the velocity in the porous structure and accounts for the conservation of mass by the ideal gas law, as expressed in Equation 5-57 and Equation 5-58 on page 153 of the *Chemical Engineering Module User's Guide*.

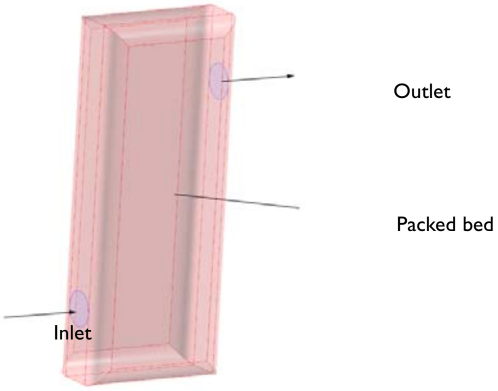


Figure 2-18: Depiction of the model geometry. Inert gas enters a porous structure from the bottom-left and leaves at the top-right.

The system you study is a packed bed reactor of the type used, for example, in small-scale reforming or catalytic combustion processes. The model investigates pressure loss, flow field, and reactor properties by pumping an inert gas through it.

Model Definition

Darcy's law in combination with the continuity equation and the ideal gas law gives the following equation:

$$\nabla \cdot \left(-\frac{kM}{\eta RT}\, p\nabla p\right) = 0 \qquad (2\text{-}17)$$

Here k denotes the permeability of the porous medium (m^2), M the molar mass (kg/mol), η the fluid viscosity (Pa·s), R the gas constant (J/(mol·K)), T the temperature (K), and p the pressure (Pa).

As for boundary conditions, the pressure is 1.5 atm at the inlet and equal to the atmospheric pressure at the outlet, $p = p_0$. All other boundaries are impervious, corresponding to the condition

$$-\frac{k}{\eta}\nabla p \cdot \mathbf{n} = 0$$

The input data for the model is listed in the following table.

PROPERTY	**VALUE**
k	$1 \cdot 10^{-13}$ m^2
M	32 g/mol
η	$3.0 \cdot 10^{-5}$ Pa·s
R	8.314 J/(mol·K)
T	355 K
p_{atm}	$1.013 \cdot 10^{5}$ Pa

Results

Figure 2-19 below shows the pressure on the outer surface of the packed bed. Pressure losses are greatest close to the inlet and the outlet where the flow is large.

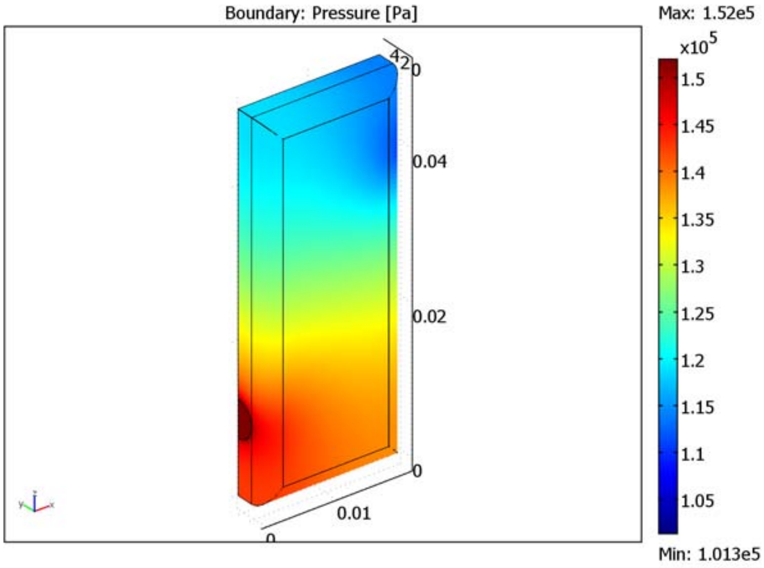


Figure 2-19: Pressure on the walls of the structure. The local pressure gradient is greatest in the inlet and outlet regions.

Because the gas density is proportional to pressure, the gas expands as it flows from the inlet to the outlet. This is clearly visible in Figure 2-20, where the flow tube's radius and color depend on the magnitude of the velocity vector.

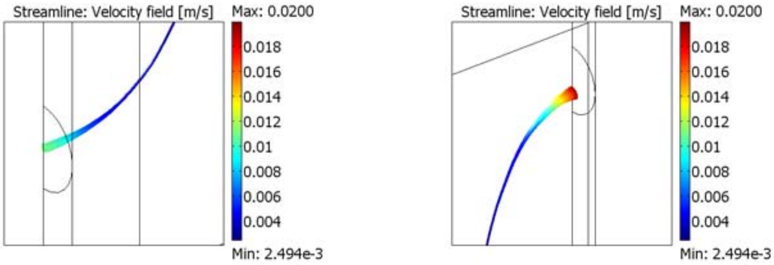


Figure 2-20: Depiction of the velocity field's streamlines at the inlet (left) and the outlet (right). The tangent to the streamline gives the direction of the vector, while its color scale and thickness indicate the velocity magnitude.

Modeling in COMSOL Multiphysics

Because the density appears inside the derivatives in the continuity equation, you must use a weak implementation. Chapter 2, "Application Mode Implementations," in the *Chemical Engineering Module User's Guide* summarizes the relevant equations. You can also inspect them on the **Weak** tab in the **Subdomain Settings - Equation System** dialog box that you open by selecting **Physics>Equation System>Subdomain Settings**.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/darcy_3d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, select **3D** from the **Space dimension** list.
3. From the list of application modes, choose **Chemical Engineering Module>Momentum Transport>Porous Media Flow> Darcy's law>Steady-state analysis**.

4 Click **OK**.

OPTIONS AND SETTINGS

Start by defining the constants and expressions below.

1 From the **Options** menu, choose **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`eta`	`3e-5[Pa*s]`	`Viscosity`
`kappa`	`1e-13[m^2]`	`Permeability`
`p_o`	`1.013e5[Pa]`	`Outlet pressure`
`p_i`	`1.5*p_o`	`Inlet pressure`
`M`	`32[g/mol]`	`Molar mass`
`R`	`8.314[J/(mol*K)]`	`Gas constant`
`T`	`355[K]`	`Temperature`

3 Choose **Options>Expressions>Scalar Expressions**.

4 Define the following expression:

NAME	EXPRESSION	DESCRIPTION
`rho`	`p*M/(R*T)`	`Density`

5 Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu, select **Work-Plane Settings**.

2 Click **OK** to accept the default settings.

3 Press the Shift key and click the **Rectangle/Square** button on the Draw toolbar.

4 Set the **Width** of the rectangle to `0.02`, the **Height** to `0.0025`, and the lower-left corner position to (`0`, `0.0025`). Click **OK** to create the rectangle R1.

5 Click the **Zoom Extents** button on the Main toolbar.

6 From the **Options** menu, select **Axes/Grid Settings**. On the **Grid** page, clear the **Auto** check box and type `0.0025` in the **x spacing** and **y spacing** edit fields. Click **OK**.

7 Click the **2nd Degree Bézier Curve** button on the Draw toolbar.

8 Click, in order, the points (0, 0.0025), (0, 0), and (0.0025, 0).

9 Click the **Line** button, then click the point (0.0175, 0).

10 Click the **2nd Degree Bézier Curve** button.

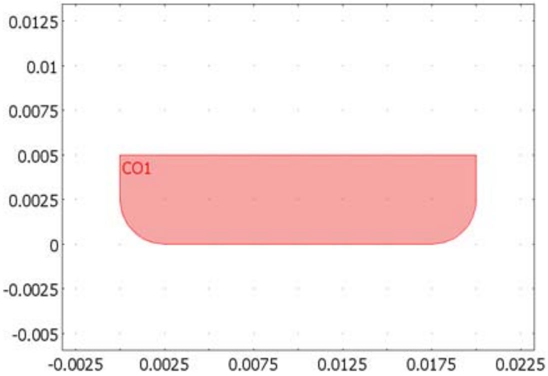
11 Click first the point (0.02, 0) and then the point (0.02, 0.0025).

12 Click the right mouse button to create a solid object, CO1.

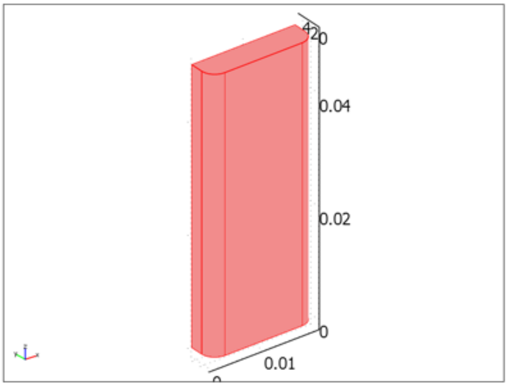
13 Press Ctrl+A to select both solid objects, R1 and CO1, then click the **Union** button on the Draw toolbar to create the composite object CO2.

14 Click the **Delete Interior Boundaries** button.

The geometry in the drawing area on your screen should now look like that in the picture below.



15 From the **Draw** menu, select **Extrude**. In the **Distance** edit field, type `0.05`. Click **OK**.



16 From the **Draw** menu, select **Work-Plane Settings**. Click the **y-z** button, then click **OK**.

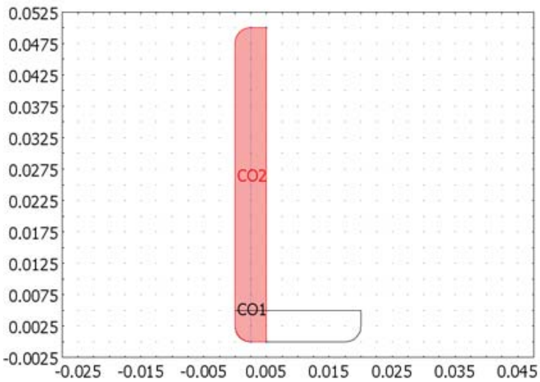
17 Click the **Zoom Extents** button on the Main toolbar.

18 Click the **2nd Degree Bézier Curve** button. Click, in order, the points (0, 0.0025), (0, 0), and (0.0025, 0).

19 Click the **Line** button. Click, in order, the points (0.005, 0), (0.005, 0.05), and (0.0025, 0.05).

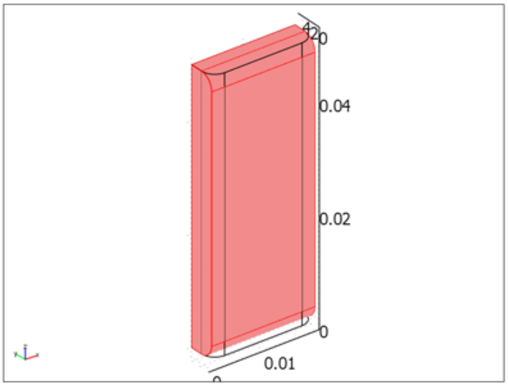
20 Click the **2nd Degree Bézier Curve** button. Click, in order, the points (0, 0.05) and (0, 0.0475).

21 Click the right mouse button to create a solid object, CO2.



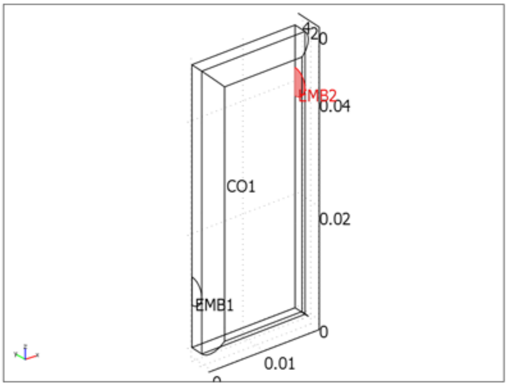
22 From the **Draw** menu, select **Extrude**. In the **Distance** edit field, type `0.02`. Click **OK**.

23 Click the **Zoom Extents** button on the Main toolbar.



24 Press Ctrl+A to select the two extruded objects, then click the **Intersection** button on the Draw toolbar.

25. Click the **Geom 2** tab to return to the work plane.
26. Draw a half circle by first clicking the **2nd Degree Bézier Curve** button on the Draw toolbar, and then clicking the points (0.005, 0.0075), (0.0025, 0.0075), (0.0025, 0.01), (0.0025, 0.0125), and (0.005, 0.0125).
27. Create a solid object by clicking the right mouse button.
28. With the solid object selected, select **Embed** from the **Draw** menu.
29. Click **OK**.
30. Press Ctrl+C to copy the object EMB1.
31. Press Ctrl+V. In the **Paste** dialog box enter an *x* displacement of `0.02` and a *z* displacement of `0.03`.
32. Click **OK**.



PHYSICS SETTINGS

Subdomain Settings

1. From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1, then specify density, permeability, and viscosity according to the table below.

PROPERTY	**VALUE**
ρ	`rho`
κ	`kappa`
η	`eta`

The expression for the density includes the dependent variable p, which makes the problem nonlinear. The initial value for the pressure is zero by default, which results in a zero density in the continuity equation. To obtain convergence, you must give a physical guess for the pressure. In this case, use the outlet pressure, p_0 (1 atm).

3 Click the **Init** tab. In the **p(t$_0$)** edit field, type `p_o`.

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table:

SETTINGS	**BOUNDARY 14**	**BOUNDARY 6**	**ALL OTHERS**
Type	Pressure	Pressure	Insulation/Symmetry
p_0	`p_o`	`p_i`	

3 Click **OK**.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

First plot the absolute value of the velocity vector to study the effects of expansion.

1 Click the **Plot Parameters** button on the Main toolbar.

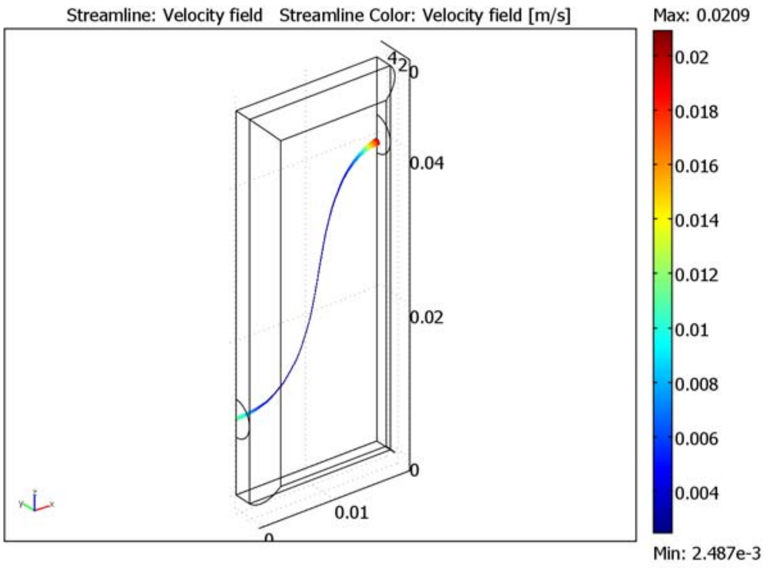
2 Clear the **Slice** check box in the **Plot type** area.

3 Click the **Streamline** tab and select the **Streamline plot** check box.

4 Select **Darcy's Law (chdl)>Velocity field** from the **Predefined quantities** list in the **Streamline data** area.

5. Click the **Specify start point coordinates** button and type the coordinates `1e-6`, `4.9e-3`, and `1e-2` in the **x**, **y**, and **z** edit fields, respectively.
6. To set the streamline color, click the **Line Color** tab, then click the **Use expression** button, and click the **Color Expression** button. Select **Darcy's Law (chdl)>Velocity field** from the **Predefined quantities** list, then click **OK**.
7. From the **Line type** list, select **Tube**.
8. Click the **Tube Radius** button. In the **Tube Radius Parameters** dialog box, select the **Radius data** check box. After verifying that the selection in the **Predefined quantities** list is **Darcy's Law (chdl)>Velocity field**, click **OK** to close the dialog box.
9. Back in the **Plot Parameters** dialog box, click **OK** to generate the plot.

The resulting plot shows a single flow line from the inlet to the outlet. You can use the **Zoom Window** tool to magnify the plot close to the inlet or the outlet.



Next, reproduce the pressure plot shown in Figure 2-19.

1. Click the **Plot parameters** button on the Main toolbar.
2. Click the **General** tab.
3. Clear the **Geometry edges** and **Streamline** check boxes. Select the **Boundary** check box.

4. Click the **Boundary** tab. From the **Predefined quantities** list, select **Darcy's Law>Pressure**.
5. Click **OK**.
6. Click the **Scene Light** button on the Camera toolbar.

Coupled Free and Porous Media Flow

Introduction

This is a model of the coupling between flow of a gas in an open channel and in a porous catalyst attached to one of the channel walls. The flow is described by the Navier-Stokes equation in the free region and the Brinkman equations in the porous region.

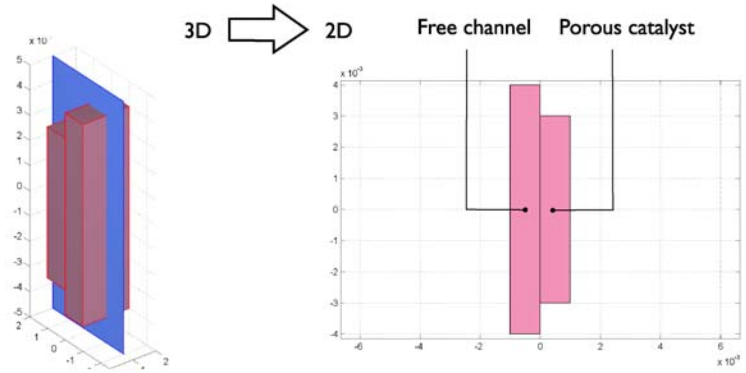


Figure 2-21: Depiction of the modeling geometry and domain. The 3D geometry can be reduced to a 2D representation assuming that changes through the thickness are negligible.

The coupling of free media flow with porous media flow is common in the field of chemical engineering. This problem type arises in filtration and separation and in chemical reaction engineering, for example in the modeling of porous catalysts in monolithic reactors. The most common way to deal with coupled free and porous media flow in a system is to incorporate Darcy's law. Yet, this does not account for viscous effects, arising from the free media flow, that may still have an effect in the region close to the free-porous structure interface. Depending on pore size and distribution as well as the fluid's properties, it can be an over-simplification to employ Darcy's law. The Brinkman equations account for momentum transport through viscous effects and through pressure gradients in porous media and can be considered an extension of Darcy's Law.

The system studied in this example is that of a 2D cross section of a rectangular reactor with a catalyst layer attached to one of its walls. Flow enters the reactor with a uniform velocity profile and develops throughout the length of the channel.

Model Definition

The modeled domain and notations for the boundary conditions are shown in the figure below.

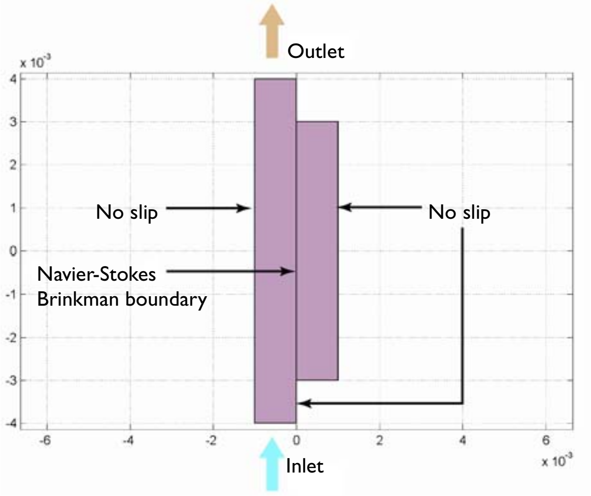


Figure 2-22: Modeled domain and boundary notations. Flow enters at the bottom and leaves at the top. The region of porous structure is not as long as the free channel.

Flow in the free channel is described by the Navier-Stokes equations:

$$\begin{gathered}\rho\frac{\partial \mathbf{u}}{\partial t} + \nabla\cdot[-\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+p\mathbf{I}] = -\rho(\mathbf{u}\cdot\nabla)\mathbf{u} \\ \nabla\cdot\mathbf{u} = 0\end{gathered} \qquad (2\text{-}18)$$

where η denotes the dynamic viscosity (Pa·s), $\mathbf{u}$ refers to the velocity in the open channel (m/s), ρ is the fluid's density (kg/m^3), and p is the pressure (Pa). In the porous domain, the Brinkman equations describe the flow:

$$\begin{gathered}\frac{\rho}{\varepsilon_p}\frac{\partial \mathbf{u}}{\partial t} + \nabla\cdot\left[-\frac{\eta}{\varepsilon_p}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+p\mathbf{I}\right] = -\frac{\eta}{k}\mathbf{u} \\ \nabla\cdot\mathbf{u} = 0\end{gathered} \qquad (2\text{-}19)$$

Here k denotes the permeability of the porous medium (m^2), and ε_p is the porosity (dimensionless). As can be seen from Equation 2-18 and Equation 2-19, the momentum transport equations are closely related. The term on the right-hand side of the Navier-Stokes formulation corresponds to momentum transported by convection in free flow. In the Brinkman formulation, this term is replaced by a contribution associated with the drag force experienced by the fluid flowing through a porous medium. In COMSOL Multiphysics, free flow and porous media flow are effortlessly combined.

The boundary conditions are

$$\begin{array}{rl} \mathbf{u}\cdot\mathbf{n} = u_0 & \text{inlet} \\ \mathbf{u} = \mathbf{0} & \text{no slip} \\ p = 0,\ \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})\mathbf{n} = \mathbf{0} & \text{outlet} \end{array} \tag{2-20}$$

where the pressure level at the outlet is used as a reference value.

The following table lists the input data for the model.

PROPERTY	VALUE	DESCRIPTION
η	10^{-5} kg/(m·s)	Dynamic viscosity
ρ	1 kg/m^3	Density
k	10^{-8} m^2	Permeability
v_0	1 cm/s	Inlet velocity

Results

The velocity field in the open channel and porous structure is shown in Figure 2-23. It shows that there are slight disturbances in the velocity at the porous wall, which suggests momentum transport by viscous effects.

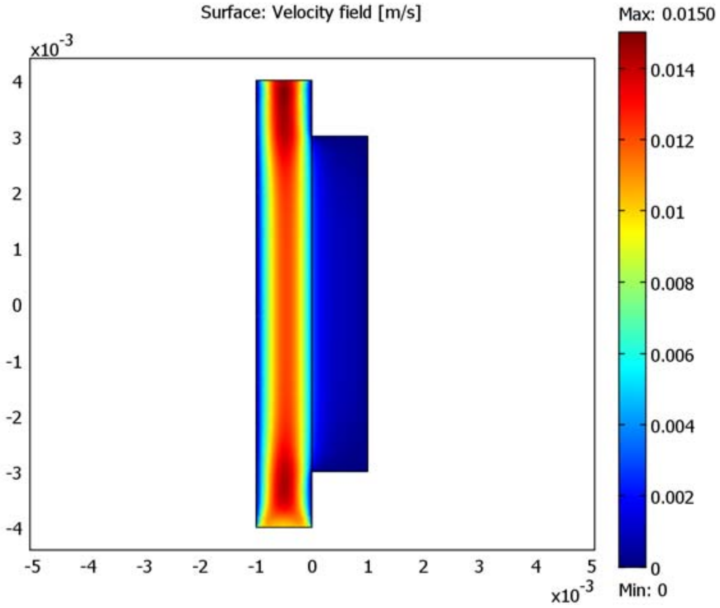


Figure 2-23: Velocity field in both the free channel and the porous media.

The velocity profile along a horizontal cross section in the middle of the channel is depicted in Figure 2-24. The plot confirms the existence of velocity gradients in the porous structure in that the velocity is continuous across the interface between the free channel and the porous structure. Further postprocessing would show that the shear rate perpendicular to the flow is also continuous. This implies that there is significant viscous momentum transfer across the interface and into the porous media, a transport that would not be accounted for by Darcy's law. If you would couple Darcy's law to the Navier-Stokes equations in this example, the profile would look substantially different. The velocity in the free channel would fall to a much smaller value in the free channel. Furthermore, a constant velocity equal to the flat part of the curve in Figure 2-24 would describe all transport in the porous media.

Assuming that Darcy's law describes the porous media flow adequately would be erroneous in this situation. This could be impractical if the velocity vector calculated here is coupled to a convective term in a material balance for a reacting species. The regions of the porous wall close to the channel interface would be subjected to a larger supply of reactants than otherwise assumed if Darcy's law would have been used.

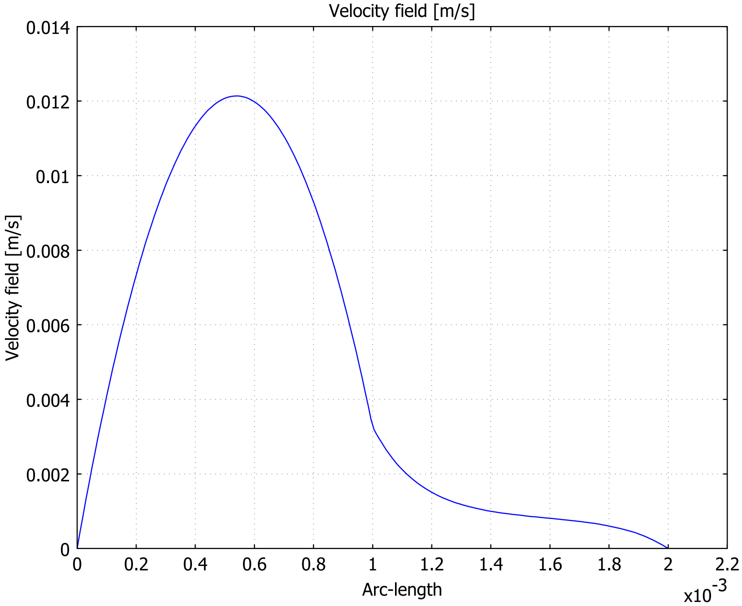


Figure 2-24: Cross section of the velocity field (modulus of velocity) in the middle of the modeling domain. The gradual reduction of viscous-dominated momentum transport to pressure-driven is evident in the region of the porous media close to the interface.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/porous_free`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. From the **Space dimension** list, select **2D**.

3 From the list of application modes, choose **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1[kg/m^3]`	`Density`
`eta`	`1e-5[Pa*s]`	`Viscosity`
`epsilon`	`0.4`	`Porosity`
`k`	`1e-8[m^2]`	`Permeability`
`v0`	`1[cm/s]`	`Inlet velocity`

GEOMETRY MODELING

1 Press the Shift key and click the **Rectangle/Square** button on the Draw toolbar.

2 Specify the following parameters in the corresponding edit fields:

PROPERTY	VALUE
Width	`1e-3`
Height	`6e-3`
Base	Corner
x	0
y	`-3e-3`

3 Click **OK**.

4 Press the Shift key and click the **Rectangle/Square** button.

5 Draw a second rectangle by entering the values below:

PROPERTY	VALUE
Width	`1e-3`
Height	`8e-3`
Base	Corner
x	`-1e-3`
y	`-4e-3`

6 Click **OK**.

7 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1.

3 Set ρ to `rho` and η to `eta`.

4 Select Subdomain 2.

5 Select the **Flow in porous media (Brinkman equations)** check box.

6 Set ρ to `rho`, η to `eta`, ε_p to `epsilon`, and **k** to `k`.

7 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select the appropriate entry from the **Boundary selection** list and enter boundary conditions according to the following table:

SETTINGS	BOUNDARY 2	BOUNDARY 3
Boundary type	Inlet	Outlet
Boundary condition	Velocity	Pressure, no viscous stress
u_0	0	
v_0	v0	
p_0		0

3 Click **OK**.

MESH GENERATION

In order to resolve the velocity profile close to the interface between the open channel and the porous domain, a finer mesh is required at this boundary.

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** option button.

3 In the **Maximum element size** edit field, type `2e-4`.

4 Click the **Boundary** tab.

5 Select Edge 5, then type `1e-4` in the **Maximum element size** edit field.

6 Click the **Remesh** button.

7 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

Postprocessing and Visualization

The default plot shows the velocity field, as illustrated in Figure 2-23. To visualize the velocity in a horizontal cross-section across the channel and the porous domain, follow these steps:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 Specify the following **Cross-section line data**:

PROPERTY	VALUE
x0	`-1e-3`
x1	`1e-3`
y0	0
y1	0

3 Click **OK** to reproduce Figure 2-24.

Turbulent Flow Through a Bending Pipe

Introduction

This example models the fluid flow through a bending pipe at high Reynolds number. It compares results obtained using both the k-ε and k-ω turbulence models with experimental data. The example contains detailed descriptions of how to make the modeling as accurate as possible.

Model Definition

Figure 2-25 shows the geometry of a generic bending pipe (Ref. 1). The pipe has a diameter of 1 meter and a total length of 6.71 m.

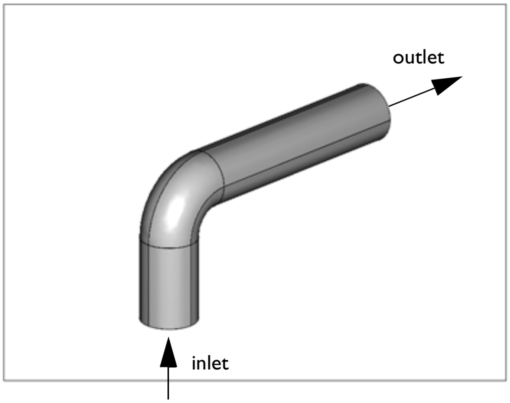


Figure 2-25: Geometry of the bending pipe. The pipe diameter is 1 m.

Because of the way the geometry is generated, the modeling domain is a union of three subdomains as shown in Figure 2-26.

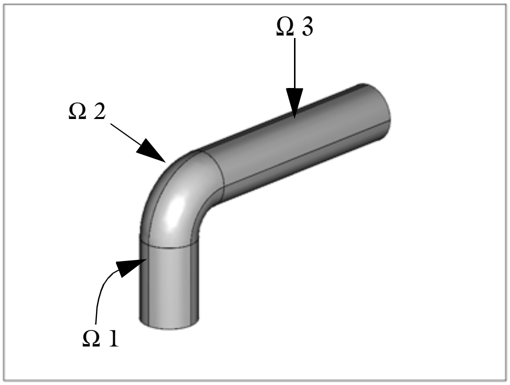


Figure 2-26: Subdomain decomposition of the geometry.

The flow characteristics are determined by the Reynolds number, which is defined as

$$\mathrm{Re} = \frac{\rho U_{\mathrm{ref}} L_{\mathrm{ref}}}{\eta}.$$

Here, ρ is the density and η denotes the dynamic viscosity, while U_{ref} and L_{ref} are the reference velocity and length, respectively. For this example it is suitable to choose U_{ref} as the inlet velocity and L_{ref} as the pipe diameter. Experimental data is available from Ref. 1 for $\mathrm{Re} = 3\cdot 10^5$. At such high Reynolds number, the flow is turbulent and a turbulence model must be used. The Chemical Engineering Module supplies two RANS models: the standard k-ε turbulence model and the Wilcox revised k-ω turbulence model from 1998. In this model, you compare the velocity profiles obtained using these two turbulence models to the experimental data.

You model the fluid as a generic fluid with $\rho = 1\ \mathrm{kg/m^3}$ and $\eta = 1/(3\cdot 10^5)$ Pa·s. The closest physical correspondence is air with rather low viscosity.

BOUNDARY CONDITIONS

At the inlet there is a uniform flow of velocity 1 m/s in the z direction. The turbulent length scale is $0.07D$, where $D = 1$ m is the pipe diameter, and the turbulent intensity is set to 5%, which is typical for fully turbulent internal flows. A constant pressure is specified at the outlet, and the flow vector is constrained to be normal to the outlet.

The model uses wall functions as boundary conditions on all other boundaries. The wall functions implemented in COMSOL Multiphysics are so called “lift off wall functions," that is, the computational domain is displaced a small distance, δ_w, from the surface. In this case, this is handled by drawing a domain with a smaller radius than the radius of the modeled pipe. The wall functions assume that the displacement expressed in viscous units, δ_w^+, falls between 30 and some upper limit dependent on the Reynolds number, in this case roughly 300. The correct procedure is for you to guess a displacement distance, δ_w, so that $30 \le \delta_w^+ \le 300$. If this is not the case, you must redraw the computational domain, choosing another value for δ_w. In this model, you set the initial guess for δ_w to be 1 cm, giving the computational domain a radius of 0.49 m compared to 0.50 m for the modeled pipe. For more information on wall functions, see "Logarithmic Wall Function" on page 141 of the *Chemical Engineering Module User's Guide*.

CORNER SMOOTHING

All nodes on the circles bounding the interior boundaries (see Figure 2-26) have two wall normals, one for each subdomain. The no-penetration condition of the wall functions results in two distinct directions in which there can be no mass flux. If this is not considered, the existing equations fulfill the constraints by forcing the flow to be stagnate at the points of intersection, which is of course unphysical. COMSOL Multiphysics provides *corner smoothing* as an application mode property for the k-ε and k-ω turbulence models to deal with this issue. An extra vectorial equation is introduced on the boundaries, and its solution is a smoothly varying wall normal. This smoothed wall normal is then used in the boundary conditions for the velocities.

Results and Discussion

Figure 2-27 shows a boundary plot of the application mode variable `dwplus_chns` for δ_w^+. The scale is restricted to $30 \le \delta_w^+ \le 300$, and by rotating the plot, you can see that the wall is complete. If δ_w^+ would have fallen outside the permitted range, there would have been areas in the boundary plot with no results. Because there are none, you can conclude that the choice of $\delta_w = 0.01$ m fulfills the above mentioned assumption for the wall functions.

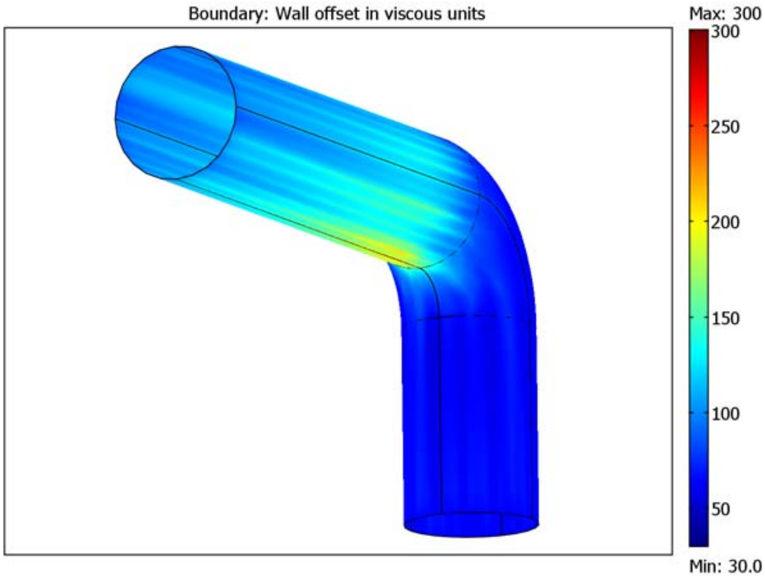


Figure 2-27: Boundary plot of δ_w^+ *from the* k-ε *solution.*

Figure 2-28 compares the velocity, U, along the line from $(1.58, 0, 0.3)$ to $(1.58, 0, 1.3)$ computed with the k-ε and k-ω turbulence models to experimental data. While both methods give fair results, the k-ω turbulence model is slightly more accurate at the wall. This implies that *k*-ω gives a better prediction of the drag and hence of the friction loss in the pipe.

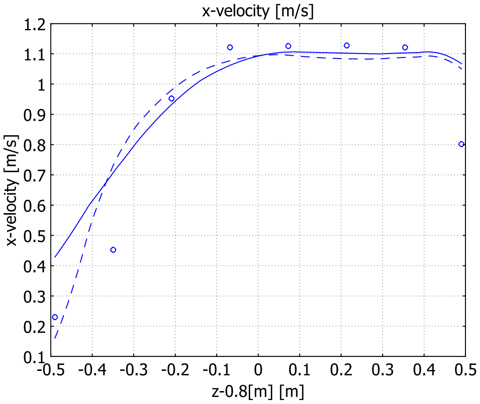


Figure 2-28: Streamwise velocity profile along the line between the points (1.58, 0, 0.3) and (1.58, 0, 1.3). The lines represent results from the k-ε (solid line) and k-ω (dashed line) models. The circles correspond to experimental data (Ref. 1).

Reference

1. I. E. Idelchik, *Handbook of Hydraulic Resistance*, 1996, Begell House Publishers.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/bending_pipe`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. From the **Space dimension** list, select **3D**.
3. From the list of application modes choose **Chemical Engineering Module>Momentum Transport>Turbulent Flow> k-ε Turbulence Model**.
4. Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu, select **Work-Plane Settings**. Click **OK**.

2 Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar. In the **Radius** edit field type `0.49`, then click **OK**.

3 From the **Draw** menu select **Revolve**.

4 In the **α2** edit field type `90`. Click the radio button **Angle from x-axis**, then type `0.8` in the **x** edit field. Click **OK**.

5 In the **Model Tree** select **Geom2**.

6 Select **Extrude** from the **Draw** menu.

7 In the **Distance** edit field type `-1.45`, then click **OK**.

8 From the **Draw** menu select **Work-Plane Settings**.

9 Click the **Face Parallel** tab and select **REV1>6** from the **Face selection** list. Click **OK**.

10 Double-click the lower left circle to open the **Circle** dialog box. Type `0.49` in both the **x** and **y** edit fields. Click **OK**.

11 Select **Extrude** from the **Draw** menu.

12 In the **Distance** edit field type `4`, then click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu select **Constants**. Enter the following settings:

NAME	EXPRESSION	DESCRIPTION
`Re`	`3e5`	`Reynolds number`

2 Click **OK**.

3 Expand **Geom1** in the **Model Tree** and right-click **k-ε Turbulence Model (chns)**, then click **Properties**.

4 From the **Corner smoothing** list select **On**, then click **OK**.

MESH GENERATION

Since the flow varies significantly less in the streamwise direction than in the radial direction, swept meshes are excellent where the pipe is straight. A swept mesh would however be inefficient in the bend and Subdomain 2 is therefore meshed using an unstructured mesh.

1 From the **Mesh** menu select **Free Mesh Parameters**.

2 Set **Predefined mesh sizes** to **Coarse**.

3 Click the **Boundary** tab. Select Boundaries 3 and 16, then type `0.25` in the **Mesh curvature factor** edit field.

4 Click **Mesh Selected**, then click **OK**.

5 From the **Mesh** menu, select **Swept Mesh Parameters**.

6 Select Subdomain 1, then select the **Manual specification of element layers** check box.

7 In the **Number of element layers** edit field type `6`.

8 Click **Mesh selected**.

9 Select Subdomain 3, then select the **Manual specification of element layers** check box.

10 In the **Number of element layers** edit field type `16`.

11 Click **Mesh Selected**, then click **OK**.

12 From the **Mesh** menu, select **Free Mesh Parameters** again.

13 From the **Predefined mesh sizes** list select **Fine**.

14 Click the **Subdomain** tab. Select Subdomain 2, then click **Mesh Selected**.

15 Click **OK**.

SUBDOMAIN SETTINGS

1 From the **Physics** menu select **Subdomain Settings**.

2 Select one of the subdomains, then press Ctrl+A to select all of them.

3 In the **Dynamic viscosity** edit field, type `1/Re`.

4 Click **OK**.

BOUNDARY CONDITIONS

1 From the **Physics** menu, select **Boundary Settings**.

2 Apply boundary conditions according to the following list.

SETTINGS	BOUNDARY 3	BOUNDARY 16	ALL OTHERS
Boundary type	Inlet	Outlet	Wall
Boundary condition	Velocity	Pressure	Logarithmic wall function
w_0	1		
L_T	`0.07`		
p_0		0	
δ_w			`0.01`

3 Click **OK**.

COMPUTING THE k-ε SOLUTION

It is possible to solve this rather small problem using direct solvers.

1 Click the **Solver Parameters** button on the Main toolbar.

2 For **Group 1** click the **Linear Solver Settings** button.

3 From the **Linear system solver** list select **Direct (PARDISO)**.

4 Click **OK**.

5 For **Group 2** click the **Linear Solver Settings** button.

6 From the **Linear system solver** list select **Direct (PARDISO)**.

7 Click **OK**.

8 Click **OK.**

9 Click the **Solve** button on the Main toolbar.

POSTPROCESSING THE k-ε RESULTS

1 Click the **Plot Parameters** button on the Main toolbar.

2 Click the **Slice** tab and clear the **Slice plot** check box.

3 Click the **Boundary** tab and select the **Boundary plot** check box.

4 In the **Expression** edit field, type `dwplus_chns`.

5 Click the **Range** button.

6 Clear the **Auto** check box.

7 Type `30` in the **Min** edit field and `300` in the **Max** edit field.

8 Click **OK** twice.

This yields a plot like the one shown in Figure 2-27. Rotate the plot to verify that all of the pipe wall is represented.

Next, import the experimental data:

9 From the **Options** menu choose **Functions**.

10 Click the **New** button.

11 In the **Function name** edit field, type `exp_data`. Click the **Interpolation** button and then select **File** from the **Use data from** list.

12 Click the **Browse** button and locate the file `3Dpipe_exp-data_Re300e3.txt` in the `models/Chemical_Engineering_Module/Fluid_Flow` folder in the COMSOL Multiphysics installation directory. Click **Open**, then click **OK**.

13 From the **Extrapolation method** list, select **Constant**.

14 Click **OK** to close the **Functions** dialog box.

15 From the **Solve** menu, select **Update Model**.

16 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

17 Click the **General** tab, then select the **Keep current plot** check box.

18 Click the **Line/Extrusion** tab.

19 In the **Expression** edit field, type `exp_data(z-0.8)`.

20 In the **Cross-section line data** area, enter values according to this table:

X0	X1	Y0	Y1	Z0	Z1
`1.58`	`1.58`	`0`	`0`	`0.3`	`1.3`

21 Click the **Expression** option button, then click the **Expression** button.

22 In the **Expression** edit field, type `z-0.8`. Click **OK**, then click **OK** again.

23 Click the **Line Settings** button.

24 From the **Line style** list, select **None** and from the **Line marker** list, select **Circle**. Click **OK**.

25 Click **Apply**.

26 Go back to the **Cross-Section Plot Parameters** dialog box.

27 From the **Predefined quantities** list, select **k-ε Turbulence model (chns)>x-velocity**.

28 Click the **Line Settings** button.

29 Select **Solid line** from the **Line style** list and **None** from the **Line marker** list. Click **OK**.

30 Click **OK**.

Leave the resulting plot window open; you finish the plot later on.

COMPUTING THE k-ω SOLUTION

Next re-calculate a solution using the k-ω turbulence model. When switching turbulence models, COMSOL Multiphysics automatically adjusts the initial values so that the computation starts from the existing k-ε solution.

1 Return to the COMSOL Multiphysics user interface.

2 Right-click **k-ε Turbulence Model (chns)** in the **Model Tree**, then click **Properties**.

3 From the **Turbulence model** list, select **k-ω**. Click **OK**.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING THE k-ω SOLUTION

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 Click the **Line Settings** button. From the **Line style** list, select **Dashed line**. Click **OK**.

3 Click **OK** to obtain the plot in Figure 2-28.

Oscillating Liquid Cobalt Droplet

Introduction

Cemented tungsten carbides are hard metals used in steel cutting tools. They are produced by heating a powder consisting typically of tungsten carbide (WC) grains and cobalt (Co) grains. When the powder is heated, the cobalt melts but the tungsten carbide remains solid. The liquid cobalt glues the tungsten carbide grains together and forces air to flow out of the material. When the medium is cooled down, a solid hard metal forms. The process is called liquid phase sintering.

You can determine the character of the flow of air and liquid cobalt by simulating a droplet of cobalt surrounded by air. Such a simulation reveals the relevant time scales and shows whether the flow is dominated by inertia or viscous forces. This example shows how COMSOL Multiphysics can simulate a liquid cobalt droplet using a reinitialized mass-conserving level set method. The model studies an initially ellipsoidal droplet that starts to oscillate because of the large surface tension of liquid cobalt. The droplet's size corresponds to a typical size of the cobalt grains in liquid phase sintering, roughly 10 μm. From the results you can study the frequency and damping of the droplet's oscillations.

Model Definition

Figure 2-29 shows the initial shape of the cobalt droplet. Because of its symmetry you can use a 2D axisymmetric model. You can model the fluid flow of air and liquid cobalt with the Navier-Stokes equations in combination with a level set equation to track the interface between the air and cobalt. This model uses a reinitialized level set method both in conservative and non-conservative form.

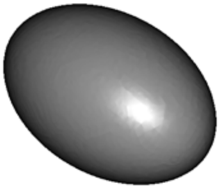


Figure 2-29: Initial droplet shape.

MASS AND MOMENTUM TRANSPORT

The Navier-Stokes equations describe the transport of mass and momentum of incompressible fluids. The Navier-Stokes equations with surface tension are

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)-\nabla\cdot(\eta(\nabla\mathbf{u}+\nabla\mathbf{u}^T))+\nabla p = \sigma\kappa\delta\mathbf{n}$$

$$\nabla\cdot\mathbf{u} = 0$$

Here, ρ denotes density (kg/m^3), η is the dynamic viscosity (Ns/m^2), $\mathbf{u}$ equals the velocity (m/s), p is the pressure (Pa), and σ represents the surface-tension coefficient (N/m). In addition, $\mathbf{n}$ is the unit vector normal to the interface, and $\kappa = -(\nabla\cdot\mathbf{n})$ is the mean curvature of the interface. Further, δ is a Dirac delta function with support only at the interface, which means that δ is zero away from the interface and that the integral of δ equal the area of the interface. You can write the surface-tension force as

$$\sigma\kappa\mathbf{n}\delta = \nabla\cdot\mathbf{T}$$

$$\mathbf{T} = \sigma(\mathbf{I}-(\mathbf{n}\mathbf{n}^T))\delta$$

where $\mathbf{I}$ is the identity matrix. By using this formulation you can include surface tension without having to calculate derivatives of the interface normal, $\mathbf{n}$.

REPRESENTATION AND CONVECTION OF THE FLUID INTERFACE

This model uses a level set method to describe and to convect the interface. The 0.5 contour of a function ϕ defines the interface. ϕ is 0 in air and 1 in cobalt. In a transition layer close to the interface, ϕ goes smoothly from 0 to 1. The normal to the interface is then

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$$

The interface moves with the fluid velocity, $\mathbf{u}$, at the interface. The following equation describes the reinitialized convection of the interface:

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}+\varepsilon\nabla\phi\right)$$

By adding the terms on the right-hand side you reinitialize the level set function. This means that you keep the thickness of the transition layer constant in time.

Note that because $\nabla\cdot\mathbf{u} = 0$, you can write the convective term in the conservative form and can thus rewrite the level set equation as

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \gamma \nabla \cdot \left(-\phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} + \varepsilon \nabla \phi \right) \tag{2-21}$$

which is important to obtain numerical conservation.

The density and the viscosity are discontinuous, and the surface-tension force is singular at the interface. To simplify the numerical calculations, let the density and viscosity go smoothly between the values for air and cobalt. This is obtained by setting

$$\rho = \rho_{\mathrm{air}} + (\rho_{\mathrm{cobalt}} - \rho_{\mathrm{air}})\phi$$

and

$$\mu = \mu_{\mathrm{air}} + (\mu_{\mathrm{cobalt}} - \mu_{\mathrm{air}})\phi$$

You can smooth the surface-tension force by letting

$$\delta = 6|\phi(1-\phi)||\nabla \phi|$$

Here it is important that you use a reinitialized level set method. The smoothing of density, viscosity, and surface tension is acceptable only if the thickness of the interface is constant.

The following table gives the physical properties of liquid cobalt and air:

	DENSITY	**DYNAMIC VISCOSITY**	**SURFACE TENSION**
cobalt	7760 kg/m^3	$5 \cdot 10^{-3}$ Pa·s	1.873 N/m
air	1.29 kg/m^3	$1.67 \cdot 10^{-5}$ Pa·s	

INITIAL CONDITIONS

Initially the droplet is at rest and has an ellipsoidal shape. The initial ϕ (see Figure 2-30) gives the correct shape of the droplet.

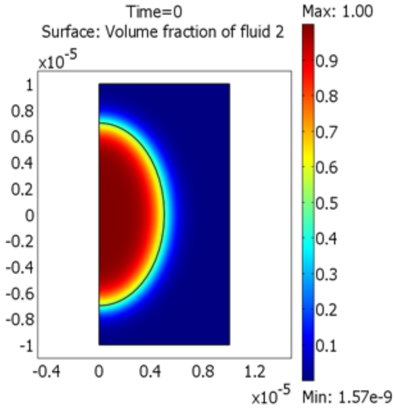


Figure 2-30: Initial ϕ .

BOUNDARY CONDITIONS

The droplet is placed in a cylindrical box using no-slip conditions, $\mathbf{u} = \mathbf{0}$, on all walls. Because there are no conditions for p on any boundary, you should fix p at a single point.

Results and Discussion

The initial ϕ appears in Figure 2-30. The model shows that the droplet immediately starts to oscillate when it is released from its initial state. Figure 2-31 and Figure 2-32 show the position of the interface and the velocity field after $5 \cdot 10^{-7}$ s and $1 \cdot 10^{-5}$ s, respectively.

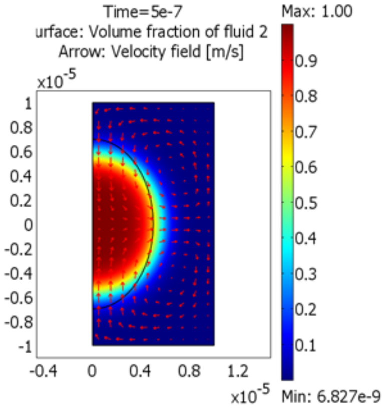


Figure 2-31: Velocity field and level set function at $t = 5 \cdot 10^{-7}$ *s.*

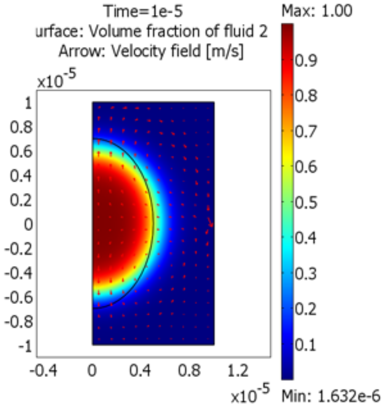


Figure 2-32: Velocity field and level set function at $t = 10^{-5}$ *s.*

Figure 2-33 shows the ratio between the two semiaxes of the ellipse as a function of time. The figure shows results using the conservative as well as the non-conservative formulation. You can see that the time scale is very small; the period of the oscillations is about $2 \cdot 10^{-6}$ s.

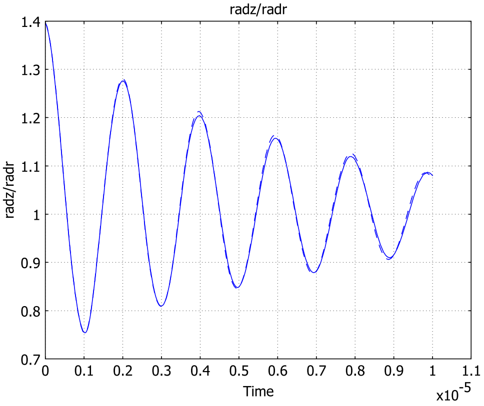


Figure 2-33: Ratio between axes as function of time. The dashed line corresponds to the conservative form and the solid line to the non-conservative form.

The total mass of the droplet is

$$M(t) = \int_{\Omega} \rho_{\mathrm{cobalt}} \phi(t) d\Omega$$

Because there is no production or flow of cobalt through the boundaries, the mass should not change with time. To check the conservation, Figure 2-34 plots the values for $M(t)$ using the conservative and the non-conservative equation forms.

Clearly, the conservative form results in exact conservation, while the non-conservative form results in a mass loss of about 0.3%.

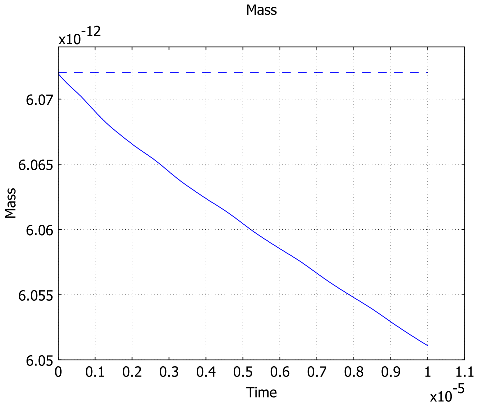


Figure 2-34: Conservation of total mass of cobalt droplet. The dashed line corresponds to the conservative form and the solid line to the non-conservative form.

References

1. C.J. Smithells, *Smithells Metals Reference Book*, Oxford, 1998.

2. E. Olsson and G. Kreiss, “A conservative level set method for two phase flow,” *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

Modeling in COMSOL Multiphysics

It is easy to set up the model using the Level Set Two-Phase Flow application mode. You only need to specify the physical parameters, boundary conditions, and the initial position of the interface. Before you can start the fluid flow calculation, you initialize the level set function. Then, store the solution, switch the analysis type from Transient initialization to Transient, and start the two-phase flow calculation.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/oscillating_droplet`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list.

2 From the list of application modes, select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Level Set Two-Phase Flow, Laminar**.

3 Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar.

2 Set the **Width** to `1e-5`, the **Height** to `2e-5`, and **z** to `-1e-5`.

3 Click **OK**, then click the **Zoom Extents** button on the Main toolbar.

4 Shift-click the **Ellipse/Circle** button. Type `5e-6` in the **A-semiaxes** edit field and `7e-6` in the **B-semiaxes** edit field. Click **OK**.

5 Click the **Create Composite Object** on the Draw toolbar.

6 In the **Set formula** edit field, type `R1*E1+R1`. Here, `R1*E1` gives the intersection between the ellipse and the rectangle. Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (units and descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
`rho_air`	`1.293[kg/m^3]`	`Density of air`
`rho_cob`	`7.760e3[kg/m^3]`	`Density of cobalt`
`eta_air`	`1.67e-5[Pa*s]`	`Viscosity of air`
`eta_cob`	`5e-3[Pa*s]`	`Viscosity of cobalt`
`sigma`	`1.873[N/m]`	`Surface tension`

3 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomains 1 and 2, then enter the following physical properties:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ_1	`rho_air`	`Density, fluid 1`
η_1	`eta_air`	`Dynamic viscosity, fluid 1`
ρ_2	`rho_cob`	`Density, fluid 2`
η_2	`eta_cob`	`Dynamic viscosity, fluid 2`

3 On the **Sources/Sinks** page, type `sigma` in the **Surface tension coefficient** edit field.

4 Go to the **Init** tab and select Subdomain 2 only. Select the option button **Fluid 2**.

5 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundaries 1, 3, and 4, then select **Symmetry boundary** from the **Boundary type** list and **Axial symmetry** from the **Boundary condition** list.

3 Select Boundaries 7 and 8. Select the **Interior boundaries** check box, then select the boundary condition **Initial fluid interface**. Click **OK**.

Point Settings

1 From the **Physics** menu, select **Point Settings**.

2 Select Point 7. Select the **Point constraint** check box. Leave the value for $\mathbf{p_0}$ at 0.

3 Click **OK**.

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar.

2 Click the **Refine Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

First make an initial calculation to obtain a good initial value for ϕ.

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, type `0 2e-6` in the **Times** edit field. Click **OK**.

3 Click the **Solve** button on the Main toolbar. This creates a good initial solution to the level set function.

Use the obtained solution as an initial condition for the simulation of the droplet motion.

1. Click the **Solver Manager** button on the Main toolbar.
2. On the **Initial Value** page, click the **Store Solution** button.
3. Select only the time **2e-6**, then click **OK**.
4. In the **Initial value** area, select **Stored solution**.
5. From the **Solution at time** list, select **2e-6**. Click **OK**.
6. From the **Physics** menu, select **Properties**. Change the **Analysis type** to **Transient**. Click **OK**.
7. Click the **Solver Parameters** button on the Main toolbar.
8. On the **General** page, type `0:2e-7:1e-5` in the **Times** edit field.
9. Click the **Time Stepping** tab. In the **Times to store in output** list, select **Time steps from solver**. Click **OK**.
10. Click the **Solve** button on the Main toolbar.

The calculations take roughly 20–40 minutes.

POSTPROCESSING AND VISUALIZATION

1. Click the **Plot Parameters** button on the Main toolbar.
2. Click the **Arrow** tab. Select the **Arrow plot** check box.
3. Select **Velocity field** from the **Predefined quantities** list.
4. Type `10` in the **Number of points/r points** edit field and type `20` in the **Number of points/z points** edit field.
5. Click the **Animate** tab.
6. In the **Solutions to use** area, select **Interpolated times** from the **Select via** list.
7. In the **Times** edit field type `0:2e-7:1e-5`.
8. Click the **Start Animation** button, then click **OK** to close the **Plot Parameters** dialog box.

To check the conservation, perform the following steps:

1. Choose **Options>Integration Coupling Variables>Subdomain Variables**.
2. Select Subdomains 1 and 2, then define a variable with the **Name** `Mass` by the **Expression** `2*pi*r*phi*rhocob`.
3. Click **OK**.
4. From the **Solve** menu, select **Update Model**.
5. From the **Postprocessing** menu, select **Domain Plot Parameters**.

6 Click the **Point** tab and select any point.

7 In the **Expression** edit field, type `Mass`.

8 Click **OK**.

To plot the ratio between the *r*- and *z*-axes of the droplet perform the following steps:

1 Click the **Line** button on the Draw toolbar.

2 Click at the coordinate point (0, 0) and then right-click the point (1e-5, 0) to draw a line between (0,0) and (1e-5,0).

3 Choose **Options>Integration Coupling Variables>Boundary Variables**.

4 Select Boundaries 1 and 3, then define a variable with the **Name** `radz` by the **Expression** `phi`.

5 Select Boundaries 5 and 8, then define a variable with the **Name** `radr` by the **Expression** `phi`.

6 Click **OK**.

7 From the **Solve** menu, select **Update Model**.

8 From the **Postprocessing** menu select **Domain Plot Parameters**.

9 Click the **Point** tab and select any point.

10 In the **Expression** edit field, type `radz/radr`.

11 On the **General** page, select **New figure** from the **Plot in** list.

12 Click **OK**.

In some cases the conservation of the non-conservative form is too poor. It is then useful to switch to the conservative form. This form results in exact mass conservation but is harder to solve numerically. To make a simulation using the conservative formulation, perform the following steps:

1 From the **Physics** menu, select **Properties**.

2 From the **Two-phase flow** list, select **Conservative level set**. Click **OK**.

3 A new mesh was created when you added the line along the *r*-axis to the geometry. Click the **Refine Mesh** button to refine the grid.

4 Click the **Solve** button on the Main toolbar to start a new calculation.

In this case, the calculations take about 60–120 minutes.

5 From the **Postprocessing** menu, select **Domain Plot Parameters**.

6 Click the **Point** tab and select any point.

7 In the **Expression** edit field, type `radz/radr`.

8 Click the **Line Settings** button. From the **Line style** list, select **Dashed line**. Click **OK**.

9 Click the **General** tab. From the **Plot in** list, select **Figure 2**.

10 Select the **Keep current plot** check box, then click **Apply**.

11 From the **Plot in** list, select **Figure 1**.

12 Click the **Point** tab and select any point.

13 In the **Expression** edit field, type `Mass`, then click **OK**.

The plots in Figure 1 and Figure 2 correspond to Figure 2-33 and Figure 2-34, respectively.

Turbulent Flow over a Backward-Facing Step

Introduction

The backward-facing step is an interesting case for studying the performance and solution strategy of a turbulence model, because it presents both turbulent channel flow and recirculation. In this case, the flow is subjected to a sudden increase of the cross section, resulting in a separation of flow starting at the point of expansion. Spatial variations in the velocity field cause a production of turbulence outside the wall region and its interaction with the mean flow influences the size of the separation zone. The size of the zone, or the reattachment length, is one of the quantities that must be predicted accurately by a turbulence model.

The Reynolds number and the expansion ratio are two numbers that can be used to characterize the flow. Existing data indicate that the length of the reattachment zone increases with the expansion ratio. The Reynolds numbers are calculated based on the step height and the inlet free stream velocity. The reattachment length increases with Reynolds number until 1200, where it then decreases between $1200 < \mathrm{Re} < 6600$, to then be relatively constant for higher Reynolds numbers, when the flow is in state of fully developed turbulence.

Model Definition

This model treats the backward-facing step for a flow configuration with an area expansion ratio of 3/2. Assuming that the channel is deep enough, you can neglect variations in the z direction and reduce the problem from 3D to 2D. The step height, h, is chosen as the length scale, the inlet is set to $2h$, the initial channel length to $8h$, and the length of the channel after the expansion is set to $35h$ (see Figure 2-35). Do not confuse this h with the predefined variable h for the mesh element diameter, which you use in the model when specifying the logarithmic wall function.

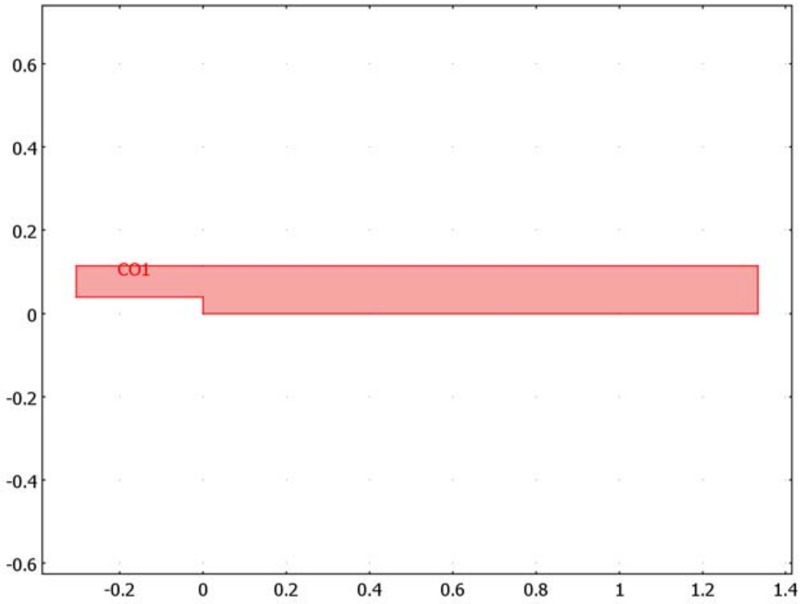


Figure 2-35: Model geometry.

The k-ε model describes turbulent flow in the domain. The equations for the momentum transport and continuity are the following:

$$\rho\frac{\partial\mathbf{U}}{\partial t}-\nabla\cdot\left[\left(\eta+\rho\frac{C_\mu k^2}{\sigma_k\ \varepsilon}\right)\cdot(\nabla\mathbf{U}+(\nabla\mathbf{U})^T)\right]+\rho\mathbf{U}\cdot\nabla\mathbf{U}+\nabla P = 0 \qquad (2\text{-}22)$$

$$\nabla\cdot\mathbf{U} = 0$$

where ρ denotes the density of the fluid (kg/m^3), **U** represents the averaged velocity (m/s), η the dynamic viscosity (N·s/m^2), P the pressure (Pa), k the turbulence energy (m^2/s^2), and ε the dissipation rate of turbulence energy (m^2/s^3). The turbulence energy equation is given by

$$\rho\frac{\partial k}{\partial t}-\nabla\cdot\left[\left(\eta+\rho C_\mu\frac{k^2}{\varepsilon}\right)\nabla k\right]+\rho\mathbf{U}\cdot\nabla k = \frac{1}{2}\rho C_\mu\frac{k^2}{\varepsilon}(\nabla\mathbf{U}+(\nabla\mathbf{U})^T)^2-\rho\varepsilon \qquad (2\text{-}23)$$

and the dissipation equation by

$$\rho\frac{\partial\varepsilon}{\partial t}-\nabla\cdot\left[\left(\eta+\rho C_\mu\frac{k^2}{\varepsilon}\right)\nabla\varepsilon\right]+\rho\mathbf{U}\cdot\nabla\varepsilon = \frac{1}{2}\rho C_{\varepsilon 1}k(\nabla\mathbf{U}+(\nabla\mathbf{U})^T)^2-\rho C_{\varepsilon 2}\frac{\varepsilon^2}{k} \qquad (2\text{-}24)$$

The model constants in the above equations are determined from experimental data and are set to the values in Table 2-2.

TABLE 2-2: CONSTANTS USED IN THE TURBULENCE ENERGY AND DISSIPATION EQUATIONS

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

At the inlet, set the velocity component in the x direction, u, to $u_0 = 18.2$ m/s, and that in the y direction, v, to zero. Further, specify a constant pressure value of 0 at the outlet and logarithmic wall functions at the solid walls.

Results

Figure 2-36 shows the velocity field. The low flow speed near the lower corner after the step indicates the presence of a recirculation zone.

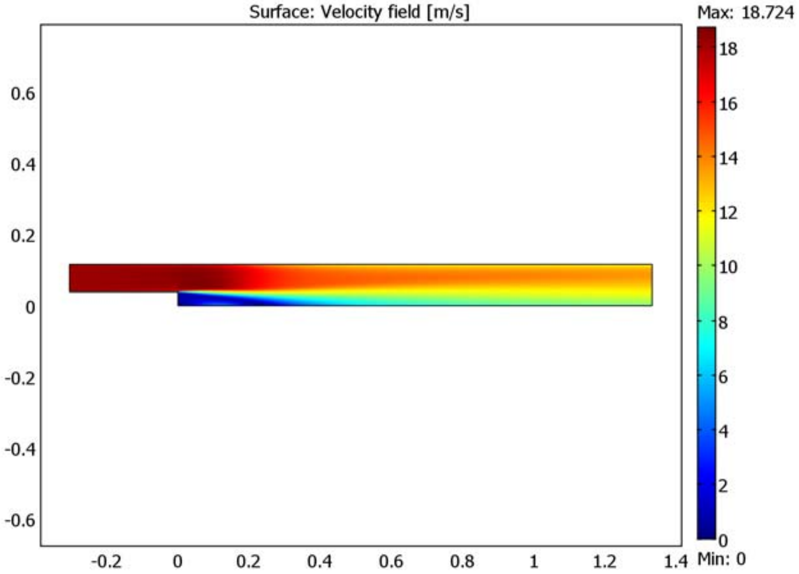


Figure 2-36: Velocity field (modulus of the velocity vector) of flow over a backstep.

Figure 2-37 zooms in on the region around the backstep. The plot, displaying the magnitude of the velocity together with velocity streamlines, shows that a recirculation zone appears after the backstep.

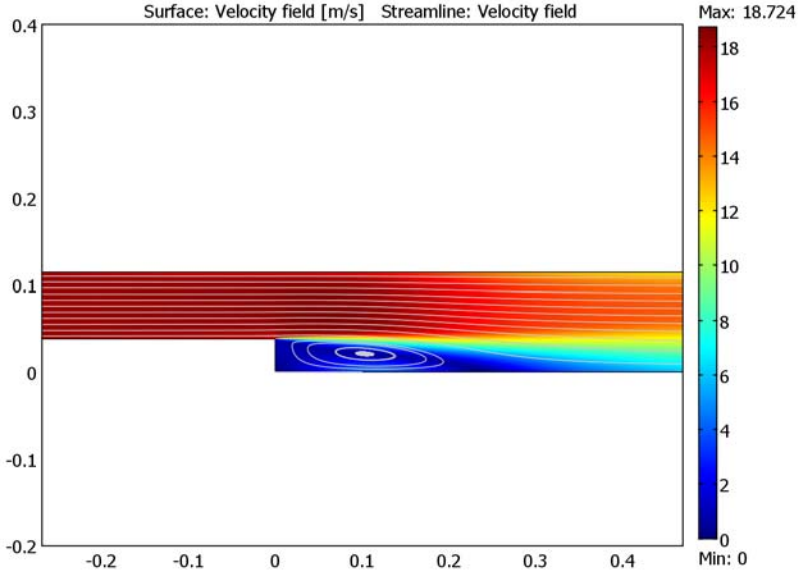


Figure 2-37: Magnitude and streamline plot of the velocity field. The figure shows a recirculation region after the backstep.

You can determine the size of the recirculation zone by plotting the zero contour of the x-velocity and coloring it with x/h. The maximum of x/h along that contour gives the size of the recirculation zone. Figure 2-38 shows the corresponding plot. The figure shows that the obtained reattachment length is 6.3. Compare this to results presented in Ref. 1. There, the reattachment length is experimentally determined to be 7.1, while numerical results using a k-ε turbulence model yield 6.1.

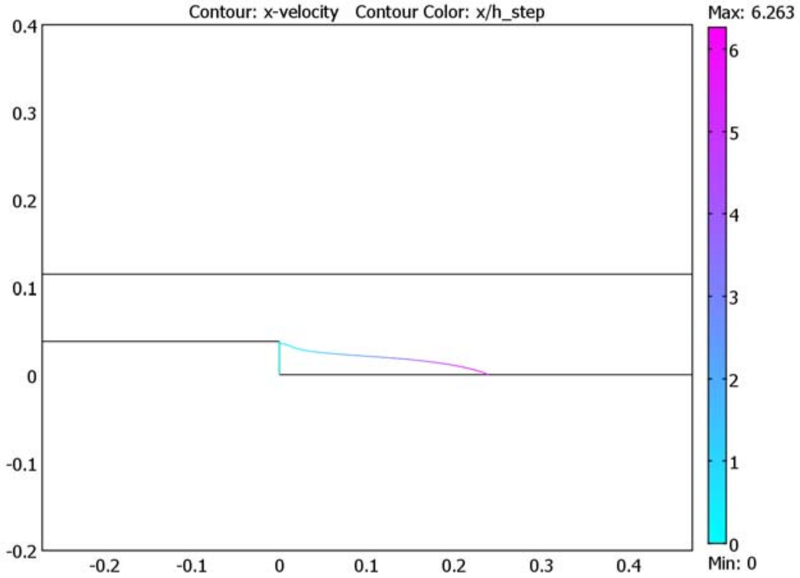


Figure 2-38: Calculation of the recirculation zone. The plot shows the contour corresponding to zero velocity in the x direction. The contour is colored by the scaled distance from the step, x/h. Its maximum value gives the recirculation length, in this case 6.3.

The section below explains in detail how to create this model in the Chemical Engineering Module.

Reference

1. *1st NAFEMS Workbook of CFD Examples. Laminar and Turbulent Two-Dimensional Internal Flows*, NAFEMS, 2000.

Model Library path:

`Chemical_Engineering_Module/Fluid_Flow/turbulent_backstep`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **2D** from the **Space dimension** list.

3 From the **Application Modes** tree, select **Chemical Engineering Module>Momentum Transport>Turbulent Flow>k-ε Turbulence Model**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Enter the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1.23[kg/m^3]`	`Density`
`eta`	`1.79e-5[Pa*s]`	`Viscosity`
`v0`	`18.2[m/s]`	`Inlet peak velocity`
`h_step`	`3.81[cm]`	`Step height`
`Re`	`rho*v0*h_step/eta`	`Reynolds number (step)`

The Reynolds number value 47,648 appears in the **Value** column for `Re`.

GEOMETRY MODELING

1 Press the Shift key and click the **Rectangle/Square** button.

2 Enter rectangle dimensions according to the table below in the appropriate edit fields. When done, click **OK**.

OBJECT DIMENSIONS	EXPRESSION
Width	`0.3048`
Height	`0.0762`
x	`-0.3048`
y	`0.0381`

3 Repeat the procedure for another rectangle with the following dimensions:

OBJECT DIMENSIONS	EXPRESSION
Width	`1.3335`
Height	`0.1143`
x	0
y	0

4 Click the **Zoom Extents** button on the Main toolbar.

5 Click the **Create Composite Object** button on the Draw toolbar.

6 In the **Set formula** edit field, type `R1+R2`.

7 Clear the **Keep interior boundaries** check box, then click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1.

3 Type `rho` in the ρ edit field and `eta` in the η edit field.

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Setting**.

2 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3, 4, 5, 6	BOUNDARY 7
Boundary type	Inlet	Wall	Outlet
Boundary condition	Velocity	Logarithmic wall function	Pressure
u_0	`v0`		
v_0	0		
p_0			0
δ_w		`h/2`	

The variable `h` is a predefined variable for the mesh element diameter.

3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** option button.

3 Type 3 in the **Resolution of narrow regions** edit field, then click **OK**.

4 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button. Select the **Adaptive mesh refinement** check box.

2 Click the **Adaptive** tab.

3 Type 4 in the **Maximum number of refinements** edit field.

4 From the **Refinement method** list, select **Meshinit**.

5 Click **OK** to close the **Solver Parameters** dialog box.

6 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The first plot, shown in Figure 2-36, is generated automatically and shows a surface plot of the velocity field.

1 To visualize the mesh, click the **Mesh Mode** button on the Main toolbar.

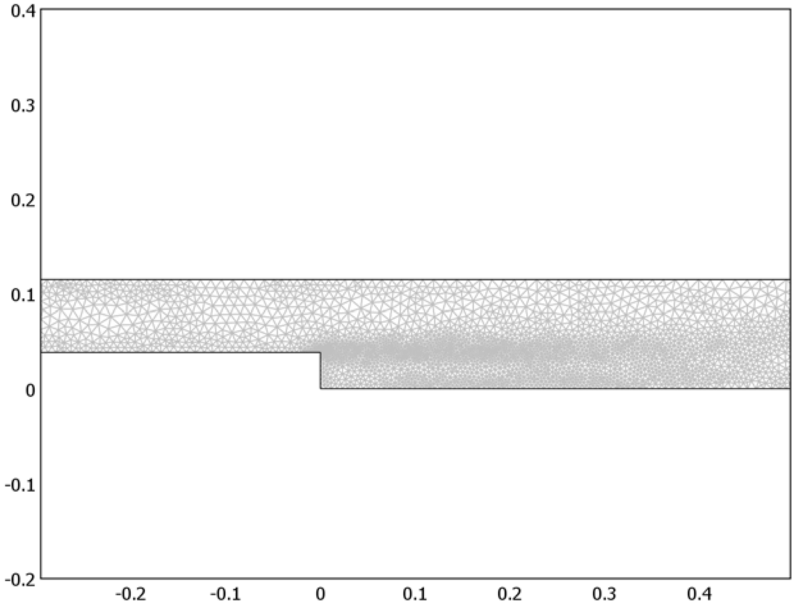


Figure 2-39: Plot of the mesh obtained using adaptive mesh refinement. Note that the mesh can vary slightly on different computers.

2 Click the **Plot Parameters** button on the Main toolbar.

3 On the **General** page, clear the **Surface** check box and select the **Contour plot** check box.

4 On the **Contour** page, type `u` in the **Expression** edit field.

5 Click the **Vector with isolevels** option button and type `0` in the associated edit field.

6 Click the **Color Data** tab and select the **Color data** check box. Type `x/h_step` in the **Expression** edit field.

7 Click **Apply**.

You should now obtain the plot in Figure 2-38.

8 Back in the **Plot Parameters** dialog box, click the **General** tab.

9 In the **Plot type** area, select the **Streamline** and the **Surface** check boxes and clear the **Contour** check box.

10 Click the **Streamline** tab.

11 Click the **Specify start point coordinates** option button. Type `0.1` in the **x** edit field and `linspace(0,0.13,20)` in the **y** edit field.

12 Click **OK** to generate the plot in Figure 2-37.

3

Heat Transfer and Non-Isothermal Flow—Tutorials and Benchmarks

This chapter contains examples of fluid flow models where the temperature varies, that is, non-isothermal flow models. Both laminar and turbulent flows are treated, and several examples demonstrate how you can set up a model accounting for heat transfer in solid as well as fluid domains.

Forced Turbulent Convection Cooling of a Hot Plate

Introduction

The following model demonstrates how to model a conjugate heat and mass transfer problem with COMSOL Multiphysics. The model uses the Non-Isothermal Flow predefined multiphysics coupling from the Chemical Engineering Module.

Figure 3-1 depicts the geometry: a horizontal stream of air that cools a thin and infinitely wide horizontal plate. The plate is at a uniform temperature at the bottom, and the flow is turbulent. This is a well-studied case of convection cooling that works well as a benchmark that demonstrates the accuracy of the modeling methods.

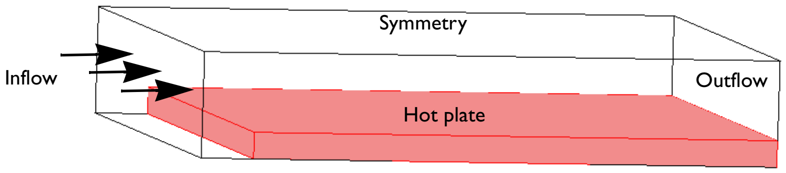


Figure 3-1: Forced convection cooling of a horizontal plate.

Model Definition

The model works with the following equations:

- Reynolds-averaged Navier-Stokes (RANS) equations in the air domain.
- The conductive and convective heat equation in the air and the solid (copper) wall.

The Non-Isothermal Flow predefined multiphysics coupling sets up these application modes together with applicable couplings, making it easy to model the fluid-thermal interaction.

The material properties for the fluid are those of air at atmospheric pressure, and for the solid plate those of copper. You can load these properties from the built-in materials library where the air properties are temperature dependent.

It is necessary to correct the fluid's thermal conductivity to take into account the effect of mixing due to eddies. The turbulence results in an effective thermal conductivity, k_{eff}, according to the equation

$$k_{\text{eff}} = k + k_T \qquad k_T = C_p \eta_T .$$

Here k is the physical thermal conductivity of the fluid (W/(m·K)), k_T is the turbulent conductivity (W/(m·K)), η_T denotes the turbulent viscosity (kg/(m·s)), and C_p equals the heat capacity (J/(kg·K)). With COMSOL Multiphysics you can easily obtain the effective conductivity by using the ready-made fluid group in the fluid domain. In the group, the variable for turbulent conductivity is already given in the Convection and Conduction application mode for the fluid.

Figure 3-2 depicts the model with its boundary conditions.

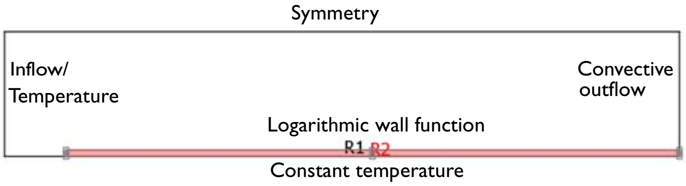


Figure 3-2: Modeled 2D geometry with boundary conditions.

The boundary conditions for the problem are:

- k-ε equations in the fluid domain
  - Specified velocity at the inlet
  - Specified pressure at the outlet
  - Symmetry at the top boundary
  - Logarithmic wall function at the plate's surface boundaries
- Heat transport equations
  - Room temperature at the inlet
  - Convection-dominated transport at the outlet
  - Symmetry at the top boundary
  - Thermal wall function at the plate/air interface
  - Fixed temperature at the bottom of the heated plate

To model the solid-fluid interfaces, the model uses the logarithmic wall function boundary condition for turbulent flow, in which an algebraic relationship—the logarithmic wall function—describes the momentum transfer at the solid-fluid interface. This means that the modeled domain ends at the top of the laminar boundary layer where the fluid experiences a significant wall-tangential velocity. This is an important aspect to consider when modeling the heat transfer. Like the fluid velocity, the temperature is not modeled in the laminar sublayer. Instead of assuming the temperature to be continuous across the layer, the model uses a thermal wall function. This creates a jump in temperature between the solid surface and the fluid due to the omitted laminar sublayer. The predefined group for the wall domains defines this wall function in the following way.

To implement the thermal wall function, the model uses two heat transfer application modes: one for the solid and one for the fluid. These are connected through a heat flux boundary condition, the thermal wall function. This means that the resistance to heat transfer through the laminar sublayer is related to that for momentum transfer for the fluid. You therefore determine the heat flux, $q(\mathrm{W/m^2})$, from the equation

$$q = \frac{\rho C_p C_\mu^{1/4} k_\mathrm{w}{}^{1/2}(T_\mathrm{w} - T)}{T^+}$$

where ρ and C_p are the fluid's density and heat capacity, respectively; C_μ is a numerical constant of the turbulence model; and k_w is the value of the turbulent kinematic energy at the wall. Furthermore, T_w equals the temperature (K) of the solid at the wall, while T is the fluid temperature on the other side of the omitted laminar sublayer (K).

The dimensionless quantity T^+ is related to the dimensionless wall offset, $\delta_\mathrm{w}{}^+$, through the definition

$$T^+ = \frac{\mathrm{Pr}_T}{\kappa}\ln(\delta_\mathrm{w}{}^+) + \beta \tag{3-1}$$

where the turbulent Prandtl number Pr_T is fixed to 1.0; κ is the von Karman constant, which is set to 0.41; and β is a model constant set to 3.27. The dimensionless wall offset is defined as

$$\delta_\mathrm{w}{}^+ = \frac{\delta_\mathrm{w} C_\mu^{1/4} k_\mathrm{w}^{1/2}}{\nu} \tag{3-2}$$

where δ_w is the specified wall offset, which in COMSOL Multiphysics defaults to the local mesh size at the boundary, and $\nu = \eta/\rho$ denotes the kinematic viscosity.

At the front of the hot plate a stagnation point for the flow develops. Typical for two-equation turbulence models such as the k-ε model is an unphysical production of turbulence at stagnation points. The remedy is to apply a *realizability constraint*, which is a physical constraint on the turbulent viscosity. The realizability constraint makes the simulation less stable and is therefore applied only when necessary.

Results

The example solves the problem for a set of inlet velocities between 1 m/s and 100 m/s. Figure 3-3 depicts the temperature distribution for the inlet velocity 1 m/s.

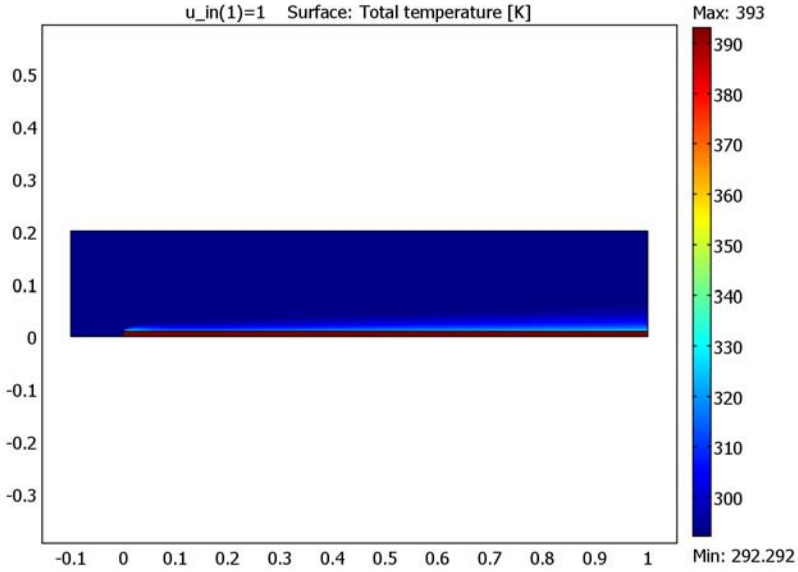


Figure 3-3: Temperature distribution at an inlet velocity of 1 m/s.

The heated layer of air at the plate surface is rather thick considering the relatively high velocity. This is an effect of the turbulent thermal conductivity caused by the eddies in the flow. The next figure depicts the turbulent thermal conductivity of the air.

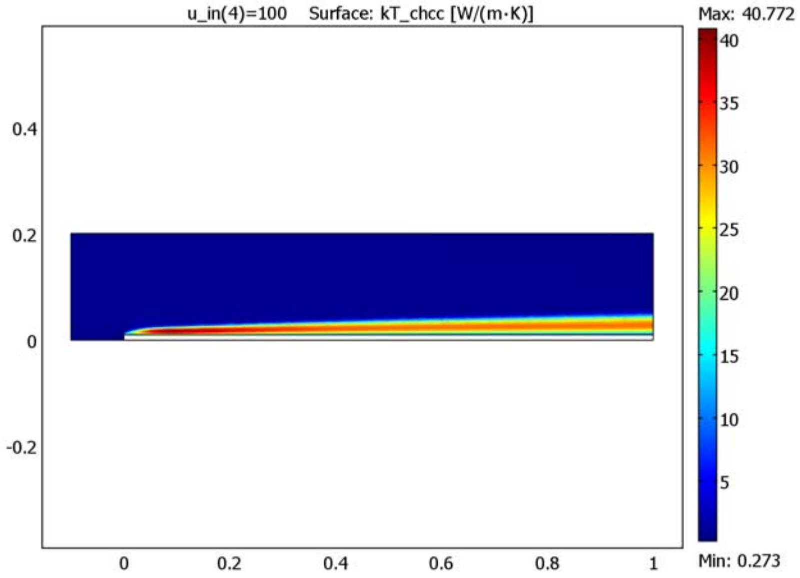


Figure 3-4: Turbulent thermal conductivity of the air at an inlet velocity of 100 m/s.

The turbulent conductivity is very much higher than the physical thermal conductivity of air, which is 0.03 W/(m·K) at 323 K. This means that the added turbulent conductivity dominates over the laminar conductivity, and hence that the turbulent eddies cause a significantly higher heat flux at the cooled surface compared to a laminar flow.

In this example you also modify the turbulent flow model to take density variations into account. The density of air decreases with temperature; the following figure shows its variation at an inlet velocity of 1 m/s.

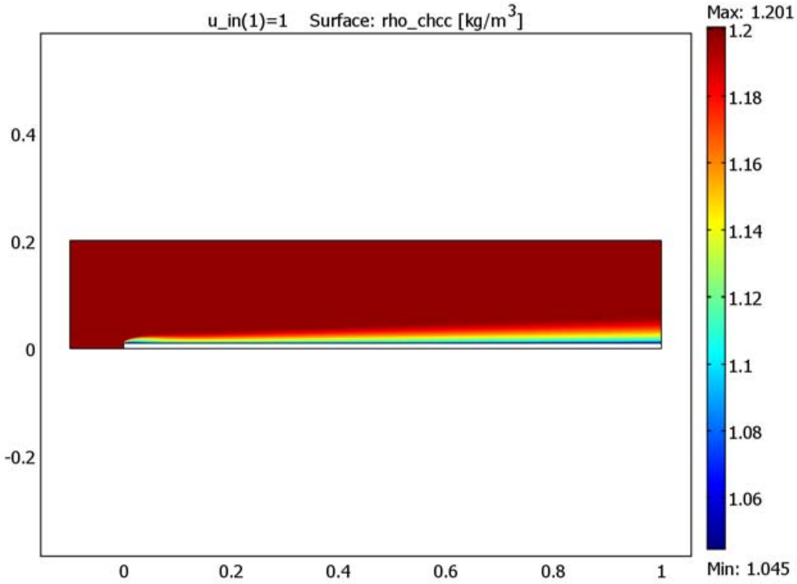


Figure 3-5: Fluid density at an inlet velocity of 1 m/s.

These results point out the importance of taking density variations into account. As the density decreases, the fluid velocity increases. This effect becomes apparent in the next figure, which shows the velocity distribution at the same inlet velocity.

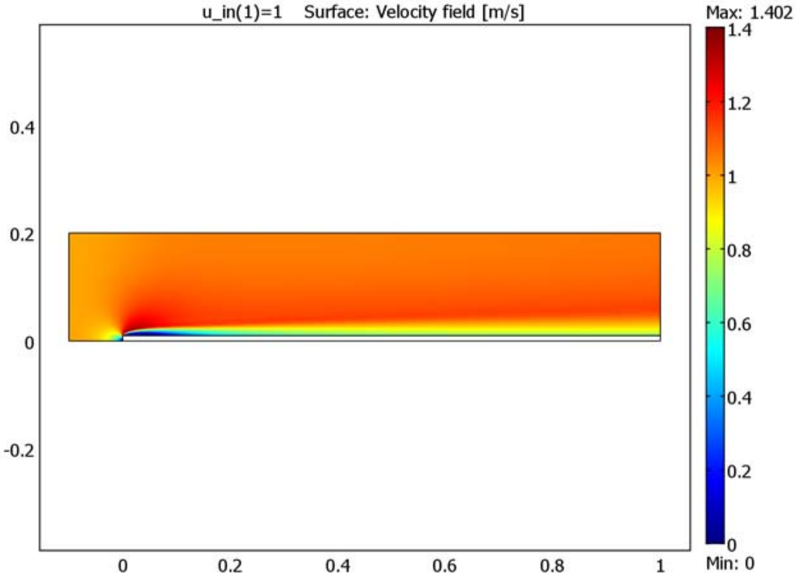


Figure 3-6: Velocity field at an inlet velocity of 1 m/s.

If you had treated the flow as being isothermal, the average would not have varied between the inlet and the outlet. However, for a non-isothermal flow the average velocity is inversely proportional to the average density, and it varies with changing average temperature. This means that the flow field for the fluid is different when taking density variations into account.

As the fluid heats up, its velocity increases slightly. Thus the boundary layer decreases and the local heat transfer coefficient should become larger. So if you neglect density variations when modeling forced convection cooling, the model slightly underestimates the cooling/heating power.

The accuracy in predicting the heat transfer coefficient in this example is dictated by the accuracy of the Reynolds analogy and the accuracy of the flow model. The situation this example models is very well studied, so you can readily verify the results in terms of heat transfer coefficient predictions. The following figure compares the local

h coefficient from the model with an empirical expression valid for the geometry and conditions studied (assuming turbulent flow).

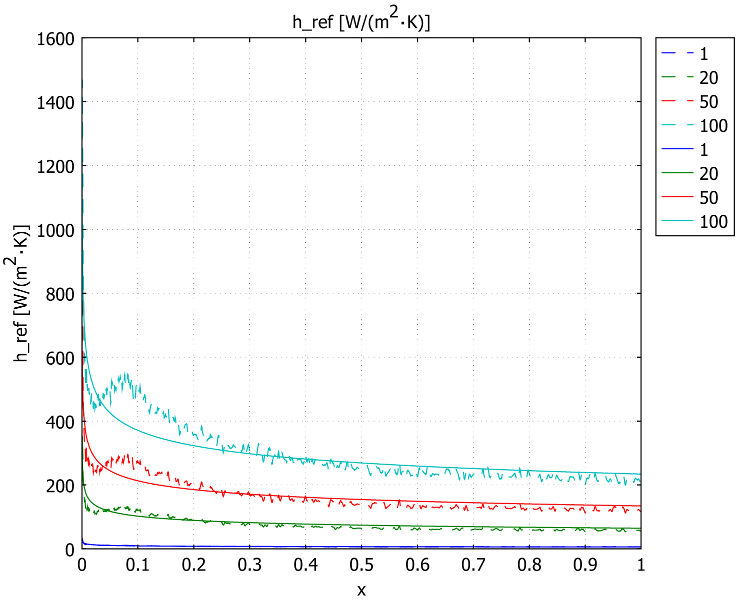


Figure 3-7: Local heat transfer coefficient as determined empirically (solid) and with the model (dashed) for various inlet velocities.

The model agrees well with empirical data for low to intermediate inlet velocities. The deviations at the leading edge of the plate are due to the correlation which assumes that the boundary layer is fully developed for all x. However, the region where the results deviates from the correlation increases in size as the inlet velocity increases. The logarithmic wall function in COMSOL Multiphysics is valid under certain conditions that depend on the resolution, the velocity, and the viscosity. As displayed in Equation 3-1, the wall function uses the dimensionless wall offset, δ_w^+ (defined in Equation 3-2). For the wall function to be an accurate approximation, δ_w^+ for the first internal node should be larger than 30 but less than some upper limit dependent on the Reynolds number (for more details see the section "Logarithmic Wall Function" on page 141 of the *Chemical Engineering Module User's Guide*). Figure 3-8 depicts the parameter δ_w^+ against plate surface for various inlet velocities.

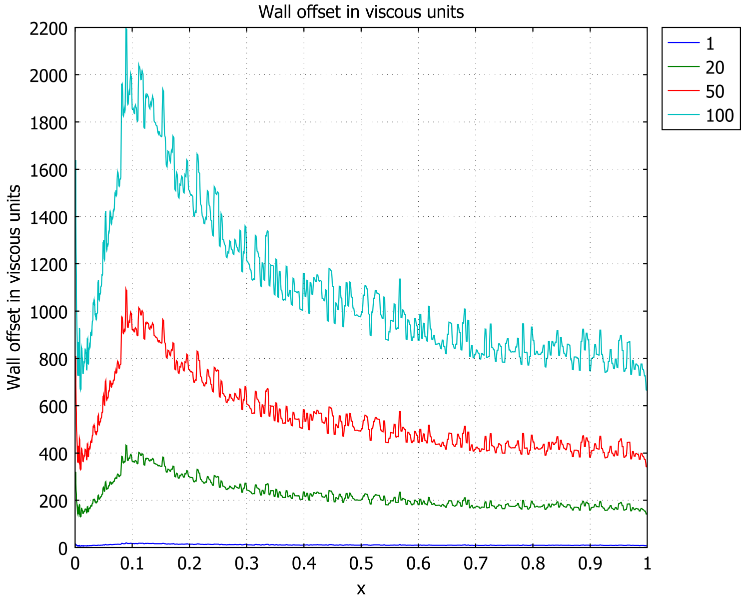


Figure 3-8: Dimensionless wall offset at the plate surface for various inlet velocities.

A maximum δ_w^+ value of a few hundreds is always acceptable, whereas a value above 1000 is always questionable. Note that the value of δ_w^+ exceeds 1000 when the inlet velocity is 50 m/s or higher. Hence, the mesh is too coarse for these cases. As a consequence, both the fluid velocity at the boundary and the heat transfer coefficient become less accurate. You can easily correct this situation by making the mesh finer at the boundary at the leading edge of the plate.

References

1. A. Bejan, *Heat Transfer*, 1993, John Wiley.

2. B. Sundén, “Kompendium i Värmeöverföring,” Department of Heat Transfer, LTH, Lund University, Sweden, p. 137, 2004 (in Swedish).

Modeling in COMSOL Multiphysics

The COMSOL Multiphysics implementation is straightforward using the Chemical Engineering Module's Non-Isothermal Flow multiphysics coupling, combining the Convection and Conduction and *k*-ε Turbulence Model application modes.

Model Library path: `Chemical_Engineering_Module/Heat_Transfer_and_Nonisothermal_Flow/forced_turbulent_convection`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Open the **Model Navigator**, and in the **Space dimension** list select **2D**.
2. In the list of application modes, select **Chemical Engineering Module>Flow With Variable Density>Non-Isothermal Flow>k-ε Turbulence Model**.
3. Click **OK**.

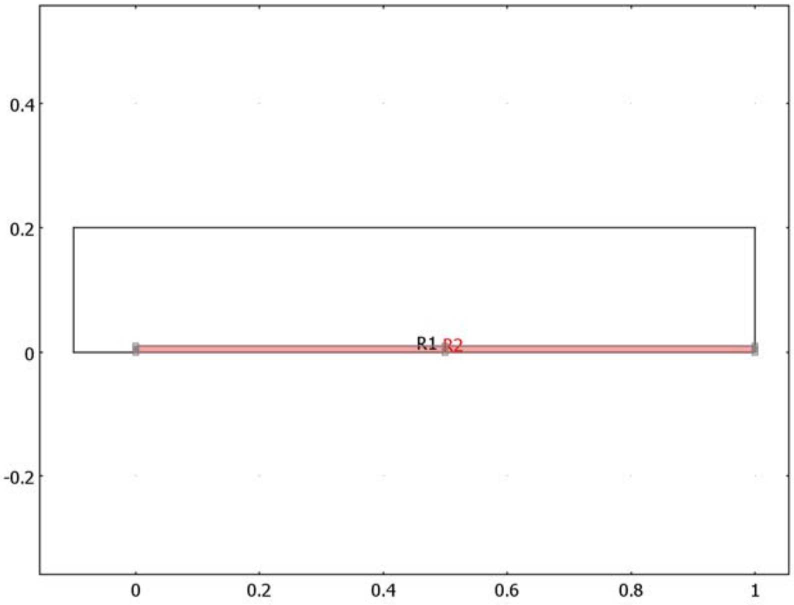
GEOMETRY

1. Using the **Rectangle** dialog box, create two rectangles with specifications according to the following table. You launch the **Rectangle** dialog box by shift-clicking the **Rectangle/Square** button on the Draw toolbar or by choosing **Specify Objects>Rectangle** from the Draw menu.

OBJECT	WIDTH	HEIGHT	BASE	X	Y
R1	`1.1`	`0.2`	Corner	`-0.1`	0
R2	1	`0.01`	Corner	0	0

2. Click the **Zoom Extents** button on the Main toolbar.

You should now see the following geometry:



CONSTANTS, EXPRESSIONS, AND VARIABLES

1 From the **Options** menu, open the **Constants** dialog box. Specify the following names, expressions, and descriptions (optional); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`T_amb`	`293[K]`	`Surrounding air temperature`
`delta_T`	`100[K]`	`Plate-to-air temperature difference`
`T_av`	`T_amb+delta_T/2`	`Average temperature`
`p_ref`	`1.013e5[Pa]`	`Reference pressure`
`u_in`	`1[m/s]`	`Inlet velocity`

2 Choose **Options>Expressions>Scalar Expressions**. Specify the following names, expressions, and descriptions (optional); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`L`	`x`	`Distance from leading edge`
`ReL_ref`	`u_in*L/mat1_nu0(T_av[1/K])[m^2/s]`	`Reference Reynolds number`

NAME	EXPRESSION	DESCRIPTION
`Pr_ref`	`mat1_eta(T_av[1/K])[Pa*s]* mat1_Cp(T_av[1/K])[J/(kg*K)]/ mat1_k(T_av[1/K])[W/(m*K)]`	`Reference Prandtl number`
`NuL_ref`	`0.037*ReL_ref^0.8*Pr_ref^0.33`	`Reference Nusselt number`
`h_ref`	`mat1_k(T_av[1/K])[W/(m*K)]* NuL_ref/L`	`Handbook h coefficient`

PHYSICS SETTINGS

Now it is time to set up the physics in the subdomain and the boundary settings. In this model you load the material properties from the built-in material library.

Fluid-Flow Settings (k-ε Turbulence Model)

1 From the **Multiphysics** menu, select **3 k-ε Turbulence Model**.

2 From the **Physics** menu, select **Properties**.

3 Set **Realizability** to **On**, then click **OK**.

4 Choose **Physics>Subdomain Settings**. Select Subdomain 2 (the plate).

5 Select **Solid domain** from the **Group** list underneath the **Subdomain selection** list.

6 Select Subdomain 1 (the fluid). Select **Fluid domain** in the **Group** list.

7 Then click the **Load** button to open the **Materials/Coefficients Library** dialog box. Select **Basic Material Properties>Air, 1 atm**, then click **OK**.

8 Next, edit the predefined entry for the dynamic viscosity. To do so, click in the **Dynamic viscosity** edit field replace `T` with `Tf`.

9 The expression for the density must also be edited. Click on the **Density** tab.

10 Click in the **Density** edit field, and replace `p` with `p_ref` and `T` with `Tf`; the entry should read `rho(p_ref[1/Pa],Tf[1/K])[kg/m^3]`.

11 Clear the **Pressure p** check box and click **OK** to close the **Subdomain Settings** dialog box.

12 Choose **Physics>Boundary Settings**. Then apply the following boundary settings:

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3	BOUNDARIES 4, 6	BOUNDARY 8
Boundary type	Inlet	Symmetry boundary	Wall	Outlet
Boundary condition	Velocity	-	Logarithmic wall function	Pressure
u_0	`u_in`			
v_0	`0`			
L_T	`0.001`			
I_T	`0.01`			
δ_w			h	
p_0				0

The small values of L_T and I_T are appropriate for essentially non turbulent free-stream flows.

13 Click **OK**.

Heat Transfer Settings

Now set up the parameters for the heat transfer:

1. From the **Multiphysics** menu, select **1 Convection and Conduction (chcc)**.
2. From the **Physics** menu, select **Subdomain Settings**.
3. Select Subdomain 2. Then select **Solid domain** from the **Group** list.
4. Select Subdomain 1. Select **Fluid domain** from the **Group** list.
5. From the **Library material** list, select **Air, 1 atm**.
6. For that material, edit the expressions for the **Thermal Conductivity,** the **Density**, and the **Heat capacity** by replacing `p` with `p_ref` and `T` with `Tf`.
7. Click the **Init** tab. In the **Tf(t_0)** edit field type `T_amb`, then click **OK**.
8. From the **Physics** menu, open the **Boundary Settings** dialog box.
9. Specify boundary settings according to the following table. When finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3	BOUNDARIES 4, 6	BOUNDARY 8
Group			wall	
Boundary condition	Temperature	Thermal insulation		Convective flux
T_0	`T_amb`			

10 From the **Multiphysics** menu, select **2 Convection and Conduction (chcc2)**.

11 From the **Physics** menu, select **Subdomain Settings**.

12 Select Subdomain 1, then select **Fluid domain** from the **Group** list.

13 Select Subdomain 2, then select **Solid domain** from the **Group** list.

14 Click the **Load** button.

15 From the **Materials** tree, select **Basic Material Properties>Copper**. Click **OK**.

16 Click **OK**.

17 From the **Physics** menu, select **Boundary Settings**.

18 Specify the following boundary conditions; when finished, click **OK**.

SETTINGS	BOUNDARY 5	BOUNDARIES 4, 6
Group		wall
Boundary condition	Temperature	
T_0	`T_amb+delta_T`	

MESH GENERATION

To solve the problem and get an accurate solution, the mesh must be fine at the solid/fluid interface, especially at the point of first contact. Generate such a mesh with the following steps:

1. Choose **Mesh>Free Mesh Parameters**. In the list of **Predefined mesh sizes** select **Coarse**.
2. Go to the **Boundary** page and select Boundaries 4 and 6. Set the **Maximum element size** to `3e-3` and the **Element growth rate** to `1.2`.
3. Go to the **Point** page and select Point 4. Set the **Maximum element size** to `1e-3`.
4. Click **Remesh** to generate the mesh. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

To solve this model for a range of inlet velocities, use the parametric solver.

1. Click the **Solver Parameters** button on the Main toolbar.
2. From the **Solver** list, select **Parametric Segregated**.
3. In the **Parameter name** edit field type `u_in`, and in the **Parameter values** edit field type `1 20 50 100`.
4. Select the **Manual specification of segregated steps** check box.
5. Set the **Damping** for **Group 1** to `0.25`.
6. Click the **Parametric** tab. From the **Predictor** list, select **Constant**.

7 Select the **Manual tuning of parameter step size** check box. In the three edit fields (**Initial step size**, **Minimum step size**, and **Maximum step size**) type `9`, `5`, and `50`, respectively. These settings force the parameter solver to take larger steps than it would do by default, which in turn reduces the solution time.

8 Click **OK**, then click the **Solve** button on the Main toolbar. The software needs roughly 30 minutes to solve this setup on a 3-GHz PC.

POSTPROCESSING AND VISUALIZATION

Reproduce the plots in Figure 3-3–Figure 3-6 using the **Plot Parameters** dialog box.

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select **1** from the **Parameter value** list.

3 Click **Apply** to generate the plot in Figure 3-3.

Proceed to generate the plot in Figure 3-4 of the turbulent thermal conductivity, k_T with the following steps:

4 On the **General** page, select **100** from the **Parameter value** list.

5 Click the **Surface** tab. Type `kT_chcc` in the **Expression** edit field on the **Surface Data** page, then click **Apply** to generate the plot.

Next reproduce Figure 3-5 as follows:

6 While still on the **Surface** page, type `rho_chcc` in the **Expression** edit field on the **Surface Data** page.

7 On the **General** page, select **1** from the **Parameter value** list. Click **Apply**.

To generate Figure 3-6 execute the following instructions:

8 Click the **Surface** tab. From the **Predefined quantities** list on the **Surface Data** page, select **k-ε Turbulence Model (chns)>Velocity field**.

9 Click **OK**.

Use the **Domain Plot Parameters** dialog box to generate Figure 3-7 and Figure 3-8:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 On the **Line/Extrusion** page, select Boundary 6.

3 In the **y-axis data** area, type `abs(ntflux_Tf_chcc/(Ts-Tf))` in the **Expression** edit field. From the **x-axis data** list, select **x**.

4 Click the **Line Settings** button. From the **Line style** list, select **Dashed line**. Select the **Legend** check box, then click **OK**.

5 Click **Apply** to generate the first lines of the plot.

6. On the **General** page, select the **Keep current plot** check box.
7. Return to the **Line/Extrusion** page. In the **Expression** edit field, type `h_ref`.
8. Click the **Line Settings** button. From the **Line style** list, select **Solid line**. Click **OK**.
9. Click **Apply** to finalize the plot in Figure 3-7.

   Next, turn to the plot in Figure 3-8:
10. On the **General** page, clear the **Keep current plot** check box.
11. On the **Line/Extrusion** page, type `dwplus_chns` in the **Expression** edit field.
12. Click **OK**.

Heating of a Finite Slab

Introduction

This simple example covers the heating of a finite slab, modeling how the temperature varies with time. You first set up the problem in COMSOL Multiphysics and then compare it to the analytical solution given in Ref. 1.

Model Definition

The model domain is defined between $x = -b$ and $x = b$. The initial temperature is constant, equal to T_0, over the whole domain; see the figure below. At time $t = 0$, the temperature at both boundaries is lowered to T_1.

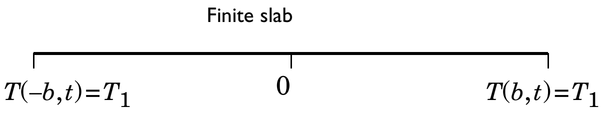


Figure 3-9: Depiction of the modeling domain.

To compare the modeling results to the literature (Ref. 1), introduce new dimensionless variables according to the following definitions:

$$\Theta = \frac{T_1 - T}{T_1 - T_0}, \qquad \eta = \frac{x}{b}, \qquad \tau = \frac{\alpha t}{b^2} \tag{3-3}$$

The model equation then becomes

$$\frac{\partial\Theta}{\partial\tau} = \frac{\partial^2\Theta}{\partial\eta^2} \tag{3-4}$$

with the associated boundary and initial conditions

$$\begin{aligned} \tau &= 0 & \Theta &= 1 \\ \eta &= \pm 1 & \Theta &= 0 \end{aligned} \tag{3-5}$$

Results

Figure 3-10 on page 115 shows the temperature as a function of position at the dimensionless times τ = 0.01, 0.04, 0.1, 0.2, 0.4, and 0.6. In this plot, the slab's center is situated at $x = 0$ with its end faces located at $x = -1$ and $x = 1$. The temperature profiles shown in this graph are identical to the analytical solution given in Carslaw and Jaeger (Ref. 1).

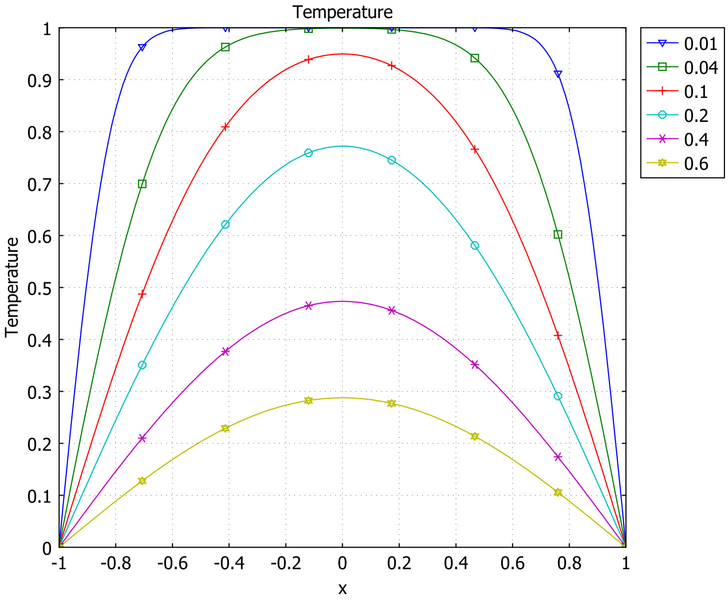


Figure 3-10: Results from the simulation at different times.

Reference

1. H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids*, 2nd ed., Oxford University Press, p. 101, 1959.

Model Library path: `Chemical_Engineering_Module/ Heat_Transfer_and_Nonisothermal_Flow/slab`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 From the **Space dimension** list, select **1D**.

3 Select **Chemical Engineering Module>Energy Transport>Conduction>Transient analysis** from the application modes list.

4 Click **OK**.

GEOMETRY MODELING

1 Choose **Draw>Specify Objects>Line**.

2 In the **Coordinates** area, type `-1 1` in the **x** edit field.

3 In the **Name** edit field, type `slab`.

4 Click **OK**.

5 Click the **Zoom Extents** button.

PHYSICS SETTINGS

Model Settings

Because the model uses dimensionless variables, disable unit handling.

1 From the **Physics** menu, select **Model Settings**.

2 From the **Base unit list**, select **None**.

3 Click **OK**.

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1.

3 Enter PDE coefficients according to the following table:

PROPERTY	VALUE
k	1
ρ	1
C_p	1

4 On the **Init** page, set **T(t_0)** to 1.

5 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select both boundaries and choose **Zero temperature** in the **Boundary condition** list.

3 Click **OK**.

MESH GENERATION

1 Click the **Mesh** button to initialize the mesh.

2 Click the **Refine Mesh** button once.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, type `0:0.01:1` in the **Times** edit field.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default plot shows the temperature distribution along the slab for $\tau = 1$.

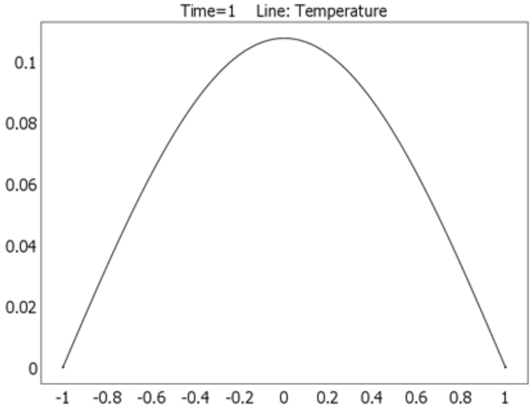


Figure 3-11: Temperature distribution along the slab at $\tau = 1$.

You can compare the COMSOL Multiphysics solution to that of Ref. 1 by plotting the temperature for a given set of output times, as in Figure 3-10. To reproduce this plot, following these steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 On the **General** page, select the **Line/extrusion plot** check box in the **Plot type** area.

3. From the **Solutions to use** list, select the time steps **0.01**, **0.04**, **0.1**, **0.2**, **0.4**, and **0.6** by holding down the Ctrl key.
4. On the **Line/Extrusion** page, click the **Line Settings** button
5. From the **Marker type** list, select **Cycle**.
6. Select the **Legend** check box, then click **OK** to close the **Line Settings** dialog box.
7. Click **OK** to close the **Domain Plot Parameters** dialog box and generate the plot.

A 3D Model of a MEMS Heat Exchanger

Introduction

The model in this study deals with a micro heat exchanger made of stainless steel. These type of heat exchangers are found in lab-on-a-chip devices in biotechnology and in microreactors, for example for micro fuel cells. Because of its cross-flow construction, you model the heat exchanger in 3D. The model takes heat transferred through both convection and conduction into account. The geometry and material conditions of the heat exchanger are taken from Ref. 1.

Model Definition

Figure 3-12 shows the geometry of the heat exchanger. A square cross-section is used for the fluid channels instead of circular cross-sections, often used in macroscopic heat exchangers. The heat exchanger is of cross-flow configuration and can consist of about 20 unit cells. Because the unit cells are almost identical except for edge effects in the outer cells, you can restrict the model to a single unit cell.

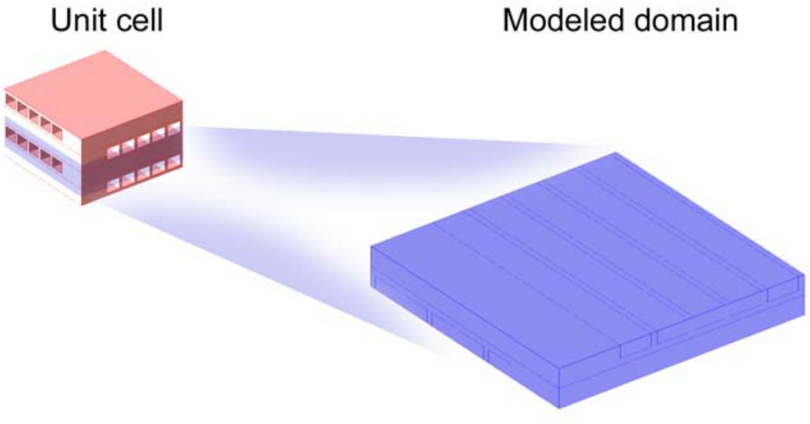


Figure 3-12: Depiction of the modeled part of the micro heat exchanger.

The model equation is a stationary energy transport taking into consideration heat transfer through convection and conduction:

$$\rho C_p u \cdot \nabla T - \nabla \cdot (k \nabla T) = 0 \qquad (3\text{-}6)$$

where C_p denotes the specific heat capacity (J/(kg·K)), T is the temperature (K), k is the thermal conductivity (W/(m·K)), ρ is the density (kg/m^3), **u** is the velocity (m/s), and Q is a sink or source term that is set to zero, since there is no production or consumption of heat in the device.

Because the model uses the Convection and Conduction application mode, you set the velocity, $\mathbf{u} = (u, v, w)$, to zero in all directions in the solid parts of the reactor. In the channels, you set the velocity field to an analytical expression that approximates fully developed laminar flow for a channel of square cross-section. For both the hot and cold streams, set the velocity component in the z direction to zero. For the cold stream, the y-component of the velocity is zero while the x-component is given by the expression below:

$$u = 16u_{\max}\frac{(z-z_0)(z_1-z)}{(z_1-z_0)^2}\frac{(y-y_0)(y_1-y)}{(y_1-y_0)^2} \qquad (3\text{-}7)$$

The following figure explains the notation used in Equation 3-7.

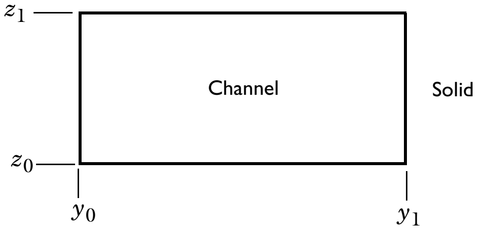


Figure 3-13: Representation of the cross-section in the x-plane of a channel. The y and z coordinates in the figure appear in the analytical expression for the velocity vector; see Equation 3-7.

By analogy, the velocity component in the hot stream is zero in the x direction while the y-component is given by the following expression:

$$v = 16v_{\max}\frac{(z-z_0)(z_1-z)}{(z_1-z_0)^2}\frac{(x-x_0)(x_1-x)}{(x_1-x_0)^2} \qquad (3\text{-}8)$$

The boundary conditions are insulating for all outer surfaces except for the inlet and outlet boundaries in the fluid channels. At the inlets for both the cold and hot streams the temperatures are constant:

$$\begin{aligned} T &= T_{\text{cold}} \\ T &= T_{\text{hot}} \end{aligned} \tag{3-9}$$

At the outlets, the transport of heat is dominated by convection, so the Convective flux boundary condition is suitable:

$$k\nabla T\cdot\mathbf{n} = 0 \tag{3-10}$$

This expression sets the conduction term in the outflow direction to zero.

Results

Figure 3-14 shows a few temperature isosurfaces in the device, which clearly reveal the influence of the convective term.

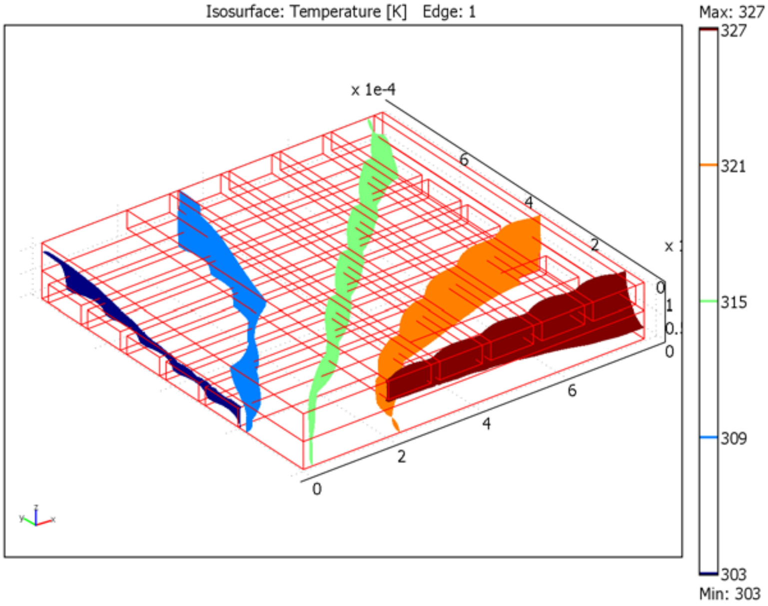


Figure 3-14: Isotherms through the cell unit's geometry.

Temperature differences between the different outlets in both the hot and cold streams imply that the hot stream is not uniformly cooled in the different channels, see Figure 3-15.

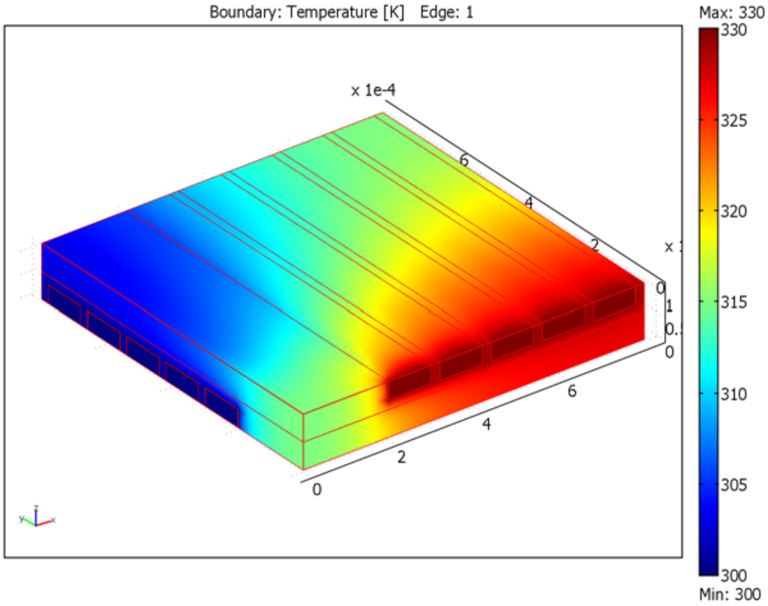


Figure 3-15: Boundary plot of the temperature in the heat exchanger. The distribution of the temperature in the region of the respective outlets leads to the conclusion that the cooling is not uniform.

In order to visualize the velocity field in the flow channels, you can look at a sequence of cross-section plots perpendicular to the direction of the plot. The velocity profile is almost identical to a fully developed velocity profile. The flow in the figure is normalized and the value 1 corresponds to a maximum velocity of 5 mm/s.

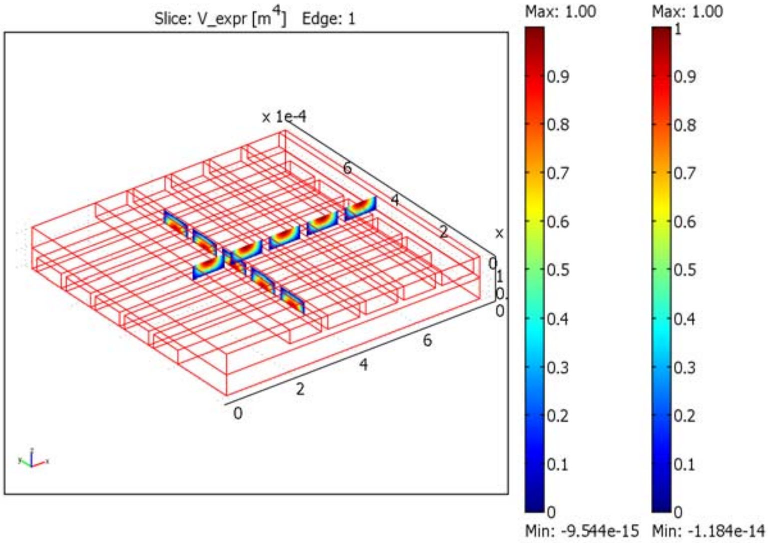


Figure 3-16: Normalized velocity profiles in the flow channels.

Reference

1. W. Ehrfeld, V. Hessel, and H. Löwe, *Microreactors*, Weinheim, 2000.

Model Library path: `Chemical_Engineering_Module/`
`Heat_Transfer_and_Nonisothermal_Flow/mems_heat_exchanger_3d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. From the **Space dimension** list, select **3D**.

3 Select the **Chemical Engineering Module>Energy Transport>Convection and Conduction** application mode.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define constants according to the table below.

NAME	EXPRESSION	DESCRIPTION
`k1`	`0.6[W/(m*K)]`	`Thermal conductivity, fluid`
`C_p1`	`4200[J/(kg*K)]`	`Heat capacity, fluid`
`rho1`	`1000[kg/m^3]`	`Density, fluid`
`k2`	`15[W/(m*K)]`	`Thermal conductivity, steel`
`C_p2`	`420[J/(kg*K)]`	`Heat capacity, steel`
`rho2`	`7800[kg/m^3]`	`Density, steel`
`T0`	`300[K]`	`Inlet temperature, cold stream`
`T1`	`330[K]`	`Inlet temperature, hot stream`
`u_max`	`5[mm/s]`	`Maximum flow velocity, x direction`
`v_max`	`5[mm/s]`	`Maximum flow velocity, y direction`

GEOMETRY MODELING

1 From the **Draw** menu, select **Work-Plane Settings**.

2 Click the **Quick** tab and select **y-z plane**.

3 Click **OK**.

4 From the **Options** menu, select **Axes/Grid Settings**.

5 Clear the **Auto** check box.

6 Enter axis values according to the following table:

x min	-10
x max	810
y min	-10
y max	110

7 Click the **Grid** tab.

8 Clear the **Auto** check box.

9 Set both **x spacing** and **y spacing** to 20.

10 Click **OK**.

11 Click the **Rectangle/Square** button, then click the coordinates (0, 0) and (800, 60).

12 Make another rectangle with opposite corners at the points (200, 0) and (300, 40).

13 Click the **Array** button on the Draw toolbar.

14 Set **x displacement** to `120` and **Array size x** to `5`.

15 Click **OK**.

16 Select all geometry objects by pressing Ctrl+A.

17 Click the **Create Composite Object** button on the Draw toolbar.

18 In the **Set formula** edit field, type `R1+R2+R3+R4+R5+R6`.

19 Make sure that the **Keep interior boundaries** check box is selected, then click **OK**.

The 2D cross-section is now ready, and you can extrude it to 3D:

1 From the **Draw** menu, select **Extrude**.

2 In the **Distance** edit field, type `800`. Click **OK**.

3 Make a copy of the 3D object by pressing Ctrl+C.

4 Paste the copy with Ctrl+V.

5 Click the **Rotate** button on the Draw toolbar.

6 Set the **Rotation angle** to `180`.

7 In the **Point on rotation axis** edit field, enter the following settings:

x	0
y	0
z	60

8 Specify the **Rotation axis direction vector** according to:

x	1
y	1
z	0

9 Click **OK**.

10 Select all geometry objects by pressing Ctrl+A.

11 Click the **Scale** button.

12 Set the **Scale factor** to `1e-6` in all directions.

13 Click **OK**.

14 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

You need a number of expression variables to express the velocity profile in the channels.

1. From the **Options** menu, choose **Expressions>Subdomain Expressions**.
2. Specify expressions according to the tables below.

NAME	SUBDOMAINS 3–7	SUBDOMAINS 8–12
U_expr	16*(z-z0)*(z1-z)/(z1-z0)^2*(y-y0)*(y1-y)/(y1-y0)^2	-
V_expr		16*(z-z0)*(z1-z)/(z1-z0)^2*(x-x0)*(x1-x)/(x1-x0)^2
z0	-40[um]	80[um]
z1	80[um]+z0	80[um]+z0
x1	-	100[um]+x0
y1	100[um]+y0	-

NAME	SUBDOMAIN 8	SUBDOMAIN 9	SUBDOMAIN 10	SUBDOMAIN 11	SUBDOMAIN 12
x0	200[um]	200[um]+1*120[um]	200[um]+2*120[um]	200[um]+3*120[um]	200[um]+4*120[um]

NAME	SUBDOMAIN 3	SUBDOMAIN 4	SUBDOMAIN 5	SUBDOMAIN 6	SUBDOMAIN 7
y0	200[um]	200[um]+1*120[um]	200[um]+2*120[um]	200[um]+3*120[um]	200[um]+4*120[um]

3. Click **OK**.
4. From the **Physics** menu, select **Subdomain Settings**.
5. Enter subdomain properties according to the following table:

SETTINGS	SUBDOMAINS 1, 2	SUBDOMAINS 3–7	SUBDOMAINS 8–12
k (isotropic)	k2	k1	k1
ρ	rho2	rho1	rho1
C_p	C_p2	C_p1	C_p1
Q	0	0	0
u	0	u_max*U_expr	0
v	0	0	v_max*V_expr
w	0	0	0

6 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARIES 8, 14, 20, 26, 32	BOUNDARIES 41, 48, 55, 62, 69	BOUNDARIES 44, 51, 58, 65, 72, 77–81	ALL OTHERS
Boundary condition	Temperature	Temperature	Convective flux	Thermal insulation
T_0	T0	T1		

3 Click **OK**.

MESH GENERATION

Initialize the mesh by pressing the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, verify the that the **Linear system solver** is set to **GMRES**.

3 Set the **Preconditioner** to **Algebraic multigrid**.

4 In the **Quality of multigrid hierarchy** edit field, type 2.

5 Click **OK**.

6 Click the **Solve** button on the Main toolbar.

The model is of a size close to 78,000 degrees of freedom and may need 1 Gigabyte of RAM in order to solve.

POSTPROCESSING AND VISUALIZATION

The default plot shows slices of the temperature. You reproduce the plots in Figure 3-14 on page 121 with the following steps.

1 From the **Postprocessing** menu, select **Plot Parameters**.

2 On the **General** page, clear the **Slice** check box and select the **Isosurface** and **Edge** check boxes in the **Plot type** area.

3 On the **Isosurface** page, choose **Convection and Conduction (chcc)>Temperature** from the **Predefined quantities** list.

4 On the **Edge** page, type 1 in the **Expression** edit field.

5 Click **OK**.

Generate the plot in Figure 3-15 as follows:

1 From the **Postprocessing** menu, select **Plot Parameters**.
2 On the **General** page, clear the **Isosurface** check box and select the **Boundary** check box.
3 On the **Boundary** page, select **Convection and Conduction (chcc)>Temperature** from the **Predefined quantities** list.
4 Click **OK**.

Finally, execute the following instructions to reproduce the plots in Figure 3-16:

1 On the **General** page, clear the **Boundary** check box and select the **Slice** check box.
2 On the **Slice** page, type `U_expr` in the **Expression** edit field in the **Slice data** area.
3 Set **x-levels** to `1`, and **y-levels** and **z-levels** to `0`.
4 Click **Apply**.
5 On the **General** page, check the **Keep current plot** check box.
6 Return to the **Slice** page and change the **Expression** to `V_expr`.
7 Set **y-levels** to `1`, and **x-levels** and **z-levels** to `0`.
8 Click **OK**.

Non-Isothermal Flow in a Cooling Process

Introduction

This model highlights the predefined multiphysics coupling Non-Isothermal flow. The momentum transport is described by the Weakly Compressible Navier-Stokes application mode, which is applicable to flow with velocities less than Mach 0.3 (approximately 100 m/s for atmospheric air). Below Mach 0.3 pressure expansion work done by the gas is negligible.

The following example models the flow of air over a hot fin. The fin heats the fluid, and both density and viscosity vary significantly due to the heating. The heat transport is defined in both the fin and the air whereas the momentum transport is applied only in the air.

Model Definition

The geometry of the domain is shown below. The depth of the flow domain is large making a 2D approximation valid, assuming negligible gradients in the depth.

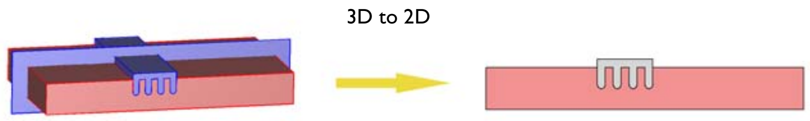


Figure 3-17: Modeling domain of a cooling device. Air enters at the left boundary, flows over the fin, and the gas heats up.

The model is described by weakly compressible Navier-Stokes equations and an energy transport equation with both convection and conduction; see Equation 3-11 and Equation 3-12:

$$\begin{gathered}\rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\eta\,(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-(2\eta/3)(\nabla\cdot\mathbf{u})\mathbf{I}]+\rho\mathbf{g}\\ \nabla\cdot(\rho\mathbf{u}) = 0\end{gathered} \tag{3-11}$$

$$\rho C_p\mathbf{u}\nabla\cdot T - \nabla\cdot(k\nabla T) = 0 \tag{3-12}$$

In these equations, η denotes the viscosity of the solution (kg/(m·s)), $\mathbf{u}$ is the velocity (m/s), ρ represents density (kg/m^3), p is the pressure (Pa), k equals the thermal conductivity (W/(m·K)), and C_p is the heat capacity (J/(kg·K)).

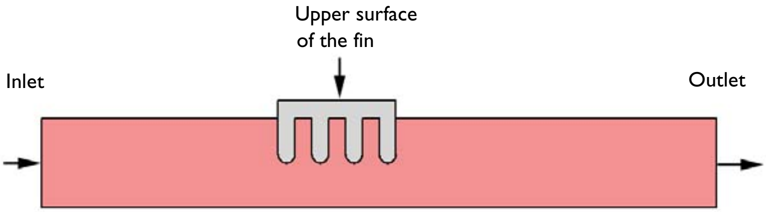


Figure 3-18: Definition of boundary conditions.

At the inlet, apply a laminar profile with a maximum velocity of 0.1 m/s. The corresponding average velocity is then

$$u_{\text{average}} = \frac{2}{3}u_{\max}. \tag{3-13}$$

At the outlet, the viscous stress is assumed to be zero, and the pressure is set according to the atmospheric conditions:

$$p = 10^5 \text{ Pa} \tag{3-14}$$

At all other boundaries, use a no-slip condition:

$$\mathbf{u} = \mathbf{0} \tag{3-15}$$

For the energy transport, set the inlet temperature to 298 K, and at the top surface of the fin to 398 K.

$$\begin{gathered} T = T_{0,\,\text{inlet}} \\ T = T_{0,\,\text{fin}} \end{gathered} \tag{3-16}$$

At the outlet, apply convective flux as a boundary condition. It assumes that heat transport is dominated by convection and follows from

$$\mathbf{n} \cdot (k\nabla T) = 0 \tag{3-17}$$

This implies that the gradient of T in the direction perpendicular to the outlet boundary is negligible. At all other boundaries, insulating conditions apply:

$$\mathbf{n} \cdot (-k\nabla T + \rho C_p T \mathbf{u}) = 0 \qquad (3\text{-}18)$$

Use material properties of atmospheric air for the fluid and those of copper for the fin. The viscosity varies with temperature and the density follows from the ideal gas law, varying with temperature and pressure. The model loads material properties from the built-in materials database.

Results

Results from the simulation show a clear influence of temperature on the velocity profile emerging from variations in density. Figure 3-19 shows a temperature distribution in the gas phase that is fairly large and will give rise to a significant effect on the flow profile.

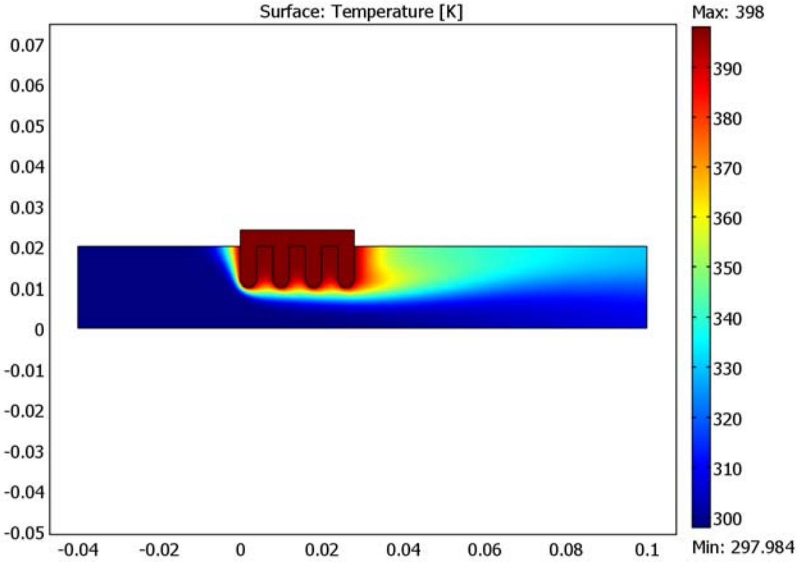


Figure 3-19: Temperature distribution in both the flowing gas and the fin.

Density varies with the inverse of the temperature, as seen in Figure 3-20.

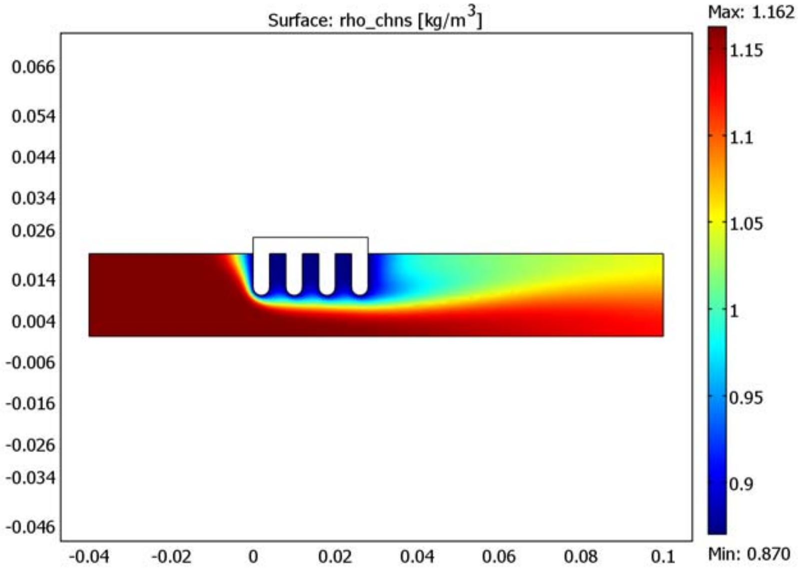


Figure 3-20: Gas density distribution in the cooling device.

This variation has a direct influence on the velocity profile seen in Figure 3-21. At the outlet the flow reaches an almost fully developed profile but with an average velocity that is approximately 6.4% higher than the inlet value. The increased velocity is a consequence of the thermal gas expansion caused by the density decrease.

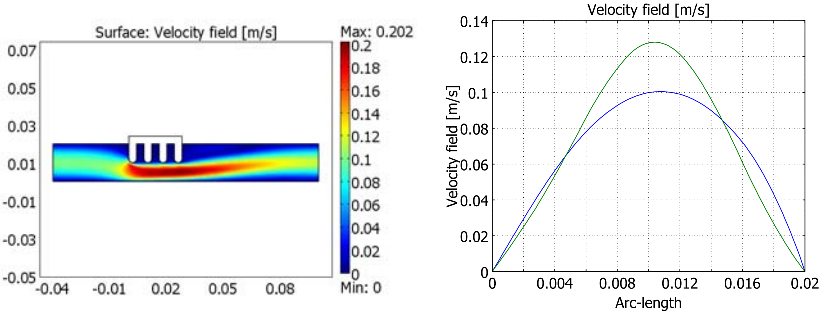


Figure 3-21: Velocity field distribution (left) in the cooling device and cross-sectional plots of the velocity field (right) at the inlet (solid line) and outlet (dashed line).

Accounting for the temperature effects on fluid flow can be important. In this example, you can observe the effect of expansion as an increase in velocity.

Model Library path: `Chemical_Engineering_Module/Heat_Transfer_and_Nonisothermal_Flow/nonisothermal_flow`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 From the list of application modes, select **Chemical Engineering Module>Flow with Variable Density>Non-Isothermal Flow>Laminar**.

3 Click **OK**.

OPTIONS AND SETTINGS

1 Open the **Axes/Grid Settings** dialog box from the **Options** menu and specify **x-y limits** according to the table below.

PROPERTY	VALUE
x min	`-0.1e-2`
x max	`2.9e-2`
y min	`0.5e-2`
y max	`2.5e-2`

2 Click the **Grid** tab. Clear the **Auto** check box and specify **x spacing** and **y spacing** values according to the table below.

PROPERTY	VALUE
x spacing	`0.2e-2`
y spacing	`0.2e-2`

3 Click **OK**. These axis/grid settings produce a suitable grid for drawing the geometry.

4 From the **Options** menu, select **Constants**.

5 Define the following constants (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
`u_max`	`0.1[m/s]`	`Maximum inlet velocity`
`p0`	`1e5[Pa]`	`Outlet pressure`
`T_in`	`298[K]`	`Inlet temperature`
`T_hot`	`398[K]`	`Fin hot side temperature`

6 Click **OK**.

GEOMETRY MODELING

To draw the cooling fin, combine the **Line** and the **2nd Degree Bézier Curve** tools.

1 Select the **Line** tool on the Draw toolbar and click the coordinates $(0, 2.4 \cdot 10^{-2})$ and $(0, 1.2 \cdot 10^{-2})$.

2 Switch to the **2nd Degree Bézier Curve** tool and click $(0, 1 \cdot 10^{-2})$, $(0.2 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(0.4 \cdot 10^{-2}, 1 \cdot 10^{-2})$, and $(0.4 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

3 Switch back to the **Line** tool and click $(0.4 \cdot 10^{-2}, 2 \cdot 10^{-2})$, $(0.8 \cdot 10^{-2}, 2 \cdot 10^{-2})$, and $(0.8 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

4 Click the **2nd Degree Bézier Curve** tool again and click on the coordinates (0.8, 1), $(1 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(1.2 \cdot 10^{-2}, 1 \cdot 10^{-2})$, and $(1.2 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

5 Click the **Line** tool and the coordinates $(1.2 \cdot 10^{-2}, 2 \cdot 10^{-2})$, $(1.6 \cdot 10^{-2}, 2 \cdot 10^{-2})$, and $(1.6 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$

6 Click the **2nd Degree Bézier Curve** tool followed by the coordinates $(1.6 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(1.8 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(2 \cdot 10^{-2}, 1 \cdot 10^{-2})$, and $(2 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

7 Click the **Line** tool followed by the coordinates the coordinates (2e-2, 2e-2), $(2.4 \cdot 10^{-2}, 2 \cdot 10^{-2})$, and $(2.4 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

8 Click the **2nd Degree Bézier Curve** tool followed by the coordinates $(2.4 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(2.6 \cdot 10^{-2}, 1 \cdot 10^{-2})$, $(2.8 \cdot 10^{-2}, 1 \cdot 10^{-2})$, and $(2.8 \cdot 10^{-2}, 1.2 \cdot 10^{-2})$.

9 Click the **Line** tool, click $(2.8 \cdot 10^{-2}, 2.4 \cdot 10^{-2})$ and click the right mouse button.

This creates the composite object CO1.

10 Press the Shift key and click the **Rectangle/Square** button. The **Rectangle** dialog box appears.

11 Specify properties according to the following table:

PROPERTY	**VALUE**
Width	`14e-2`
Height	`2e-2`
x position	`-4e-2`
y position	`0`

12 Click **OK**.

13 Select the object CO1 and copy it by clicking the **Copy** button or by pressing Ctrl+C.

14 Click the **Create Composite Object** button and type `R1-CO1` in the **Set formula** edit field.

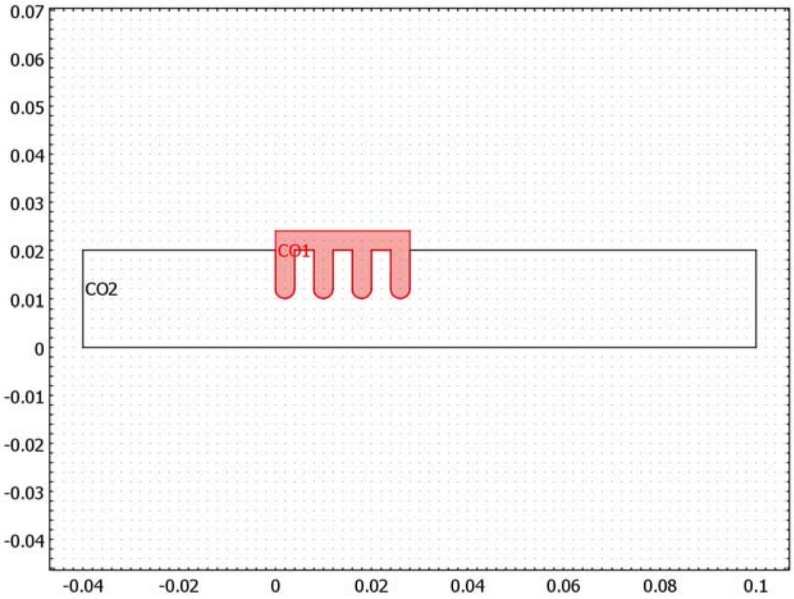
15 Click **OK**.

16 Click the **Paste** button.

17 Click **OK** in the **Paste** dialog box.

18 Click the **Zoom Extents** button on the Main toolbar.

The final geometry is now ready.



PHYSICS SETTINGS

Subdomain Settings—Weakly Compressible Navier-Stokes

1. From the **Multiphysics** menu, select **Weakly Compressible Navier-Stokes (chns)**.
2. From the **Physics** menu, select **Subdomain Settings**.
3. Select Subdomain 2, then clear the **Active in this domain** check box**.** This action disables the flow application in the solid fin part of the geometry.
4. Select Subdomain 1, then click the **Load** button. This opens the **Materials/Coefficients Library** dialog box.
5. From the **Materials** list, select **Basic Material Properties>Air, 1 atm**. Click **OK**.
6. On the **Init** page, type `p0` in the **p(t_0)** edit field to specify the initial pressure value.
7. Click **OK**.

Boundary Conditions—Weakly Compressible Navier-Stokes

1. From the **Physics** menu, select **Boundary Settings**.
2. Specify boundary conditions according to the table below.

SETTINGS	BOUNDARY 1	BOUNDARY 19	ALL OTHERS
Type	Inlet	Outlet	Wall
Condition	Laminar inflow	Pressure, no viscous stress	No slip
U_0	`2/3*u_max`		
p_0		`p0`	

Note that the default boundary condition is **No slip** at exterior boundaries.

3. Click **OK**.

Subdomain Settings—Heat Transfer

1. In the **Multiphysics** menu, switch to **Convection and Conduction (chcc)**.
2. From the **Physics** menu, select **Subdomain Settings**.
3. Select Subdomain 1, then select **Air, 1 atm** from the **Library material** list.
4. Select Subdomain 2, then select **Solid domain** from the **Group** list.
5. Click the **Load** button. In the **Materials** list, select **Basic Material Properties>Copper**, then click **OK**.
6. Click the **Init** tab.
7. Select both subdomains. Set **T(t_0)** to `T_in`, then click **OK**.

Boundary Conditions—Heat Transfer

In the same way as just done, define the boundary conditions according to the table below in the **Boundary Settings** dialog box.

SETTINGS	BOUNDARY 1	BOUNDARY 6	BOUNDARY 19	ALL OTHER BOUNDARIES
Boundary condition	Temperature	Temperature	Convective flux	Thermal insulation
T_0	`T_in`	`T_hot`		

MESH GENERATION

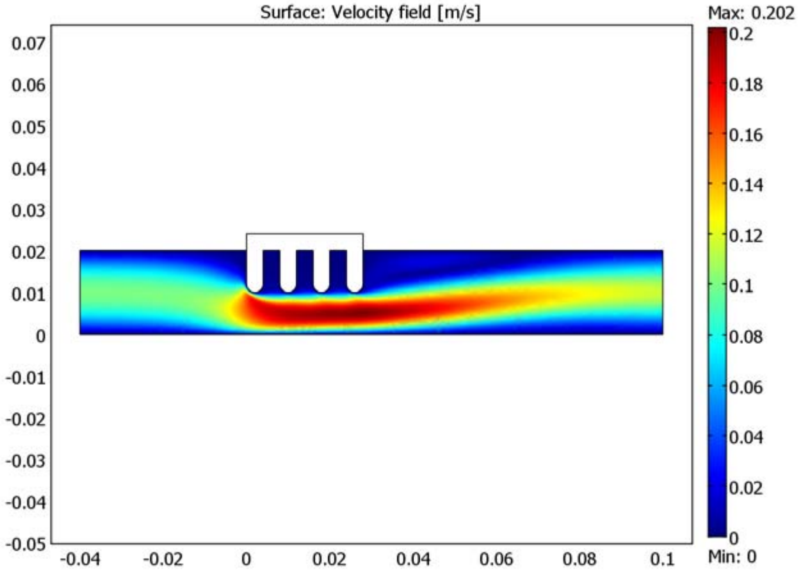
1. From the **Mesh** menu, select **Free Mesh Parameters**.
2. From the **Predefined mesh sizes** list, select **Finer**. Click **Remesh**. This produces a mesh of approximately 2800 elements.
3. Click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default plot shows the velocity field as seen in the following figure. Because of the reduced cross section, the velocity increases in the vicinity of the fin. Thermal expansion caused by the heating also accelerates the air.



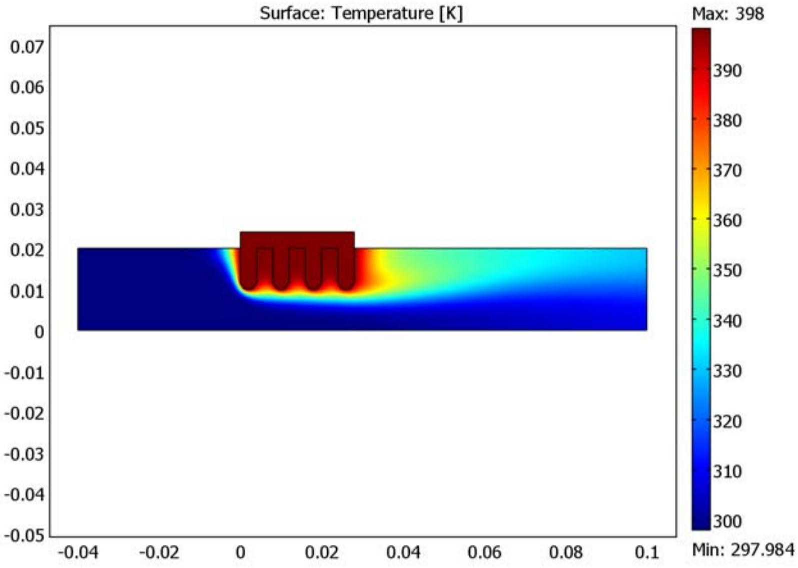
To visualize the temperature field, follow these steps:

1 Select **Postprocessing>Plot Parameters**.

2 Click the **Surface** tab.

3 From the **Predefined quantities** list on the **Surface Data** page, select **Convection and Conduction (chcc)>Temperature**.

4 Click **OK** to get the following plot:

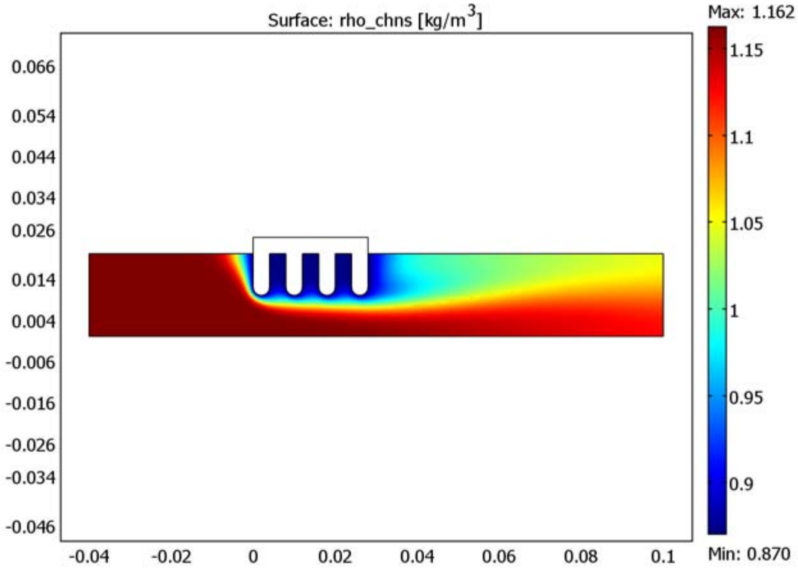


The air heats up as it passes the fin. This temperature increase causes the density and viscosity to decrease. To visualize the density of the air follow these steps:

1 Click the **Plot parameters** button on the Main toolbar.

2 On the **Surface** page, type `rho_chns` in the **Expression** edit field. The variable `rho_chns` is the flow applications variable for density.

3 Click **OK** to produce the following plot:



The density variation leads to a slight expansion of the air and a higher outlet velocity. You can visualize the velocity profile upstream and downstream the fin by creating a multiple-line cross-section plot according to the following instructions:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

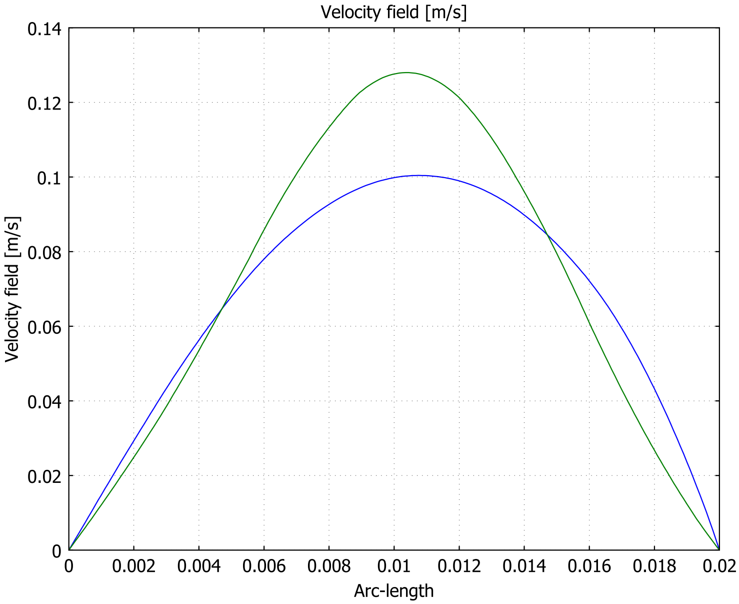
2 On the **Line/Extrusion** page enter the **Cross-section line data** given in the following table.

x0	`-2e-2`
x1	`-2e-2`
y0	`2e-2`
y1	`0`

3 Select the **Multiple parallel lines** check box.

4 Click the **Vector with distances** button and type `0 10e-2` in the associated edit field.

5 Click **OK**.



The figure shows that the velocity profile is unsymmetrical and that the maximum velocity shifts toward the top wall as the air passes the fin.

To investigate the influence of the density variation on the average flow rate, that is, the fluid expansion, integrate the velocity divided by the channel width to compute the average velocity at the inlet and outlet. Use the following steps:

1 From the **Postprocessing** menu, select **Boundary Integration**.
2 Select Boundary 1 (the inlet) and type `u/2[cm]` in the **Expression** edit field. By thus dividing the velocity with the channel height you obtain the average inlet velocity.
3 Click **Apply** to see the result displayed in the message log at the bottom of the main COMSOL Multiphysics window. The result should be approximately 0.0667 m/s, (2/3 of the maximum velocity).
4 Select Boundary 19 (the outlet), then click **OK**. This should give you a value near 0.0713 m/s for the average outlet velocity.

This means that the fluid has experienced an expansion of approximately 6.4%.

MEMS Heat Exchanger

Introduction

One of the most common devices in unit operations is the heat exchanger, which can both cool and heat fluids and solid materials. Cooling is a needed process for several reasons: materials are sensitive to high temperatures; operating conditions might not be optimal for high temperatures; or it might just be for practical or environmental reasons that you want to keep a temperature low. Heat exchangers are most often used in processes to remove heat when convective cooling from fans and fins isn't adequate. Heating is also used in many processes to keep a fluid at a given elevated temperature.

Model Definition

The model focuses on heat transport in a very small heat exchanger that is common in the field of microelectromechanical systems (MEMS). In this case, it might be a reactive processes that needs heating. The heat exchanger is constructed by stacking several pleated sheets or plates on top of each other while leaving a gap between them. The heating fluid circulates in the gaps between the corrugated walls where the fluid to be heated flows. To simplify the modeling process, this example studies only a cross section between two plates whose shapes in this case are sinusoidal to provide an optimal heat-transfer area. Figure 3-22 depicts a section of the heat exchanger.

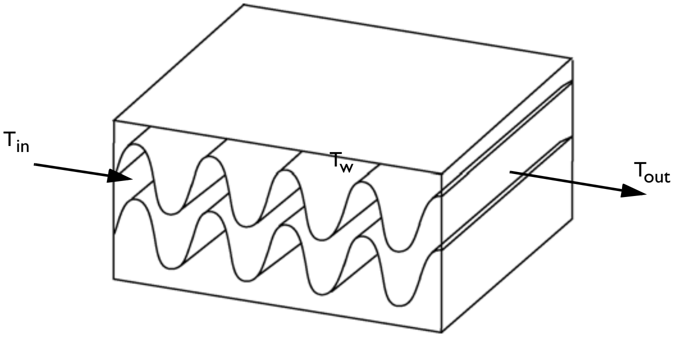


Figure 3-22: MEMS heat-exchanger geometry (Ref. 1).

The medium is plain water, and the operating temperature range spans from 0 °C to 100 °C. Because the viscosity and heat capacity change significantly in this temperature interval, their values are obtained from temperature-dependent polynomials.

The viscosity varies according to the expression

$$\eta = 0.011021 - 9.386\cdot 10^{-4}T + 2.684\cdot 10^{-6}T^2 - 2.569\cdot 10^{-9}T^3 \quad \text{Pa·s} \qquad (3\text{-}19)$$

where the temperature, T, must be expressed in kelvin (K). Similarly, the heat capacity of water is expressed by

$$C_p = 4190.86 - 0.977T + 0.019T^2 - 5.6\cdot 10^{-5}T^3 \quad \text{J/(kg·K)} \qquad (3\text{-}20)$$

Again, the temperature must be given in kelvin. The governing equations in this system are the incompressible Navier-Stokes equations accounting for the motion of the fluid:

$$\begin{gathered} -\nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 \\ \nabla\cdot\mathbf{u} = 0 \end{gathered} \qquad (3\text{-}21)$$

and the convection and conduction equation, without any heat sources, for the energy transport within the fluid:

$$\rho C_p\mathbf{u}\nabla\cdot T - \nabla\cdot(k\nabla T) = 0 \qquad (3\text{-}22)$$

At the inlet, you specify a parabolic velocity profile with a known constant temperature. The analytic solution for a fully developed laminar flow profile between two parallel plates at distance $2B$ from each other is

$$u = \frac{3}{2}u_{\text{av}}\left[1 - \left(\frac{x}{B}\right)^2\right] \qquad (3\text{-}23)$$

Here u is the local velocity and u_{av} is the average velocity. The x-origin is taken at the middle of the plates. In the model, you can make use of the dimensionless boundary length parameter s (which goes from 0 to 1 from the start to the end of a boundary) to create this profile as an inlet boundary condition. The boundary conditions then become

$$\mathbf{u}\cdot\mathbf{n} = 6u_{\text{av}}s(1-s) \qquad (3\text{-}24)$$

$$T = T_{\text{in}} \qquad (3\text{-}25)$$

The walls have no-slip conditions for velocity and a specified temperature condition for the energy transport:

$$\begin{aligned} \mathbf{u} &= 0 \\ T &= T_{\mathrm{w}} \end{aligned} \tag{3-26}$$

Finally, at the outlet boundary, the pressure (disregarding viscous stress) and the conductive heat flux are zero:

$$\begin{aligned} p &= 0 \\ \mathbf{n} \cdot (-k\nabla T) &= 0 \end{aligned} . \tag{3-27}$$

Results

Figure 3-23 shows the temperature profile along the length of the heat exchanger.

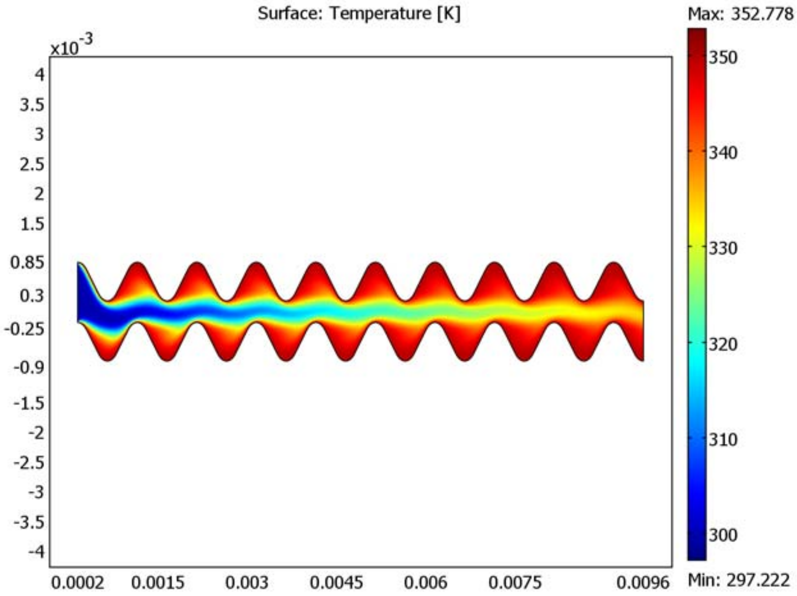


Figure 3-23: Temperature field along the length of the modeling domain.

To be able to calculate the heat exchanger's overall performance, you must find the mean temperature at the exchanger's outlet. The mixing-cup temperature of the fluid leaving the heat exchanger is calculated through

$$\langle T\rangle = \frac{\int_s T u ds}{\int_s u ds} \qquad (3\text{-}28)$$

where $s \in [0, 1]$ parameterizes the boundary. It is easy to compute the result in COMSOL Multiphysics, and the mixing cup temperature is

$$\langle T\rangle = \frac{5.058\cdot 10^{-3}}{1.50\cdot 10^{-5}} = 337\ \mathrm{K}. \qquad (3\text{-}29)$$

Reference

1. W. Ehrfeldt, V. Hessel, and H. Löwe, *Microreactors*, Wiley-VCH, 2000.

Model Library path: `Chemical_Engineering_Module/Heat_Transfer_and_Nonisothermal_Flow/sinusoidal_heat_exchanger`

Modeling Using the Graphical User Interface

1 Open COMSOL Multiphysics.

2 In the **Model Navigator**, set the **Space dimension** to **2D**.

3 From the list of application modes, select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes**.

4 Click fist the **Multiphysics** button and then the **Add** button to add the application mode to the model.

5 Select the application mode **Chemical Engineering Module>Energy Transport>Convection and Conduction**.

6 Click **Add**, then click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

1 Enter the following variable names, expressions, and (optionally) descriptions.

NAME	EXPRESSION	DESCRIPTION
`rho_c`	`985[kg/m^3]`	`Fluid density`
`k_c`	`0.6[W/(m*K)]`	`Fluid thermal conductivity`
`T_w`	`350[K]`	`Wall temperature`
`T_in`	`300[K]`	`Inlet temperature`
`u_av`	`15[mm/s]`	`Average inlet velocity`

2 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

3 Set **x min** to `-5e-5`, **x max** to `105e-5`, **y min** to `-5e-5`, and **y max** to `105e-5`.

4 On the **Grid** page, clear the **Auto** check box.

5 Type `5e-5` in both the **x spacing** and **y spacing** edit fields, then click **OK**.

GEOMETRY MODELING

1 Double-click the **SOLID** button in the status bar near the bottom of the user interface to clear the solidification option. This allows you to create open-ended line segments.

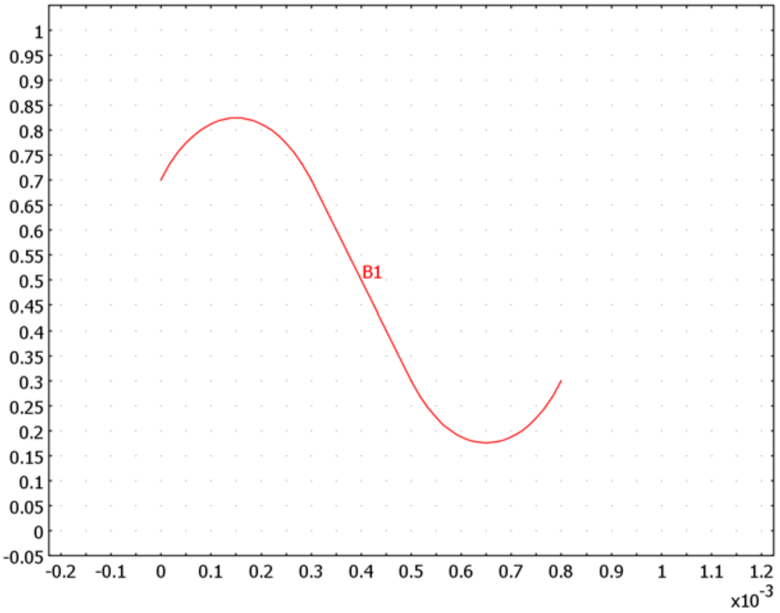
2 Click the **2nd Degree Bézier Curve** button on the Draw toolbar.

3 Click on the points (0, 0.7e-3), (0.15e-3, 1e-3), and (0.3e-3, 0.7e-3).

4 Click the **Line** button on the Draw toolbar.

5 Draw a straight line from (0.3e-3, 0.7e-3) to (0.5e-3, 0.3e-3). Right-click to terminate the line.

6 Draw a second Bézier curve through the points (0.5e-3, 0.3e-3), (0.65e-3, 0), and (0.8e-3, 0.30e-3).



7 Finish by drawing a line with the endpoints (0.8e-3, 0.30e-3), (1e-3, 0.70e-3).

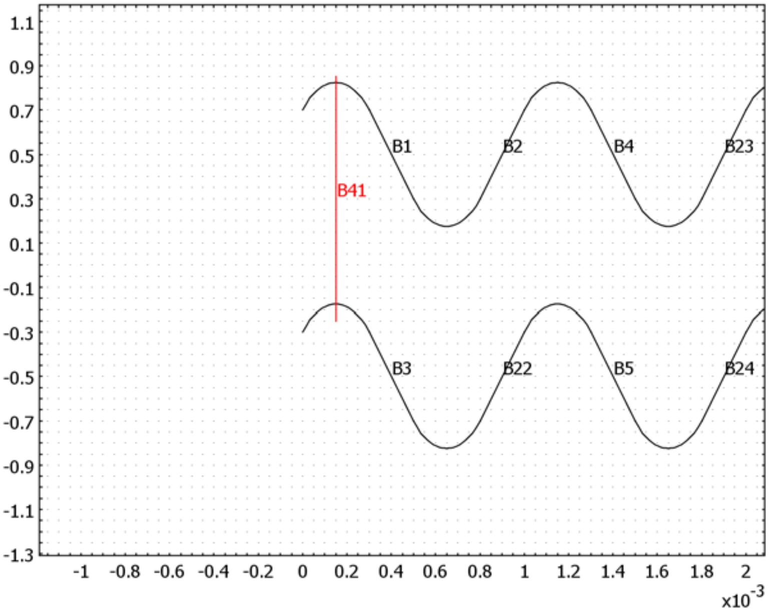
8 Press Ctrl+A to select all segments. Click the **Array** button and specify the following values; when done, click **OK**.

COMPONENT	DISPLACEMENT	ARRAY SIZE
x	`1e-3`	`10`
y	`-1e-3`	`2`

9 Open the **Axes/Grid Settings** dialog box under the **Options** menu. On the **Axis** page, select the **Axis equal** check box. On the **Grid** page clear the **Auto** check box, then type `5e-5` in both the **x-spacing** and **y-spacing** edit fields. Using a space-separated format, enter `1.5e-4 0.00965` in the **Extra x** edit field and then `-9e-4 -2.5e-4 3e-4 8.5e-4` in the **Extra y** edit field. Click **OK**.

10 Click the **Zoom Window** button on the Main toolbar and zoom in on the left-most few bends of the heat exchanger.

11 Click the **Line** button on the Draw toolbar and draw two straight lines, the first one from $(1.5\cdot10^{-4}, 8.5\cdot10^{-4})$ to $(1.5\cdot10^{-4}, -2.5\cdot10^{-4})$. Zoom out and the back in on the right portion of the geometry and draw the second line from $(9.65\cdot10^{-3}, 0.3\cdot10^{-3})$ to $(9.65\cdot10^{-3}, -0.9\cdot10^{-3})$.



12 Press Ctrl+A to select all the segments, then click the **Coerce to Solid** button on the Draw toolbar.

13 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Expressions

1 From the **Options** menu, select **Expressions>Subdomain Expressions**.

2 Select Subdomain 1, then enter the following variable names and expressions:

NAME	EXPRESSION
`eta`	`(0.11021-9.386e-4[1/K]*T+2.684e-6[1/K^2]*T^2 -2.569e-9[1/K^3]*T^3)[Pa*s]`
`C_p`	`(4190.86-0.977[1/K]*T+0.019[1/K^2]*T^2 -5.6e-5[1/K^3]*T^3)[J/(kg*K)]`

3 Click **OK**.

Subdomain Settings—Incompressible Navier-Stokes

1 From the **Multiphysics** menu choose **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu open the **Subdomain Settings** dialog box.

3 Select Subdomain 1, then enter material properties according to the following table:

PROPERTY	**VALUE**
ρ	`rho_c`
η	`eta`

4 Switch to the **Init** page, then enter `u_av` for the **u(t$_0$)** initial value.

5 Click **OK**.

Boundary Conditions—Incompressible Navier-Stokes

1 From the **Physics** menu open the **Boundary Settings** dialog box, select Boundary 1, and select **Inlet** from the **Boundary type** list and **Velocity** from the **Boundary condition** list. Set the parabolic velocity profile by typing `6*s*(1-s)*u_av` in the **u$_0$** edit field.

2 Select the type **Outlet** and the condition **Pressure, no viscous stress** condition for Boundary 40, and set **p$_0$** to `0`.

3 Click **OK**.

Subdomain Settings—Convection and Conduction

1 From the **Multiphysics** menu switch to the **2 Convection and Conduction (chcc)** application mode.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then specify values according to the following table:

PROPERTY	**VALUE**
k (isotropic)	`k_c`
ρ	`rho_c`
C_p	`C_p`
Q	`0`
u	`u`
v	`v`

4 Click the **Artificial Diffusion** button. Select the **Streamline Diffusion** check box. Click **OK** to accept the default settings and close the **Artificial Diffusion** dialog box.

This step adds a weak term that gives explicit streamline diffusion to the dependent variable T. This stabilizes the temperature field by damping oscillations produced by the discretization. For a more comprehensive explanation of streamline diffusion stabilization consult the *COMSOL Multiphysics User's Guide*.

5 On the **Init** page, set the initial value **T(t_0)** to `T_w`.

6 Click **OK**.

Boundary Conditions—Convection and Conduction

1 Open the **Boundary Settings** dialog box from the **Physics** menu and specify conditions according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARIES 2–39, 41–80	BOUNDARY 40
Type	Temperature	Temperature	Convective flux
T_0	`T_in`	`T_w`	

2 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Finer**. Click **OK**.

3 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar to open the **Plot Parameters** dialog box.

2 On the **Surface** page, type `T` in the **Expression** edit field (or select **Convection and Conduction (chcc)>Temperature** from the **Predefined quantities** list). Click **OK**.

To calculate the integral in Equation 3-28, proceed as follows:

3 From the **Postprocessing** menu, select **Boundary Integration**. Select Boundary 40, then type `T*u` in the **Expression** edit field. Click **Apply**. The value appears in the message log at the bottom of the user interface.

4 Change the entry in the in the **Expression** edit field to `u`, then click **OK**.

5 Divide the value from Step 3 with that from Step 4 to obtain the mean temperature.

4

Multicomponent Transport—Tutorials and Benchmarks

There are two different ways of performing multicomponent analysis in the Chemical Engineering Module. One is appropriate for diluted solutions and is found in the Diffusion and Convection application mode. The other one can be used for concentrated solutions, and is found in the Maxwell-Stefan Diffusion and Convection application mode. The use of both of these is exemplified in this section.

Separation through Dialysis

Introduction

Dialysis is a frequently used membrane separation process. An important application is hemodialysis, where membranes are used as artificial kidneys for people suffering from renal failure. Other applications include the recovery of caustic colloidal hemicellulose during viscose manufacturing, and the removal of alcohol from beer (Ref. 1).

In the dialysis process, specific components are preferentially transported through a membrane. The process is diffusion-driven, that is, components diffuse through a membrane due to concentration differences between the dialysate and the permeate sides of the membrane. Separation between solutes is obtained as a result of differences in diffusion rates across the membrane arising from differences in molecular size and solubility.

This example looks at a process aimed at lowering the concentration of a contaminant component in an aqueous product stream. The dialysis equipment is made of a hollow fiber module, where a large number of hollow fibers act as the membrane. It focuses on the transport of the contaminant in the hollow fiber and through its wall.

Figure 4-1 shows a diagram of the hollow fiber assembly. A large number of hollow fibers are assembled in a module where the dialysate flows on the fibers' insides while the permeate flows on their outsides in a co-current manner. The contaminant diffuses through the fiber walls to the permeate side due to a concentration gradient, whereas species with a higher molecular weight, those you want kept in the dialysate, are retained due to their low solubility and diffusivity in the membrane.

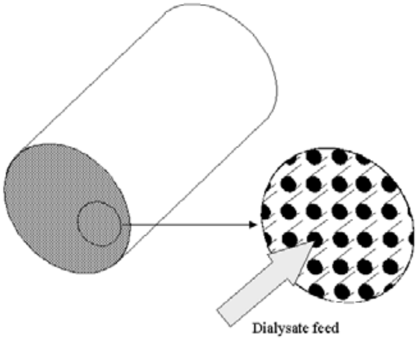


Figure 4-1: Diagram of the hollow fiber module.

Model Definition

This example models a piece of hollow fiber through which the dialysate flows with a fully developed laminar parabolic velocity profile. The fiber is surrounded by a permeate, which flows laminarly in the same direction as the dialysate. This example thus models three separate phases: the dialysate, the membrane, and the permeate. The model domain appears in Figure 4-2. Assume there are no angular gradients, so you can thus use an axisymmetrical approximation.

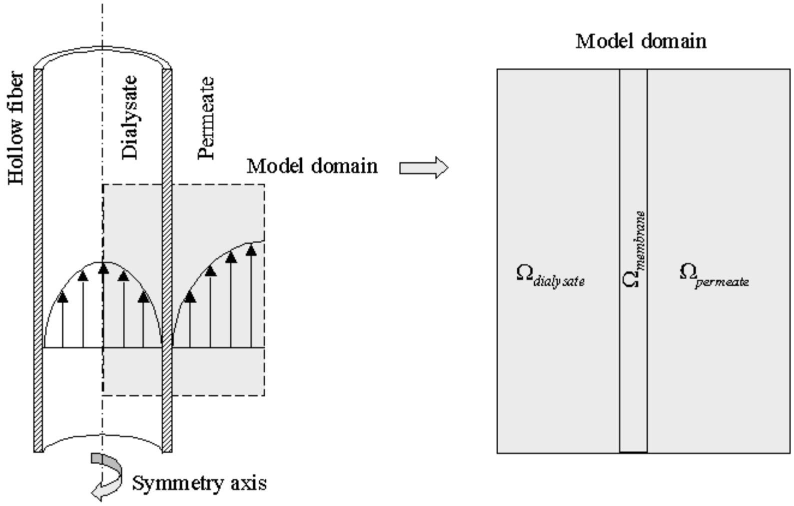


Figure 4-2: Diagram of the dialysis fiber.

The contaminant is transported by diffusion and convection in the two liquid phases, whereas diffusion is the only transport mechanism in the membrane phase. You can formulate the following mass transport equations to describe the system:

$$
\begin{aligned}
&\nabla\cdot(-D\nabla c_1 + c_1\mathbf{u}) = 0 && \text{in } \Omega_{\text{dialysate}} \\
&\nabla\cdot(-D_{\text{m}}\nabla c_2) = 0 && \text{in } \Omega_{\text{membrane}} \qquad (4\text{-}1)\\
&\nabla\cdot(-D\nabla c_3 + c_3\mathbf{u}) = 0 && \text{in } \Omega_{\text{permeate}}
\end{aligned}
$$

where c_i denotes the concentration of the contaminant (mol/m^3) in the respective phases, D denotes the diffusion coefficient (m^2/s) in the liquid phases, and D_{m} is the diffusion coefficient in the membrane, while **u** denotes the velocity (m/s) in the respective liquid phase.

The fiber is 75 times longer than its radial dimension, in this case 0.28 mm in radius and 21 mm in length. To avoid excessive amounts of elements and nodes you must scale the problem. Therefore introduce a new scaled z-coordinate, $\hat{z}$, and a corresponding differential for the mass transports:

$$\begin{aligned} \hat{z} &= \frac{z}{\mathrm{scale}} \\ dz &= \mathrm{scale}\cdot d\hat{z} \end{aligned} \qquad (4\text{-}2)$$

In the mass-transport equations, c is differentiated twice in the diffusion term, which implies that the diffusive flux vector's z-component must be multiplied by $(1/\mathrm{scale})^2$. The convective component is only differentiated once, and therefore must be multiplied by $1/\mathrm{scale}$. You can introduce the scaling of the diffusive part of the flux as an anisotropic diffusion coefficient where the diffusion in the z direction is scaled by the factor $(1/\mathrm{scale})^2$. This gives the following diffusion-coefficient matrix:

$$\overline{D} = \begin{bmatrix} D & 0 \\ 0 & \dfrac{D}{\mathrm{scale}^2} \end{bmatrix} \qquad (4\text{-}3)$$

To obtain the convective part of the flux, assume fully developed laminar flow both inside and outside the hollow fiber. This allows you to introduce the velocity distributions analytically. For the interior, this example uses the following velocity distribution (Ref. 2):

$$v_z^{\mathrm{dialysate}} = v_{\mathrm{max}}\left[1-\left(\frac{r}{R_1}\right)^2\right] \qquad (4\text{-}4)$$

where v_z is the axial component of the velocity, v_{max} is the maximum velocity in the axial direction, r represents the radial coordinate, and R_1 equals the inner radius of the hollow fiber. The velocity vector must be multiplied by $1/\mathrm{scale}$ to account for the new scaled z-coordinate.

Outside the fiber the velocity profile is more complicated. You can draw a hexagonal-shaped unit cell of the fiber assembly (Figure 4-3):

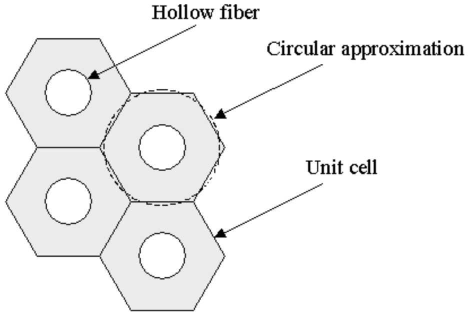


Figure 4-3: Hexagonal-shaped unit cell of the fiber assembly.

By approximating the hexagon with a circle, you can assume that the circle indicates the permeate's position of maximum velocity in the axial direction. In order to characterize the flow profile, the model twice integrates a momentum balance over a thin cylindrical shell (Ref. 2) to eventually get the following analytical expression for the permeate velocity distribution:

$$v_z^{\mathrm{permeate}} = A \cdot \left[r^2 - R_2^2 - 2 \cdot R_3^2 \cdot \ln\left(\frac{r}{R_2}\right)\right] \tag{4-5}$$

Here A (1/(m·s)) is a constant defined by

$$A = -\frac{P_0 - P_L}{4\eta L \cdot \mathrm{scale}}. \tag{4-6}$$

In these equations, R_2 and R_3 are the radial coordinates of the outer fiber wall and the approximated circle, respectively, η (Pa·s) is the permeate's dynamic viscosity, and $P_0 - P_L$ (Pa) represents the pressure drop over a length L.

The contaminant must dissolve into the membrane phase in order to be transported through it. The interface conditions between the liquid and membrane phases for the concentration are described by the dimensionless partition coefficient, K:

$$K = \frac{c_2^{\mathrm{d}}}{c_1^{\mathrm{d}}} = \frac{c_2^{\mathrm{p}}}{c_3^{\mathrm{p}}}. \tag{4-7}$$

Figure 4-4 shows a schematic concentration profile. Note that there are discontinuities in the concentration profile at the phase boundaries.

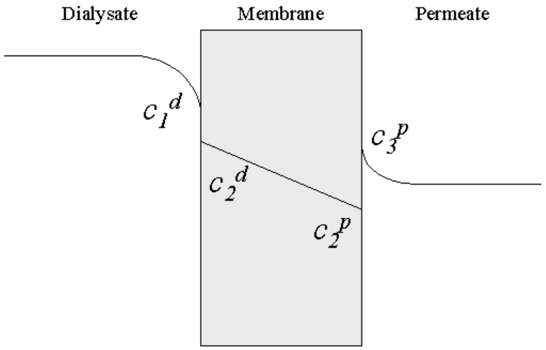


Figure 4-4: Diagram of the concentration profile across the membrane (see Equation 4-7).

To obtain a well-posed problem, you must define an appropriate set of boundary conditions; for the relevant notation, see Figure 4-5.

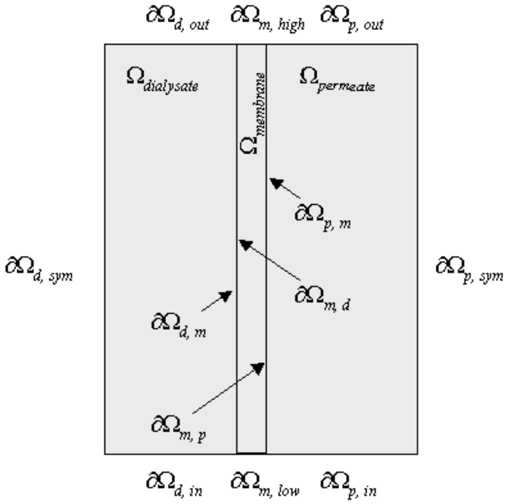


Figure 4-5: Boundaries and boundary labels for the modeled system.

At the inlet to the model domain, define concentration conditions as:

$$
\begin{aligned}
c_1 &= c_0 \qquad \text{at } \partial\Omega_{\text{d, in}} \\
c_3 &= 0 \qquad \text{at } \partial\Omega_{\text{p, in}}
\end{aligned}
\tag{4-8}
$$

At the outlet, assume that the convective contribution to the mass transport is much larger than the diffusive contribution:

$$
(-D\nabla c_i + c_i\mathbf{u})\cdot\mathbf{n} = c_i\mathbf{u}\cdot\mathbf{n} \quad \text{at } \partial\Omega_{\text{d,out}} \text{ and } \partial\Omega_{\text{p, out}} \tag{4-9}
$$

Here $\mathbf{n}$ is the normal unit vector to the respective boundary. Further, assume that you have no transport over the symmetry boundaries:

$$
(-D\nabla c_i + c_i\mathbf{u})\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{\text{d, sym}} \text{ and } \partial\Omega_{\text{p, sym}}\,. \tag{4-10}
$$

Also assume symmetry at the horizontal boundaries of the membrane:

$$
(-D_{\text{m}}\nabla c_2)\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{\text{m, high}} \text{ and } \partial\Omega_{\text{m, low}}\,. \tag{4-11}
$$

You can verify this assumption after solving the model by studying the very small vertical concentration gradient in the membrane.

MODEL DATA

The input data used in this model are listed in the following table:

PROPERTY	VALUE	DESCRIPTION
D	10^{-9} m^2/s	Diffusion coefficient, liquid phases
D_{m}	10^{-9} m^2/s	Diffusion coefficient, membrane
R_1	0.2 mm	Inner radius, hollow fiber
R_2	0.28 mm	Outer radius, hollow fiber
R_3	0.7 mm	Approximative radius, unit cell
v_{max}	1 mm/s	Maximum velocity, dialysate
A	$-2\cdot10^{-3}$ 1/(m·s)	Permeate velocity prefactor
K	0.7	Partition coefficient
c_0	1 M	Inlet concentration, dialysate
M	10^4 m/s	Stiff-spring velocity
scale	7	Axial coordinate scale factor

Results

The surface plot in Figure 4-6 visualizes the concentration distribution throughout the three model domains: the dialysate region inside the hollow fiber on the left side, the membrane in the middle, and the permeate to the right.

As the plot shows, the concentration inside the hollow fiber decreases markedly over the first 10 mm from the inlet. After this the separation process is less effective. You can also see from the plot that it takes almost 4 mm before the concentration in the core part of the fiber is influenced by the filtration process. The figure further shows the developing diffusion layers on both sides of the fiber wall.

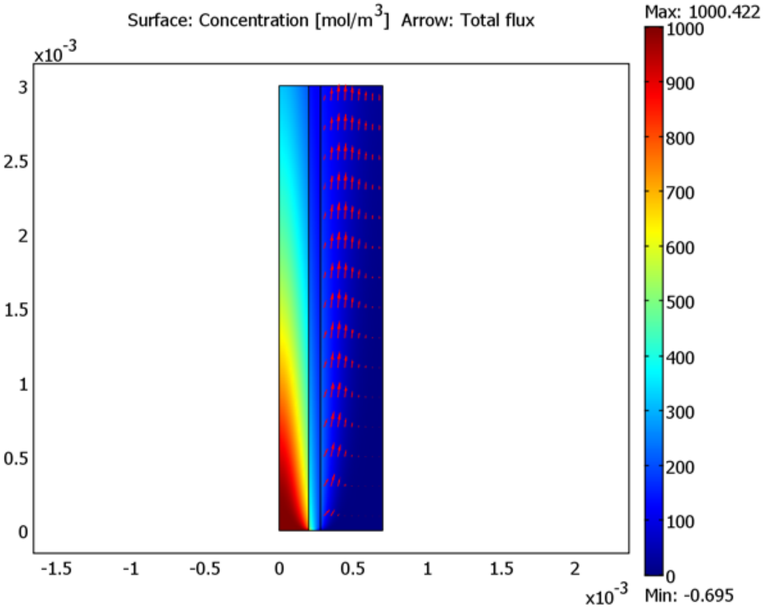


Figure 4-6: Concentration and flux in the three subdomains.

The figure also shows the concentration jump that arises at the boundary between the dialysate and the membrane. Further, the maximum concentration in the permeate occurs a few millimeters downstream from the inlet. If there is a risk of scaling on the fiber's outer surface due to high concentration of filtrated species, it is largest at the location of this maximum.

Note that this example models only a short piece at the hollow fiber's inlet end. Using a larger scale factor you can model the fiber's entire length.

Modeling in COMSOL Multiphysics

Because there are discontinuities in the concentration profile at the boundaries between liquid and membrane phases, you must use three separate variables to describe the concentration in the respective phases. To get continuous flux over the phase boundaries, apply a special type of boundary condition using the stiff-spring method. Instead of defining Dirichlet concentration conditions according to the partition coefficient K, which would destroy the continuity of the flux, you can define continuous flux conditions that, at the same time, force the concentrations to the desired values:

$$\begin{aligned}
(-D\nabla c_1 + c_1\mathbf{u}) \cdot \mathbf{n} &= M(c_2 - Kc_1) \qquad \text{at } \partial\Omega^{\mathrm{d/m}} \\
(-D_{\mathrm{m}}\nabla c_2) \cdot \mathbf{n} &= M(Kc_1 - c_2) \qquad \text{at } \partial\Omega^{\mathrm{m/d}} \\
(-D_{\mathrm{m}}\nabla c_2) \cdot \mathbf{n} &= M(Kc_3 - c_2) \qquad \text{at } \partial\Omega^{\mathrm{m/p}} \\
(-D\nabla c_3 + c_3\mathbf{u}) \cdot \mathbf{n} &= M(c_2 - Kc_3) \qquad \text{at } \partial\Omega^{\mathrm{p/m}}
\end{aligned} \tag{4-12}$$

Here M is a (nonphysical) velocity large enough to let the concentration differences in the brackets approach zero, thereby satisfying Equation 4-7. These boundary conditions also give a continuous flux across the interfaces provided that M is sufficiently large.

References

1. M. Mulder, *Basic Principles of Membrane Technology*, 2nd ed., Kluwer Academic Publishers, 1998.

2. R. B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

Model Library path:

`Chemical_Engineering_Module/Multicomponent_Transport/dialysis`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator** click the **Multiphysics** button.
3. From the space **Space Dimension** list, select **Axial symmetry (2D)**.
4. In the list of application modes select **Chemical Engineering Module>Mass Transport>Convection and Diffusion**.
5. In the **Dependent variables** edit field, type `c1`. Click the **Add** button.
6. Repeat the procedure for the application mode **Chemical Engineering Module>Mass Transport>Diffusion** and name the dependent variable `c2`.
7. Finally add a second instance of the **Chemical Engineering Module>Mass Transport>Convection and Diffusion** application mode, but this time name the variable `c3`.
8. Click **OK** to close the **Model Navigator**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Constants**.
2. Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`D`	`1e-9[m^2/s]`	`Diffusion constant, liquid phases`
`Dm`	`1e-9[m^2/s]`	`Diffusion constant, membrane`
`M`	`1e4[m/s]`	`Stiff-spring velocity`
`K`	`0.7`	`Partition coefficient`
`c0`	`1[mol/liter]`	`Inlet concentration, dialysate`
`R1`	`0.2[mm]`	`Inner radius, hollow fiber`
`R2`	`0.28[mm]`	`Outer radius, hollow fiber`
`R3`	`0.7[mm]`	`Approximate radius, unit cell`
`v1_max`	`1[mm/s]`	`Maximum velocity, dialysate`
`A`	`-2e3[1/(m*s)]`	`Permeate velocity prefactor`
`scale`	`7`	`Axial coordinate scale factor`

GEOMETRY MODELING

1. Click the **Rectangle/Square** button on the Draw toolbar and draw a rectangle of arbitrary size. Repeat this procedure once to obtain two rectangles in total.

2 Double-click on each rectangle in turn and enter the following values in the appropriate edit fields; when done, click **OK**.

PROPERTY	R1	R2
Width	`2.8e-4`	`5e-4`
Height	`3e-3`	`3e-3`
r	`0`	`2e-4`
z	`0`	`0`

3 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Expressions

For postprocessing purposes, define a concentration variable, c_{all}, that evaluates to the concentration variables c_1, c_2, and c_3, respectively, in Subdomains 1, 2, and 3.

1 Choose **Options>Expressions>Subdomain Expressions**.

2 Select Subdomain 1. Type `c_all` in the first **Name** edit field and `c1` in the **Expression** edit field.

3 Select Subdomain 2**.** Type `c2` in the **Expression** edit field for `c_all`.

4 Select Subdomain 3. Type `c3` in the **Expression** edit field for `c_all`.

5 Click **OK** to close the **Subdomain Expressions** dialog box.

Subdomain Settings—Convection and Diffusion (chcd)

1 From the **Multiphysics** menu, select **1 Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 2 and 3, then clear the **Active in this domain** check box.

4 Select Subdomain 1.

5 Click the **D (anisotropic)** button. Place the cursor in the edit field next to this button. In the diffusivity edit-field matrix that appears, type `D` in the *rr*-component (upper left) and `D/scale^2` in the *zz*-component (lower right).

6 Click the **Init** tab, then type `c0` in the **c1(t$_0$)** edit field.

7 Click **OK**.

Boundary Conditions—Convection and Diffusion (chcd)

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY 4
Type	Insulation/ symmetry	Concentration	Convective flux	Flux
$c1_0$		`c0`		
N_0				`M*(c2-K*c1)`

Subdomain Settings—Diffusion (chdi)

1 From the **Multiphysics** menu, select **2 Diffusion (chdi)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 1 and 3, then clear the **Active in this domain** check box.

4 Select Subdomain 2, then enter the anisotropic diffusivity in the same manner as for the previous application mode using the following data:

PROPERTY	VALUE
D (r direction)	`Dm`
D (z direction)	`Dm/(scale^2)`
R	`0`

Boundary Conditions—Diffusion (chdi)

1 From the **Physics** menu, select **Boundary Settings.**

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 4	BOUNDARIES 5, 6	BOUNDARY 7
Type	Flux	Insulation/Symmetry	Flux
N_0	`M*(K*c1-c2)`		`M*(K*c3-c2)`

Subdomain Settings—Convection and Diffusion (chcd2)

1 From the **Multiphysics** menu, select **3 Convection and Diffusion (chcd2)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 1 and 2, then clear the **Active in this domain** check box.

4 Select Subdomain 3, then enter the anisotropic diffusivity in the same manner as for the previous application modes using the following data:

PROPERTY	VALUE
D (r direction)	`D`
D (z direction)	`D/(scale^2)`

PROPERTY	VALUE
R	0
u	0
v	`A*((r^2)-(R2^2)-2*(R3^2)*log(r/R2))/scale`

5 Click the **Init** tab, then type `0.1*c0` in the **c3(t_0)** edit field. Click **OK**.

Boundary Conditions—Convection and Diffusion (chcd2)

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 7	BOUNDARY 8	BOUNDARY 9	BOUNDARY 10
Type	Flux	Concentration	Convective flux	Insulation/Symmetry
$c3_0$		0		
N_0	`M*(c2-K*c3)`			

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar.

2 Click the **Refine Mesh** button once to refine the mesh.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 4-6, follow these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Click the **Surface** tab. In the **Expression** edit field, type `c_all`.

3 Click the **Arrow** tab. Select the **Arrow plot** check box.

4 In the **Arrow parameters** area, select **3D arrow** from the **Arrow type** list.

5 On the **Subdomain Data** page, select **Convection and Diffusion (chcd2)>Total flux, c3** from the **Predefined quantities** list.

6 Return to the **General** page. Click the **Title** button.

7 In the **Title** dialog box, click the option button next to the edit field and enter the title `Surface: Concentration [mol/m<sup>3</sup>]  Arrow: Total flux`.

8 Click **OK** to close the **Title** dialog box.

9 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

Stefan Tube

Introduction

This example, taken from Ref. 6, illustrates the use of the Maxwell-Stefan Diffusion and Convection application mode. A multicomponent gas phase diffusion problem is solved as a 1D model. In this particular case, two of the three components experience a steady-state flux, whereas the third component has zero flux on one of the boundaries. The concentration profiles at steady state are modeled.

Model Definition

The Stefan tube, depicted in Figure 4-7, is a simple device used for measuring diffusion coefficients in binary vapors.

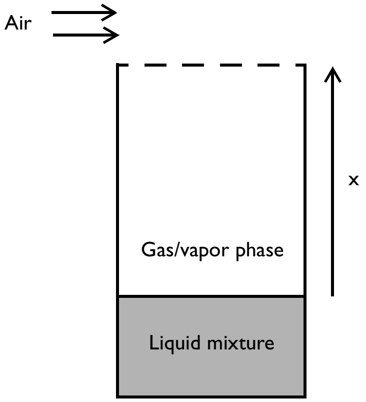


Figure 4-7: Schematic diagram of a Stefan tube.

At the bottom of the tube is a pool of mixture. The vapor that evaporates from this pool diffuses to the top of the tube, where a stream of air, flowing across the top of the tube, keeps the mole fraction of diffusing vapor there to be zero. The mole fraction of vapor above the liquid interface is in equilibrium. Because there is no horizontal flux inside the tube, you can analyze the problem using a 1D model. The system composition of acetone, methanol, and air has been extensively investigated, measuring both diffusion coefficients and composition at various positions within Stefan tubes. This makes it an ideal example for this model.

As a comparison, one experiment measured the mole fraction at the liquid interface to be $x_{\mathrm{Ac}} = 0.319$ and $x_{\mathrm{Me}} = 0.528$ where the pressure, p, was 99.4 kPa and the temperature, T, was 328.5 K. The length of the diffusion path was 0.238 m. The respective Maxwell-Stefan diffusion coefficients, D_{ij}, of the three binary pairs were calculated and are used in the model according to Table 4-1.

TABLE 4-1: LABELS AND MAXWELL-STEFAN DIFFUSION COEFFICIENTS

COMPONENT	**LABEL**	D_{ij}	**VALUE**
Acetone	1	D_{12}	$8.48\cdot10^{-6}$ m^2/s
Methanol	2	D_{13}	$13.72\cdot10^{-6}$ m^2/s
Air	3	D_{23}	$19.91\cdot10^{-6}$ m^2/s

To model this problem, use the Maxwell-Stefan Diffusion and Convection application mode for three components. It solves for the fluxes in terms of mass fractions for two of the three components. The mass fraction, ω, of the third is given by the two first. The three equations are:

$$\nabla\cdot\left[-\rho\omega_1\sum_k[D_{1\mathrm{k}}(\nabla x_k+(x_k-\omega_k)((\nabla p)/p))]+\right.$$
$$\left.D^T((\nabla T)/T)\right] = R-(\rho\mathbf{u}\cdot\nabla\omega_1) \qquad (4\text{-}13)$$

$$\nabla\cdot\left[-\rho\omega_{2(1)}\sum_k[D_{2\mathrm{k}}(\nabla x_k+(x_k-\omega_k)((\nabla p)/p))]+\right.$$
$$\left.D^T((\nabla T)/T)\right] = R-(\rho\mathbf{u}\cdot\nabla\omega_2) \qquad (4\text{-}14)$$

$$\omega_3 = 1-\omega_1-\omega_2 \qquad (4\text{-}15)$$

where D is the diffusion coefficient (m^2/s), p is the pressure (Pa), T is the temperature (K), $\mathbf{u}$ is the velocity (m/s), x and ω are mole and mass fractions, respectively, and the mixture density, ρ_{mix} (kg/m^3), is a function of the average mixture mole fraction, M_{mix} (kg/mol), according to Equation 4-17:

$$M_{\mathrm{mix}} = \sum_i x_i M_i \qquad (4\text{-}16)$$

$$\rho_{\mathrm{mix}} = \frac{p}{RT}M_{\mathrm{mix}} \qquad (4\text{-}17)$$

In this case, there is no imposed fluid velocity. However, there will appear a fluid velocity due to the diffusion fluxes. At the top of the tube the mass fractions are fixed, with the fraction of air being unity. At the bottom (at the liquid interface), the fractions are also fixed according to the previously mentioned experimental conditions. The fact that there is no air flux at the interface results in the following relation for the convective velocity, at steady state:

$$u = \frac{n_{\mathrm{diff},3}}{\omega_3\rho} \tag{4-18}$$

where $n_{\mathrm{diff},3}$ is the diffusive mass flux of air (kg/(m^2·s)).

Results

The steady-state mole fractions as a function of position is depicted in Figure 4-8. As a comparison, the results given from Ref. 6 are depicted in Figure 4-9.

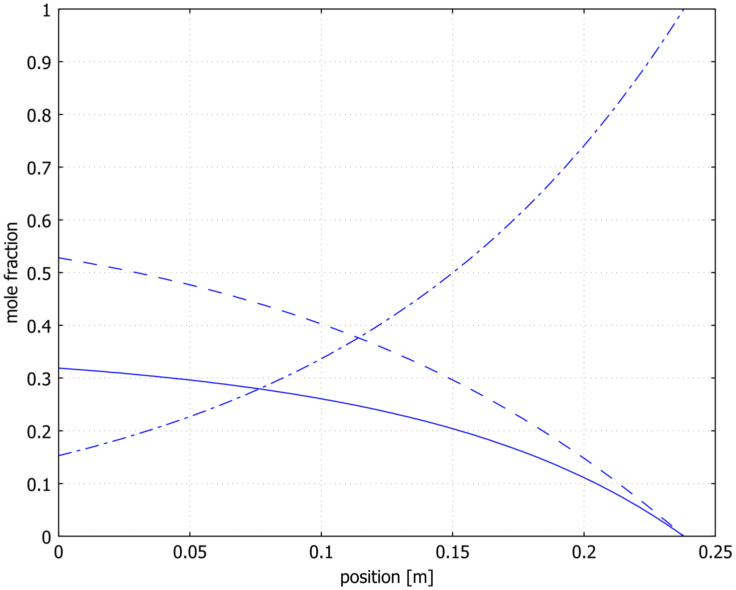


Figure 4-8: Steady-state mole fractions of: acetone(-), methanol (- -), and air(-˙-), in the Stefan tube according to the COMSOL Multiphysics model as solved using Maxwell-Stefan diffusivities.

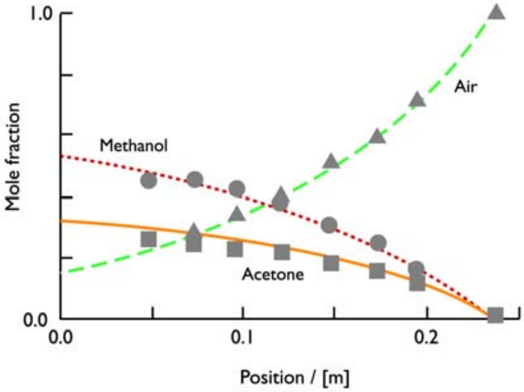


Figure 4-9: Steady-state mole fractions of: acetone(-), methanol (- -), and air(-˙-), in a Stefan tube according to experimental data (Ref. 6).

We can see that the COMSOL Multiphysics model emulates the results from Ref. 6 rather well, which means the Maxwell-Stefan equations describe the mass transport process in the system.

A significant advantage with the Maxwell-Stefan diffusion formulation, in comparison with Fick's law, is the inclusion of a conservation of mass. In the absence of chemical reactions (source terms) and convective contributions, the Maxwell-Stefan formulation results in zero net mass flux. This is not the case for the Fickian diffusion formulation. A consequence of the conservation of mass is that if there is a net mass flux. In this example, it can be described by the convective term, which you can see in Figure 4-10.

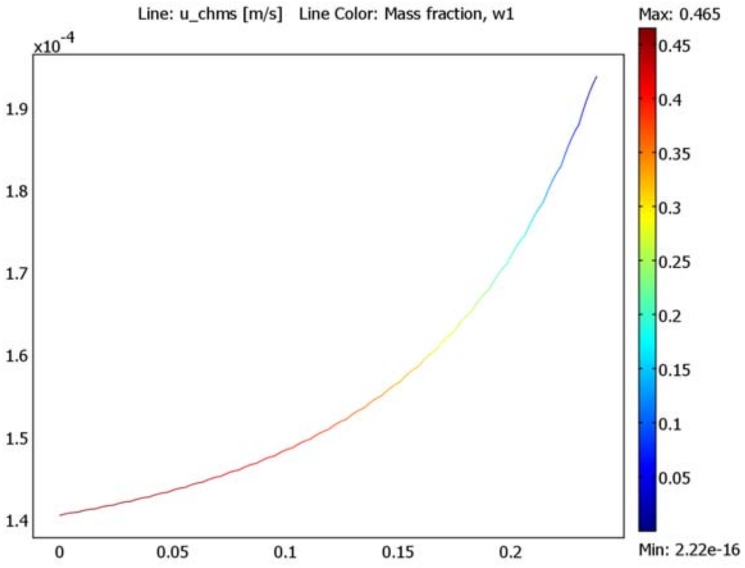


Figure 4-10: Velocity of the gas mixture in the Stefan tube from the pool surface to the outlet.

References

1. C.F. Curtiss and R.B. Bird, *Ind. Eng. Chem. Res.*, vol. 38, p. 2515, 1999.

2. R.B. Bird, W. Stewart, and E. Lightfoot, *Transport Phenomena*, John Wiley & Sons, New York, 1960.

3. G.A.J. Jaumann *Wien. Akad. Sitzungsberichte (Math.-Naturw. Klasse)*, vol. 120, p. 385, 1911.

4. J. O. Hirschfelder, C.F. Curtiss, and R.B. Bird, *Molecular Theory of Gases and Liquids*, Wiley, USA, **1954**.

5. E.N. Fuller, P.D. Schettler, and J.C. Giddings, *Ind. Eng. Chem.* 58, p. 19, **1966**.

6. R. Taylor and R. Krishna, *Multicomponent Mass Transfer,* John Wiley & Sons Inc., NY, USA, p. 21, 1993.

Model Library path:

`Chemical_Engineering_Module/Multicomponent_Transport/stefan_tube`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 On the **New** page, set the **Space dimension** to **1D**.

3 Select the application mode **Chemical Engineering Module>Mass Transport> Maxwell- Stefan Diffusion and Convection**.

4 In the **Dependent variables** edit field, type `w1`, `w2`, and `w3`. Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`p0`	`1.013e5[Pa]`	`Pressure`
`T0`	`328.5[K]`	`Temperature`
`Rg`	`8.314[J/mol]`	`Gas constant`
`D12`	`8.48e-6[m^2/s]`	`MS diffusion coefficient, acetone`
`D13`	`13.72e-6[m^2/s]`	`MS diffusion coefficient, methanol`
`D23`	`19.91e-6[m^2/s]`	`MS diffusion coefficient, air`
`M_air`	`28.8[g/mol]`	`Molar mass, air`
`M_ace`	`58[g/mol]`	`Molar mass, acetone`
`M_met`	`32[g/mol]`	`Molar mass, ethanol`
`x_ace0`	`0.319`	`Acetone mole fraction at liquid interface`
`x_met0`	`0.528`	`Methanol mole fraction at liquid interface`
`x_air0`	`1-x_ace0-x_met0`	`Air mole fraction at liquid interface`

NAME	EXPRESSION	DESCRIPTION
`w_air0`	`x_air0*M_air/(x_air0*M_air+x_ace0*M_ace+x_met0*M_met)`	`Air mass fraction at liquid interface`
`w_ace0`	`x_ace0*M_ace/(x_air0*M_air+x_ace0*M_ace+x_met0*M_met)`	`Acetone mass fraction at liquid interface`
`w_met0`	`1-w_air0-w_ace0`	`Methanol mass fraction at liquid interface`

3 Choose **Options>Expressions>Scalar Expressions**.

4 Define the following scalar expression (again, the description is optional):

NAME	EXPRESSION	DESCRIPTION
`M_mix`	`x_w1_chms*M_ace+x_w2_chms*M_met+x_w3_chms*M_air`	`Average molar mass`

5 Click **OK**.

GEOMETRY MODELING

1 Create a line between the coordinates 0 and 0.238 by using **Specify Objects>Line** in the **Draw** menu, typing `0 0.238` in the **x** edit field in the **Coordinates** area, and then click **OK**.

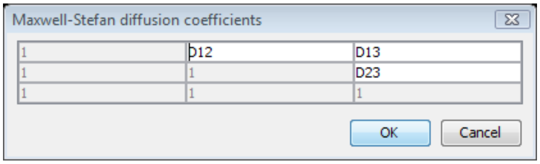
2 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**. Select subdomain 1.

2 On the **General** page, click the **Edit** button for the **Maxwell-Stefan diffusivity matrix**, and type `D12`, `D13`, and `D23`, in the edit fields for the corresponding diffusion coefficients.



1	D12	D13
1	1	D23
1	1	1

3 Click **OK** to close the **Maxwell-Stefan diffusion coefficients** dialog box.

4 Apply the following additional settings:

PROPERTY	VALUE
ρ	`M_mix*p0/(Rg*T0)`
p	`p0`
T	`T0`
u	`(-dflux_w3_chms)/(w3*rho_chms)`

5 On the **w1** page, type `M_ace` in the **M** edit field.

6 Similarly, type `M_met` and `M_air` in the **M** edit fields on the **w2** and **w3** pages.

7 Finally, type `w_ace0` and `w_met0` in the edit fields **w1** and **w2** on the **Init** page.

8 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Specify boundary conditions according to the following table.

SETTINGS	BOUNDARY 1	BOUNDARY 2
Boundary condition	Mass fraction	Mass fraction
w1	`w_ace0`	`0`
w2	`w_met0`	`0`

3 Click **OK**.

MESH GENERATION

Click the **Refine Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

In order to reproduce the plot in Figure 4-8, do the following:

1 From the **Postprocessing** menu, select **Domain plot parameters**.

2 On the **General** page, select the **Keep current plot** check box.

3 Click the **Title/Axis** button, type `position [x]` and `mole fraction` in the edit fields for **First axis label** and **Second axis label**, clearing the **Auto** button prior to typing in the entries. Click **OK**.

4 Select the **Line/Extrusion** page, select subdomain 1 and type `x_w1_chms` in the **Expression** edit field. Click **Apply**.

5 Return to the **Domain plot parameters** dialog box and type `x_w2_chms` in the **Expression** edit field.

6 Click the **Line Settings** button. From the **Line style** list, select **Dashed line**. Click **OK**.

7 Click **Apply**.

8 Similarly, plot `x_w3_chms` using line style **Dash-dot line** and click **OK**.

To reproduce Figure 4-10, proceed as follows:

9 Click the **Plot Parameters** button on the Main toolbar.

10 On the Line page, type `u_chms` in the **Expression** edit field. Select **Use expression to color lines**, then click **OK**.

Maxwell-Stefan Diffusion in a Fuel Cell Unit Cell

Introduction

In concentrated gases and liquids, where the concentrations of species are of the same order of magnitude, there is no obvious solvent-solute relationship. Fick's law for diffusion accounts only for 1-way solute-solvent interactions whereas the Maxwell-Stefan equations account for all interactions of species in a solution. In a system with three components, three pair-wise interactions are present, while for a system of four components there are six such interactions. These interactions are described as Fick-analogous Maxwell-Stefan diffusion coefficients, D_{ij}.

This example models the steady-state mass transport in the cross section of a proton exchange membrane fuel cell cathode. It models the mass transport in the 3-component gas mixture using Maxwell-Stefan diffusion. The cross section includes the channel and current collector in the bipolar plate, at the upper boundary, while the active layer defines the lower boundary.

The purpose of this model is to show how to consider Maxwell-Stefan diffusion in mass transport.

Model Definition

Figure 4-11 describes the computational domain. The insulating boundary at the top of the domain is the current-collector boundary corresponding to the position of the bipolar plate. The vertical boundaries are symmetry boundaries, while the lower boundary, denoted a reactive boundary, represents the position of the active layer.

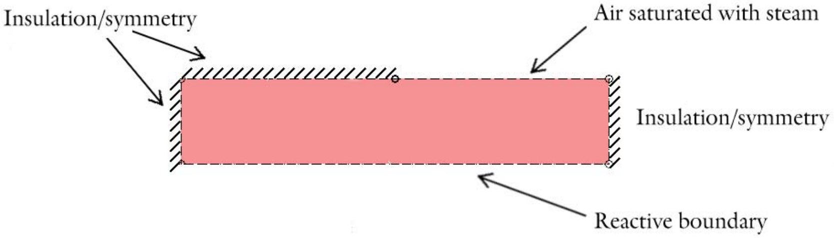


Figure 4-11: Depiction of the modeling domain with descriptions of the boundary conditions.

The model equations are defined by a simple mass transport taking the divergence of the mass flux through diffusion and convection. This yields the following expression for species i:

$$\nabla\cdot\left[-\rho\omega_i\sum_{j=1}^{N}\mathsf{D}_{ij}\left\{\frac{M}{M_j}\left(\nabla\omega_j+\omega_j\frac{\nabla M}{M}\right)+(x_j-\omega_j)\frac{\nabla p}{p}\right\}+\omega_i\rho\mathbf{u}\right] = 0 \qquad (4\text{-}19)$$

where M denotes the total molar mass of the mixture (kg/mol), M_j gives the molar mass of species j (kg/mol), and ω_j is the mass fraction of species j. M can also be expressed in terms of the mass fractions, ω_j. The symmetric diffusivities are strongly dependent on the composition and are given by these expressions (see Ref. 2 and Ref. 3):

$$\mathsf{D}_{11} = \frac{\dfrac{(\omega_2+\omega_3)^2}{x_1D_{23}}+\dfrac{\omega_2^2}{x_2D_{13}}+\dfrac{\omega_3^2}{x_3D_{12}}}{\dfrac{x_1}{D_{12}D_{13}}+\dfrac{x_2}{D_{12}D_{23}}+\dfrac{x_3}{D_{13}D_{23}}} \qquad (4\text{-}20)$$

$$\mathsf{D}_{12} = -\frac{\dfrac{\omega_1(\omega_2+\omega_3)}{x_1D_{23}}+\dfrac{\omega_2(\omega_1+\omega_3)}{x_2D_{13}}-\dfrac{\omega_3^2}{x_3D_{12}}}{\dfrac{x_1}{D_{12}D_{13}}+\dfrac{x_2}{D_{12}D_{23}}+\dfrac{x_3}{D_{13}D_{23}}} \qquad (4\text{-}21)$$

where x_j is the mol fraction of species j (which can be expressed in terms of the mass fractions ω_j), and D_{ij} is the Maxwell-Stefan diffusivities (m^2/s). Additional entries of the symmetric diffusivities are constructed by permutation of the indices, that is, $D_{12} = D_{21}$. The Maxwell-Stefan diffusivities can be described with an empirical equation (Ref. 4) based on the kinetic gas theory:

$$D_{ij} = k\frac{T^{1.75}}{p(\nu_i^{1/3}+\nu_j^{1/3})^2}\left[\frac{1}{M_i}+\frac{1}{M_j}\right]^{1/2} \qquad (4\text{-}22)$$

where k is a constant with the value $3.16\cdot10^{-8}$ Pa·m^2/s, T is the temperature expressed in kelvin, p denotes the pressure (Pa), ν_i equals the molar diffusion volume of species i expressed in m^3/mol, and M_i is the molar mass of species i expressed in kg/mol. The molar diffusion volumes are given in Table 4-2 (Ref. 1).

TABLE 4-2: DIFFUSION VOLUMES

SPECIES	DIFFUSION VOLUME
O_2	$16.6\cdot10^{-6}$ m^3/mol
H_2O	$12.7\cdot10^{-6}$ m^3/mol
N_2	$17.9\cdot10^{-6}$ m^3/mol

At the reactive boundary (the electrode), the flux of oxygen is

$$\mathbf{n}_{O_2}\cdot\mathbf{n} = \left(-\frac{i_c}{4F}\right)M_{O_2} \tag{4-23}$$

where $\mathbf{n}_j$ represents the mass flux of j, and i_c is the reaction current given by the Tafel expression:

$$i_c = \left(-\frac{S_a\delta i_0}{4F}\right)\frac{\omega_{O2}}{\omega_{O2_0}}\exp\left(\frac{0.5F\eta}{RT}\right). \tag{4-24}$$

Here S_a denotes the specific surface area (m^2/m^3), and δ is the thickness of the active layer (m). In the Tafel equation, F denotes Faraday's number (C/mol), R is the gas constant (J/(mol·K)), T represents the temperature (K), i_0 denotes the exchange current density (A/m^2), and η is the overpotential (V). The subscript zero in the mass fraction for oxygen represents the reference state.

Similarly, the flux of water is

$$\mathbf{n}_{H2O}\cdot\mathbf{n} = \frac{i_c}{F}\left(\frac{1}{2}+t_{H_2O}\right)M_{H_2O} \tag{4-25}$$

where t_{H2O} is the transport number for water (that is, the number of water molecules dragged with each proton migrating through the membrane).

At the reactive boundary there is no flux of nitrogen gas because it does not take part in the reactions. This boundary condition results in zero total flux of nitrogen in the entire subdomain at steady state. Included this fact in the model by specifying the subdomain gas velocity according to

$$\mathbf{u} = \left(-\frac{1}{\omega_{N_2}\rho}\right)\nabla\cdot\left[-\left(\rho\omega_{N_2}\sum_{j=1}^{N}D_{N_2,j}\left\{\frac{M}{M_j}\left(\nabla\omega_j+\omega_j\frac{\nabla M}{M}\right)+(x_j-\omega_j)\frac{\nabla p}{p}\right\}\right)\right] \tag{4-26}$$

At the inlet, a fixed composition is applied. This model uses a composition of air saturated with steam at 80 °C as according to the following table (Ref. 1).

TABLE 4-3: INPUT DATA FOR THE MASS FRACTIONS AT THE INLET

SPECIES	MASS FRACTION
O_2	0.1447
H_2O	0.3789
N_2	0.4764

Results

Figure 4-12 shows the mass fraction of oxygen at a 0.8 V cathode overvoltage (representing a short circuit of the fuel cell).

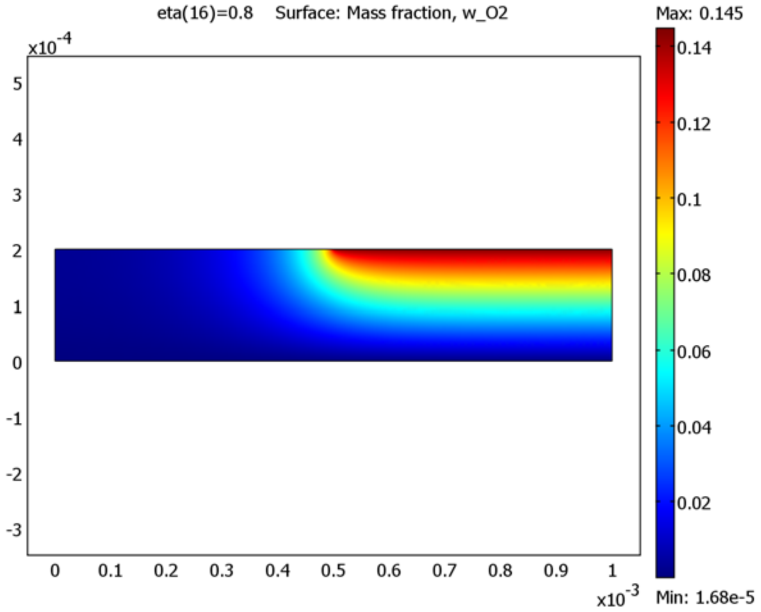


Figure 4-12: Mass fraction of oxygen at 0.8 V overvoltage of the cathode (an almost short circuit of the fuel cell).

The oxygen concentration in the active layer is close to zero in the positions far away from the inlet.

The large variation in concentration has a direct influence on the value of the diffusion coefficients for oxygen and the other involved species, nitrogen and water.

To illustrate the composition dependence in the diffusivities, you can plot the Maxwell-Stefan diffusivity of D_{22} (the water diffusivity); see Figure 4-13.

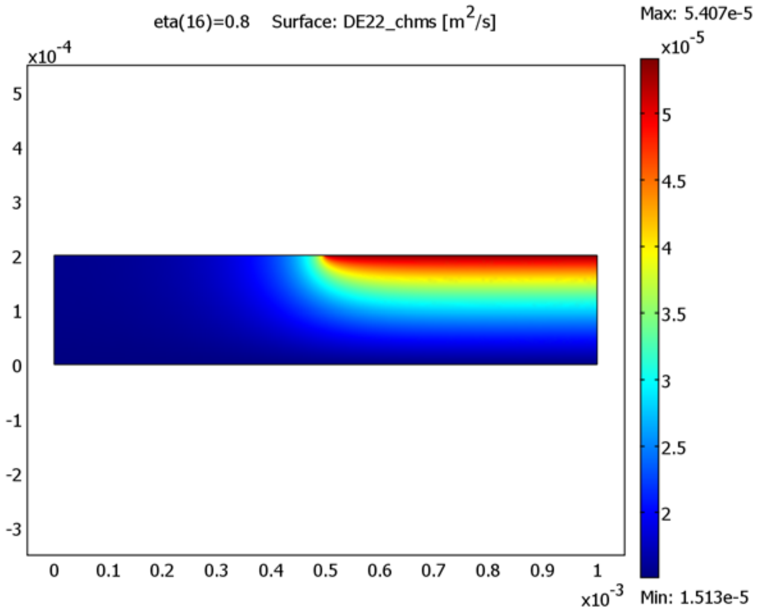


Figure 4-13: Variation of Maxwell-Stefan diffusivity of water, D_{22}*, within the gas mixture at 0.8 V overvoltage.*

The water diffusivity decreases with decreasing oxygen concentration. This is probably due to the decreased interaction among oxygen molecules.

Figure 4-14 shows the convective gas velocity induced by the drag and production of water at the reactive boundary. The induced gas velocity causes significant convective fluxes out from the reactive boundary, significantly reducing the concentration of oxygen at the boundary. This causes a poorer performance of the cell. In addition, there is a significant velocity peak at the corner of the inlet. This is caused by the close to spherical diffusion situation at that point.

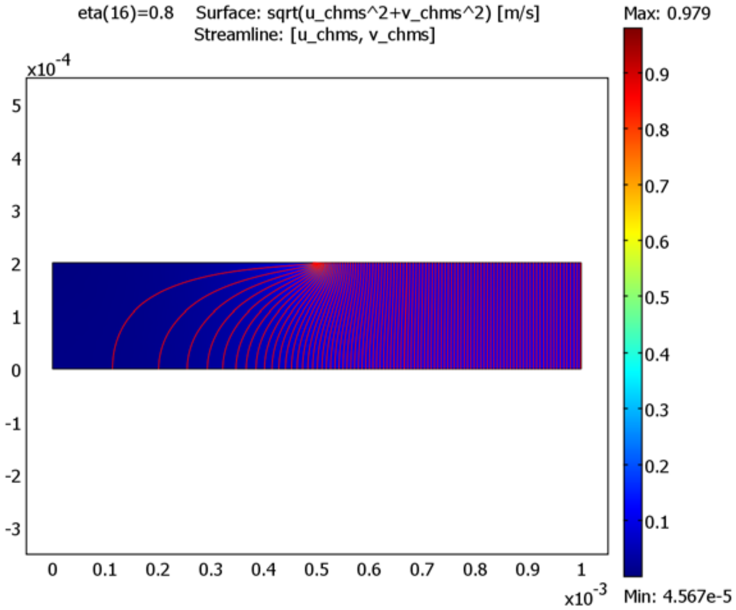


Figure 4-14: Velocity field in the fuel cell cathode gas compartment at 0.8 V cathode overvoltage.

This example also investigates cathode performance in terms of a polarization curve (Figure 4-15). At high cathode overvoltages, the total electrode current levels off. This is caused by mass transport limitations, which is important to consider when designing or operating fuel cells.

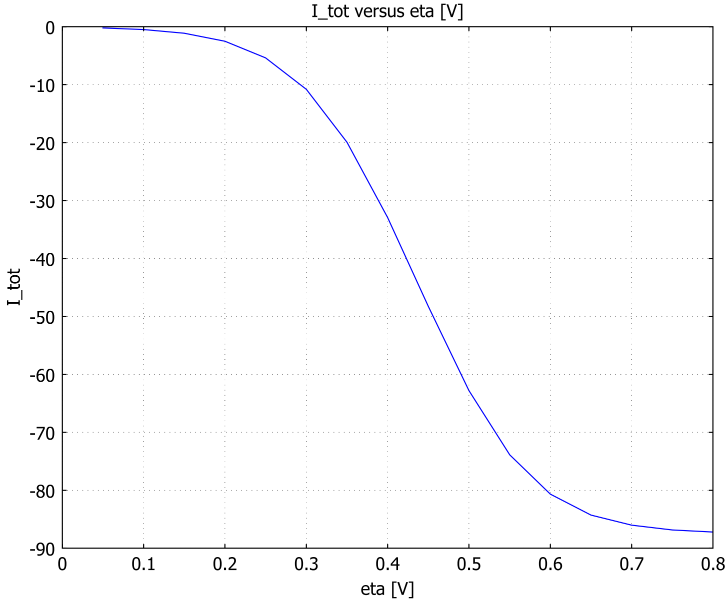


Figure 4-15: Polarization curve for the cathode.

References

1. R. Perry, D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

2. C.F. Curtiss and R.B. Bird, "Multicomponent Diffusion," *Ind. Eng. Chem. Res.*, pp. 2515–2522, vol. 38, 1999.

3. R. Bird, W. Stewart, and E. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2002.

4. J. A. Wesselingh and R. Krishna, *Mass Transfer in Multicomponent Mixtures*, Delft University Press, 2000.

Model Library path: `Chemical_Engineering_Module/Multicomponent_Transport/maxwell_stefan_diffusion`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **2D** from the **Space dimension** list.

3 In the list of application modes select the application mode **Chemical Engineering Module>Mass Transport>** **Maxwell-Stefan Diffusion and Convection**.

4 Type `w_O2 w_H2O w_N2` in the **Dependent variables** edit field.

5 Click **OK**.

Options and Settings

1 Define the following constants and expressions in the **Constants** dialog box on the **Options** menu; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
k	3.16e-8[Pa*m^2/s]	MS diffusivity prefactor
F	96485[C/mol]	Faraday’s constant
R	8.314[J/(mol*K)]	Gas constant
v_N2	17.9e-6	Molar diffusion volume, N2
v_O2	16.6e-6	Molar diffusion volume, O2
v_H2O	12.7e-6	Molar diffusion volume, H2O
M_O2	32[g/mol]	Molar mass, O2
M_H2O	18[g/mol]	Molar mass, H2O
M_N2	28[g/mol]	Molar mass N2
w_O20	0.1447	Inlet mass fraction, O2
w_H2O0	0.3789	Inlet mass fraction, H2O
T0	353[K]	Temperature
p0	101[kPa]	Pressure
D_O2_N2	k*(T0[1/K])^1.75/(p0*(v_O2^(1/3)+v_N2^(1/3))^2)*(1[kg/mol]/M_O2+1[kg/mol]/M_N2)^0.5	MS diffusivity, O2-N2 component
D_O2_H2O	k*(T0[1/K])^1.75/(p0*(v_O2^(1/3)+v_H2O^(1/3))^2)*(1[kg/mol]/M_O2+1[kg/mol]/M_H2O)^0.5	MS diffusivity, O2-H2O component
D_H2O_N2	k*(T0[1/K])^1.75/(p0*(v_H2O^(1/3)+v_N2^(1/3))^2)*(1[kg/mol]/M_H2O+1[kg/mol]/M_N2)^0.5	MS diffusivity, H2O-N2 component

NAME	EXPRESSION	DESCRIPTION
`eta`	`0.1[V]`	`Overpotential`
`S_a`	`1e7[1/m]`	`Specific surface area`
`d`	`10[um]`	`Active-layer thickness`
`i_0c`	`1[A/m^2]`	`Exchange current density`
`t_H2O`	`3`	`Drag number, H2O`

2 From the **Options** menu, select **Expressions>Scalar Expressions**.

3 Define the following expressions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION
`M`	`M_O2*x_w_O2_chms+M_H2O*x_w_H2O_chms+M_N2*x_w_N2_chms`
`i_c`	`-S_a*d*i_0c*exp(0.5*F*eta/(R*T0))*(abs(w_O2)/w_O20)`

Geometry Modeling

1 Shift-click the **Rectangle/Square** button on the Draw toolbar. Specify a rectangle by setting its **Width** to `1e-3` and its **Height** to `2e-4`. Click **OK**.

2 Click the **Zoom Extents** button on the Main toolbar.

3 Shift-click the **Point** button on the Draw toolbar. Add a point at the coordinates (`5e-4,2e-4`), then click **OK**.

Subdomain Settings

1 Select **Subdomain Settings** in the **Physics** menu.

2 Select 1 from the **Subdomain selection** list.

3 In the **General** page, type `M*p0/(R*T0)` in the **Density** edit field.

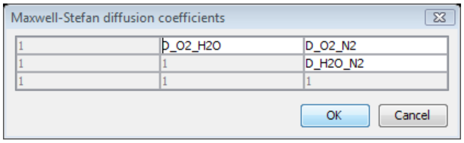
4 Type `p0` in the **Pressure** edit field

5 Type `T0` in the **Temperature** edit field.

6 In the **u** and **v** edit fields, type `-dflux_w_N2_x_chms/(w_N2*rho_chms)` and `-dflux_w_N2_y_chms/(w_N2*rho_chms)`, respectively.

7 Click the **D_{ij} Edit** button.

8 Type `D_O2_H2O`, `D_O2_N2`, and `D_H2O_N2` in the **Binary diffusion coefficients** matrix component edit fields (as in this figure).



1	D_O2_H2O	D_O2_N2
1	1	D_H2O_N2
1	1	1

9 Click **OK**.

10 Click the tabs for each species and type `M_O2`, `M_H2O`, and `M_N2` in the corresponding **Molecular weight** edit fields.

11 Click the **Init** tab, then set the initial conditions according to the following table:

VARIABLE	INITIAL VALUE
w_O2(t_0)	`wO20`
w_H2O(t_0)	`wH2O0`

12 Click **OK**.

13 From the **Physics** menu, select **Properties**. In the **Equation form** list select **Conservative**.

14 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 On the **w_O2** page, specify boundary conditions as in this table:

SETTINGS	BOUNDARIES 1, 3, 5	BOUNDARY 2	BOUNDARY 4
Type	Insulation/Symmetry	Flux	Mass fraction
n_0		`M_O2*i_c/(4*F)`	
w_O2$_0$			`w_O20`

3 On the **w_H2O** page, specify boundary conditions as in this table:

SETTINGS	BOUNDARIES 1, 3, 5	BOUNDARY 2	BOUNDARY 4
Type	Insulation/Symmetry	Flux	Mass fraction
n_0		`-M_H2O*i_c*(1/2+t_H2O)/F`	
w_H2O$_0$			`w_H2O0`

4 Click **OK**.

Mesh Generation

1. Click the **Initialize Mesh** button on the Main toolbar.
2. Click the **Refine Mesh** button to refine the mesh.

Preparing for Postprocessing

1. Choose **Options>Integration Coupling Variables>Boundary Variables**.
2. In the dialog box that opens, select Boundary 2. In the **Name** edit field, type `I_tot`, and in the **Expression** edit field, type `i_c`. Click **OK**.

Computing the Solution

1. Click the **Solver Parameters** button on the Main toolbar.
2. Select the **Parametric** solver.
3. In the **Parameter name** edit field, type `eta`. In the **Parameter values** edit field, type `0.05:0.05:0.8`. Click **OK**.
4. Click the **Solve** button on the Main toolbar.

Postprocessing and Visualization

The default plot, reproduced in Figure 4-12, shows the mass fraction of oxygen, w_{O2}. Because the solution is parametric, you can view the results as an animation by clicking the **Animate** button on the Plot toolbar.

To reproduce the plot in Figure 4-13, do as follows:

1. Click the **Plot Parameters** button on the Main toolbar.
2. Click the **Surface** tab.
3. Type `DE22_chms` in the **Expression** edit field on the **Surface Data** page.
4. Click **Apply**.

To generate Figure 4-14, follow these instructions:

1. On the **Surface** page, type `sqrt(u_chms^2+v_chms^2)` in the **Expression** edit field.
2. Click the **Streamline** tab. Select the **Streamline plot** check box.
3. On the **Streamline Data** page, type `u_chms` and `v_chms` in the edit fields for **x component** and **y component**, respectively.
4. From the **Streamline plot type** list, select **Magnitude controlled**.
5. Click **OK**.

Finally, generate Figure 4-15 with these steps:

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.

2. On the **Point** page, type `I_tot` in the **Expression** edit field inside the **y axis data** area.
3. In the **x axis data** area, click the lower option button, then click the **Expression** button.
4. In the **X Axis Data** dialog box, type `eta` in the **Expression** edit field. Click **OK**.
5. Back in the **Domain Plot Parameters** dialog box, select Point 1.
6. Click **OK**.

5

Mixers and Stirred Vessels

This chapter contains examples of mixers and stirred vessels.

Laminar Static Mixer

Introduction

In static mixers, also called motionless or in-line mixers, a fluid is pumped through a pipe containing stationary blades. This mixing technique is particularly well suited for laminar flow mixing because it generates only small pressure losses in this flow regime. This example studies the flow in a twisted-blade static mixer. It evaluates the mixing performance by calculating the concentration's standard deviation.

Model Definition

This model studies the mixing of one species dissolved in water at room temperature. The geometry consists of a tube with three twisted blades of alternating rotations (Figure 5-1).

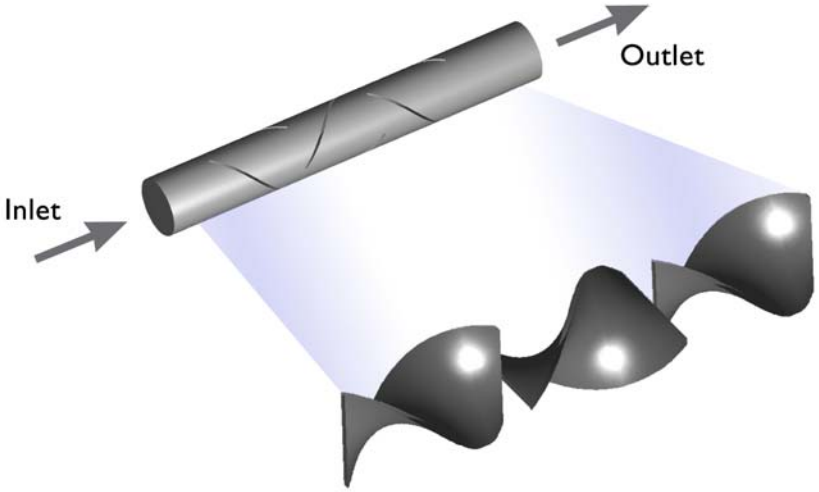


Figure 5-1: Depiction of a laminar static mixer containing three blades with alternating rotations.

The tube's radius, R, is 6 mm; the length is $14R$, and the length of each blade is $3R$. The inlet flow is laminar and fully developed with an average velocity of 1 cm/s. At the outlet, the model specifies a constant reference pressure of 0 Pa. The equations for the momentum transport are the stationary Navier-Stokes equations in 3D:

$$-\nabla\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p=0 \qquad (5\text{-}1)$$
$$\nabla\cdot\mathbf{u}=0$$

Here η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ is the velocity (m/s), ρ represents the fluid density (kg/m^3), and p denotes the pressure (Pa). The fluid's properties are not affected by the change in concentration of the dissolved species.

The model studies the mixing performance by assuming a discontinuous concentration profile at the mixer's inlet. The inlet concentration is defined as

$$c_{\text{inlet}}=\begin{cases}c_0 & x<0\\ 0 & x\geq 0\end{cases} \qquad (5\text{-}2)$$

with the line $x = 0$ separating the two inlet sides. Diffusion and convection contribute to the mass flux, and the resulting mass transport equation is:

$$\nabla\cdot(-D\nabla c+c\mathbf{u}) = 0 \qquad (5\text{-}3)$$

Here D denotes the diffusion coefficient (m^2/s), and c is the concentration (mol/m^3).

At the outlet, the mass transport is mainly driven by convection. That is, the transport by diffusion is neglected in the normal direction of the pipe's cross section. Because the convective term leads to instabilities in the solution, you need a fine mesh to obtain a stable solution for the concentration field.

The low Reynolds numbers, in the mixer implies that the Navier-Stokes equations do not require a particularly dense mesh. You can therefore first solve the Navier-Stokes equations on a coarse mesh and then map the solution onto a finer mesh. In the last solution step you use this mapped velocity field in the convective mass-transport term.

Results

Figure 5-2 shows a slice plot of the concentration in the mixer. The slice at the bottom shows the lighter and darker halves of the fluid with and without the dissolved species, respectively. As the fluid flows upward through the system, the two solutions are mixed and an almost constant concentration is obtained at the outlet.

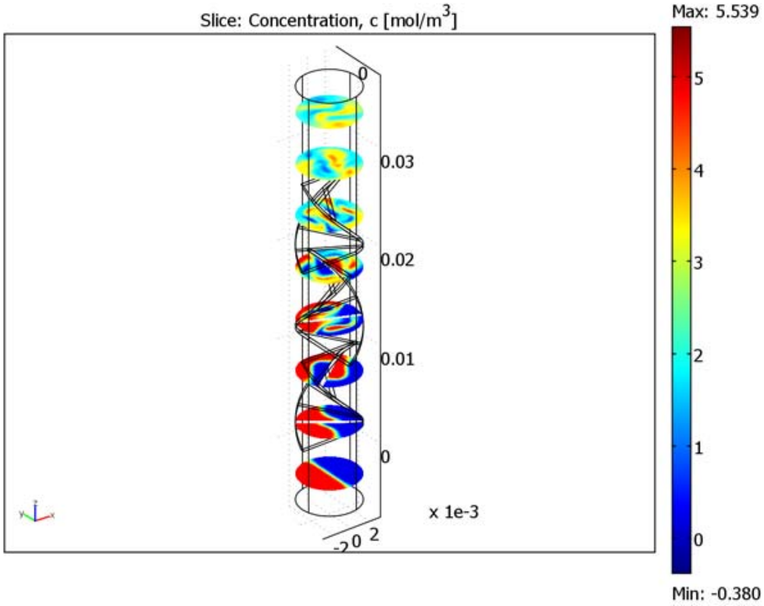


Figure 5-2: Slice plot of the concentration at different distances from the inlet.

Figure 5-3 shows the flow field responsible for the mixing. The streamlines clearly reveal the twisting motion in the fluid that is induced by the mixer blades.

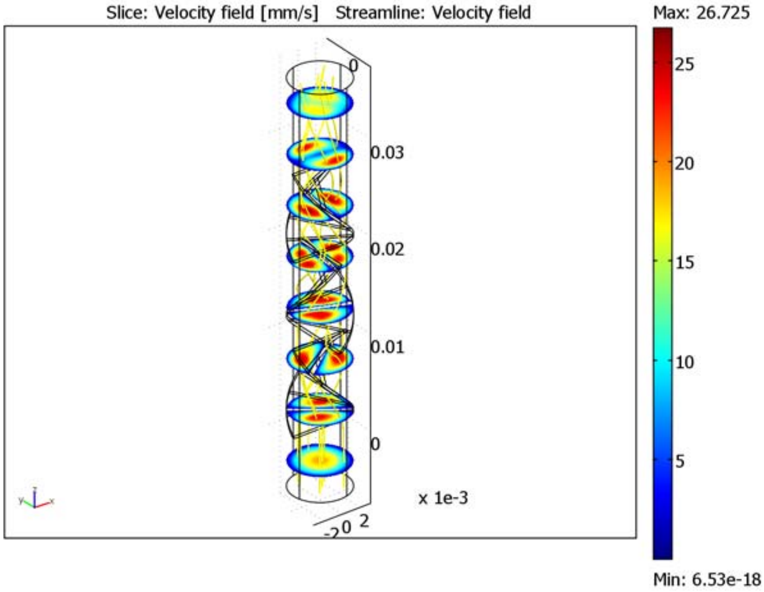


Figure 5-3: Slice plots of the velocity magnitude field inside the mixer. The streamlines show the flow direction.

You can also visualize the mixing through a series of cross-section plots. Figure 5-4 contains such a series of plots showing the concentration in the mixer's cross section along the direction of the flow. The results show that most of the mixing takes place where the blades change rotational direction (the three middle figures).

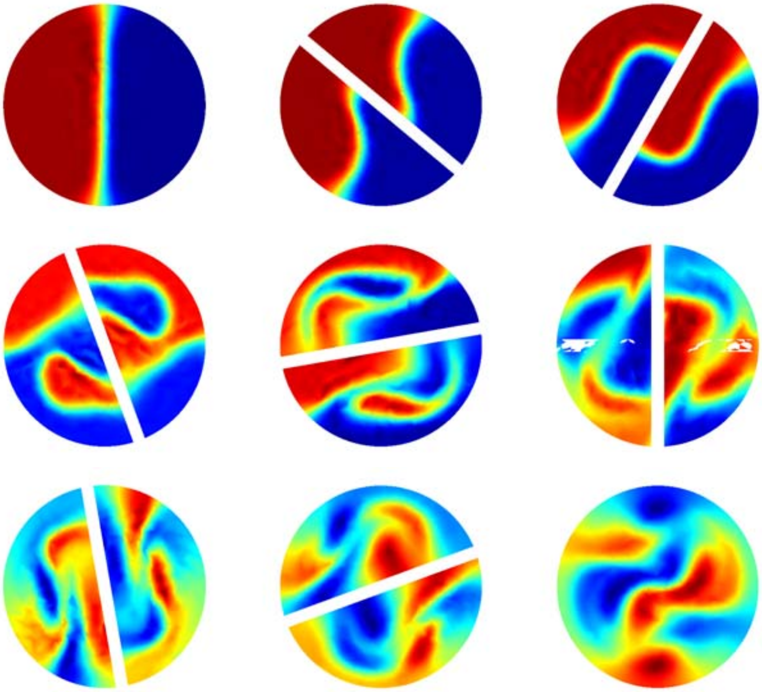


Figure 5-4: Cross-sectional plots of the concentration at different distances from the inlet. The nine plots shows the concentration at z =- 2 mm to z = 30 mm in steps of 4 mm.

References

1. R. Perry and D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

2. J.M. Coulson and J.F. Richardson, *Chemical Engineering*, vol. 1, 4th ed., Pergamon Press, 1990.

Model Library path: `Chemical_Engineering_Module/Mixers_and_Stirred_Vessels/laminar_static_mixer`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open COMSOL Multiphysics.

2 In the **Model Navigator** select **3D** from the **Space dimension** list; then click the **Multiphysics** button.

3 From the list of application modes select **Chemical Engineering>Momentum Transport>Laminar Flow.**

Incompressible Navier-Stokes and add it to the model by pressing the **Add** button.

4 In the list of application modes select **Chemical Engineering>Mass Transport>Convection and Diffusion** and add it to the model with the **Add** button.

5 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`ra`	`3[mm]`	`Tube radius`
`rho`	`1e3[kg/m^3]`	`Fluid density`
`eta`	`1e-3[Pa*s]`	`Viscosity`
`u_mean`	`10[mm/s]`	`Mean inlet velocity`
`c0`	`5[mol/m^3]`	`Inlet concentration`
`D`	`5e-8[m^2/s]`	`Diffusion coefficient`

3 From the **Options** menu, select **Visualization/Selection Settings**.

4 Change the **Visualization mesh** from **Normal** to **Fine**.

5 Click **OK**.

GEOMETRY MODELING

To create the twisted blades, start from a 2D work plane, then extrude and twist the blade cross section:

1 From the **Draw** menu, select **Work-Plane Settings**.

2 Use the default work plane by clicking **OK**.

3 Press Shift and click the **Rectangle** button on the Draw toolbar.

4 Set the **Width** to `2.4*3e-3`, the **Height** to `3e-3/8`, and **Position/Base** to **Center**.

5 Click **OK**.

6 From the **Draw** menu, select **Extrude**.

7 Set the **Distance** to `1.5e-3` and the **Twist** to `30`. Click **OK**.

The first part of the first blade in now finished.

8 Make a copy of the extrusion by pressing Ctrl+C, then paste the copy with Ctrl+V.

9 Click the **Move** button on the Draw toolbar.

10 Set the **z-displacement** to `1.5e-3`, then click **OK**.

11 Click the **Rotate** button on the Draw toolbar.

12 Set the **Rotation angle** to `-30`, then click **OK**.

13 Select both existing geometry objects by pressing Ctrl+A.

14 Copy and paste them onto the work area.

15 Move the pasted objects `3e-3` in the *z* direction.

16 Rotate `-60` degrees.

17 Click **Paste** once again. This pastes the first two parts of the blade in the original position.

18 Move the pasted selection `6e-3` in the *z* direction and rotate `-120` degrees.

You have now created the first blade. Use it as template for the other two.

19 Select all the objects that make up the first blade by pressing Ctrl+A.

20 Make a copy by pressing Ctrl+C, then press Ctrl+V to paste it.

21 Move the pasted selection `9e-3` in the *z* direction.

22 Click the **Scale** button on the Draw toolbar. Set the **x-scale** to `-1`, then click **OK**.

23 Click the **Rotate** button on the Draw toolbar. Rotate the selection `+90` degrees.

24 Press Ctrl+V once more to paste and move the pasted selection `18e-3` in the *z* direction.

You have created all three blades. Next make the tube using the cylinder tool.

25 Click the **Cylinder** button on the Draw toolbar.

26 Type `3e-3` in the **Radius** edit field and `42e-3` in the **Height** edit field.

27 In the **Axis base point** area, set the **z** position to `-6e-3`.

28 Set the **Rotation** to `15`, then click **OK**.

The final step in creating the geometry is to perform a difference operation that removes the intersection of the blades and the cylinder.

29 Select all the geometry objects defining the blades, then click the **Union** button.

30 Press Ctrl+A to select the two geometry objects present.

31 Create the final geometry by pressing the **Difference** button on the Draw toolbar.

PHYSICS SETTINGS—INCOMPRESSIBLE NAVIER-STOKES

Subdomain Settings

1. From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.
2. From the **Physics** menu, select **Subdomain Settings**.
3. Select Subdomain 1. Set the **Density** to `rho` and the **Dynamic viscosity** to `eta`.
4. On the **Init** page, set **u(t_0)** to `0`, **v(t_0)** to `0`, and **w(t_0)** to `u_mean`.
5. Click **OK**.

Boundary Settings

1. From the **Physics** menu, select **Boundary Settings**.
2. Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 20	BOUNDARY 23	ALL OTHERS
Type	Inlet	Outlet	Wall
Condition	Velocity	Pressure, no viscous stress	No slip
u_0	0	-	-
v_0	0	-	-
w_0	`2*u_mean*(1-(x^2+y^2)/ra^2)`	-	-
p_0	-	0	-

PHYSICS SETTINGS—CONVECTION AND DIFFUSION

Subdomain Settings

1. From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.
2. From the **Physics** menu, select **Subdomain Settings**.
3. Select Subdomain 1. Enter the following settings; when done, click **OK**.

PROPERTY	VALUE
D	D
R	0
u	u

PROPERTY	VALUE
v	`v`
w	`w`

Boundary Settings

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 20	BOUNDARY 23	ALL OTHERS
Type	Concentration	Convective flux	Insulation/Symmetry
c_0	`c0*flc2hs(-x[1/m],3e-4)`	-	-

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Extra fine**.

3 Click **Remesh**. When the mesher has finished, click **OK** to close the dialog box.

COMPUTING THE SOLUTION

First adjust some solver properties for a memory-efficient simulation:

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Linear system solver** list, select **Direct (SPOOLES)**.

3 Click **OK**.

Because the fluid's properties do not change with concentration, you can solve the Navier-Stokes equations independently.

1 Click the **Solver Manager** button on the Main toolbar

2 On the **Solve For** page, select **Incompressible Navier-Stokes** from the list.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar to compute the velocity field.

The next step is to solve the mass-transport equation, which requires a denser mesh than the Navier-Stokes equations.

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Normal**.

3 Click the **Custom mesh size** button, then set the **Maximum mesh size** to `7e-4`.

4 Click **Remesh**. When the mesher has finished, click **OK**.

The resulting mesh consists of approximately 57,000 elements.

1 Click the **Solver Manager** button on the Main toolbar.
2 On the **Solve For** page, select **Convection and Diffusion** from the list.
3 On the **Initial Value** page, click the **Store Solution** button.
4 In the **Initial value** area, click the **Stored solution** option button.
5 Click **OK**.
6 Click the **Solve** button on the Main toolbar to compute the solution for the concentration field.

The solution to the Navier-Stokes equations on the coarser mesh is automatically mapped to the finer mesh before the software solves the convection and diffusion equation.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 5-2 take the following steps.

1 Click the **Plot Parameters** button on the Main toolbar.
2 On the **Slice** page, select the **Slice plot** check box.
3 In the **Slice data** area, select **Convection and Diffusion (chcd)>Concentration, c** from the **Predefined quantities** list.
4 In the **Slice positioning** area, set **x-levels** and **y-levels** to `0`, and **z-levels** to `8`.
5 Click **Apply**.

   To generate the plot in Figure 5-3, continue with the following steps.

6 Still on the **Slice** page, select **Incompressible Navier-Stokes (chns)>Velocity field** from the **Predefined quantities** list on the **Slice Data** page.
7 On the **Streamline** page, select the **Streamline plot** check box.
8 In the **Predefined quantities** list in the **Streamline data** area, keep the default selection, **Incompressible Navier-Stokes (chns)>Velocity field**.
9 Click the **Advanced** button and set the **Maximum number of integration steps** to `4000`. Click **OK**.
10 On the **Line Color** page, select **Uniform color** and click the **Color** button.
11 Set the color to yellow, then click **OK**.
12 Finalize the plot by clicking **OK** in the **Plot Parameters** dialog box.

Generate the nine plots in Figure 5-4 using the cross-section plot functionality.

1. From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
2. On the **General** page, click the **Slice plot** option button in the **Plot type** area.
3. Clear the **Display cross-section in main axes** check box.
4. Click the **Slice** tab.
5. In the **Slice data** area, select **Convection and Diffusion (chcd)>Concentration, c** from the **Predefined quantities** list.
6. From the **Coordinate system to plot in** list, select **Local (slice)**.
7. Use the default settings for the *x*- and *y*-coordinates of all three points that define the cross-section plane.
8. Set **z0** = **z1** = **z2** = `-2e-3`, then click **Apply**.
9. Repeat the previous step with *z*-coordinates `2e-3` to `30e-3` with steps of `4e-3` to create the remaining eight plots.

Residence Time in a Turbulent Reactor

Introduction

Large-scale reactors usually have the economic necessity of being made out of stationary parts. The capital and running costs for motors and mixing equipment are often impediments to large-scale reactive processes such as the water treatment for metropolitan areas.

Baffled reactors are common in the process industry and are used to allow for slower reactions to fade out after an initial step. They make use of the baffled-imposed turbulence to provide mixing within the reactor. Even so, such reactors must be optimized because too much baffling can create unnecessary turbulence and pressure drops.

As in other reactors, an indication of residence time is a pointer toward the effectiveness of a reactor design. You can measure the maximum, minimum, and average time that a tracer element is present within a reactor to provide information about the reactor design and the extent of mixing. It can also show dead zones and areas of stagnation, which can themselves be problems through silt build-up and regions for secondary reactions.

This model studies the residence time in a turbulent reactor and compares a 2D approximation with a full 3D model of the reactor. It does so by first solving for a stationary turbulent flow in the reactor using the k-ε model, and then solving for a mass transport on top of this flow field in the time domain. Mass transport is described through convection and diffusion, where the turbulent viscosity from the k-ε model describes the species diffusion in the mass transport. A tracer species is introduced as a "burst" of concentration, and the model studies its journey through the reactor.

This model illustrates the use of the k-ε Turbulence Model application mode in the Chemical Engineering Module. It also shows the use of the Solver Manager in COMSOL Multiphysics, which makes it possible to solve a problem in sequential steps.

Model Definition

Figure 5-5 shows the reactor's 2D geometry. It is a cross section of a 3D geometry, showing the front view. The model is inspired by a water-treatment process where flow enters from the left and leaves the reactor at the right.

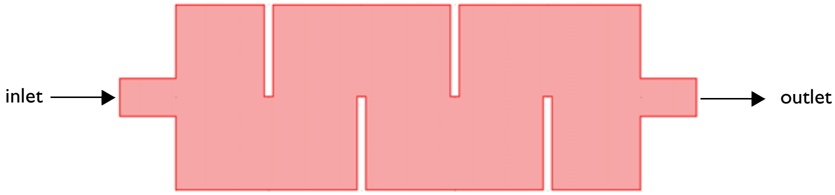


Figure 5-5: Depiction of the reactor geometry.

To describe turbulent flow in the reactor the model uses the k-ε model, for which the momentum transport and continuity equations read

$$\rho\frac{\partial\mathbf{U}}{\partial t}-\nabla\cdot\left[\left(\eta+\rho\frac{C_\mu k^2}{\sigma_k\ \varepsilon}\right)\cdot\left(\nabla\mathbf{U}+(\nabla\mathbf{U})^{\mathrm{T}}\right)\right]+\rho\mathbf{U}\cdot\nabla\mathbf{U}+\nabla P\ =\ 0 \qquad (5\text{-}4)$$

$$\nabla\cdot\mathbf{U}\ =\ 0$$

where ρ denotes the fluid's density (kg/m^3), $\mathbf{U}$ represents the average velocity (m/s), η is the dynamic viscosity (kg/(m·s)), P equals the pressure (Pa), k refers to the turbulence energy (m^2/s^2), ε is the dissipation rate of turbulent kinetic energy (m^2/s^3), and C_μ is a model constant. You find the turbulence energy by solving

$$\rho\frac{\partial k}{\partial t}-\nabla\cdot\left[\left(\eta+\rho\frac{C_\mu k^2}{\sigma_k\ \varepsilon}\right)\nabla k\right]+\rho\mathbf{U}\cdot\nabla k\ =$$

$$\frac{1}{2}\rho C_\mu\frac{k^2}{\varepsilon}\left(\nabla\mathbf{U}+(\nabla\mathbf{U})^{\mathrm{T}}\right)^2-\rho\varepsilon \qquad (5\text{-}5)$$

and the dissipation by solving

$$\rho\frac{\partial\varepsilon}{\partial t}-\nabla\cdot\left[\left(\eta+\rho\frac{C_\mu k^2}{\sigma_\varepsilon\ \varepsilon}\right)\nabla\varepsilon\right]+\rho\mathbf{U}\cdot\nabla\varepsilon\ =$$

$$\frac{1}{2}\rho C_{\varepsilon 1}C_\mu k\left(\nabla\mathbf{U}+(\nabla\mathbf{U})^{\mathrm{T}}\right)^2-\rho C_{\varepsilon 2}\frac{\varepsilon^2}{k} \qquad (5\text{-}6)$$

The model constants in the previous equations are experimentally determined. Set them to the values listed in Table 5-1.

TABLE 5-1: MODEL CONSTANTS

CONSTANT	**VALUE**
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

The inlet has a constant velocity profile in the x direction, u_0, set to 0.1 m/s, while the velocity in the y direction, v, is zero. At the outlet, apply a zero-pressure condition. At all other boundaries, logarithmic wall functions describe the boundary conditions.

Model the tracer concentration with the convection and diffusion equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c + c\mathbf{u}) = 0 \qquad (5\text{-}7)$$

where, c denotes the concentration (kg/m^3), D equals its diffusion coefficient (m^2/s), and $\mathbf{u}$ is the velocity (m/s). The velocity is given by the stationary solution of the k-ε equations, and the diffusivity is given by the turbulent viscosity ν_T given from the k-ε simulation. The assumption to decouple the velocity field and the scalar transport equation is accurate because the concentration of tracer is low and the laminar diffusivity of the tracer in water can be ignored because it is typically 1000 times lower than the turbulent transport (compare with data given in Ref. 1).

To simulate the tracer, use a time-dependent boundary condition at the inlet:

$$c = c_0 e^{-(t-3)^2} \qquad (5\text{-}8)$$

The boundary condition at the outlet is a convective-flux condition stating that all mass transport over the boundary occurs through convection. All other boundaries are insulated.

Results

The stationary velocity field appears in Figure 5-6. Regions of circulation, and therefore of mixing, increase with the number of baffles. As the figure shows, dead zones occur in the corners and in the first baffle chambers. It is also evident from the flow that a stream or "short-circuit" of velocity occurs through the middle of the reactor. The residence time in this short-circuit, compared to velocities in the recirculation areas, gives an indication of the reactor's effectiveness.

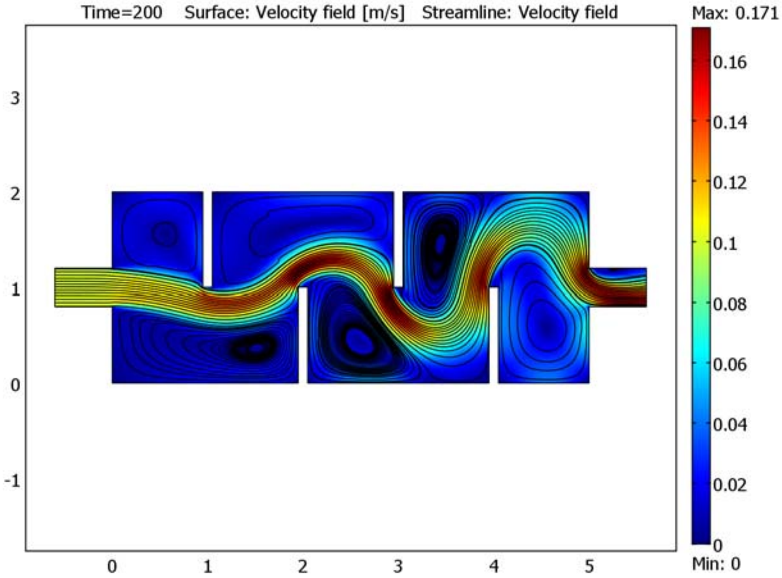


Figure 5-6: Velocity field and flow lines for the baffled reactor.

Turbulent viscosity is an important quantity in this model because it is used to simulate the diffusive properties in the mass transport; Figure 5-7 indicates that relative turbulence increases downstream in the reactor. Whereas Figure 5-6 shows the regions of recirculation, which are good for mixing, Figure 5-7 shows the chaotic behavior of the velocity vector on a smaller scale. Both figures illustrate that the mixing is far better in the last baffle chambers than in the first one.

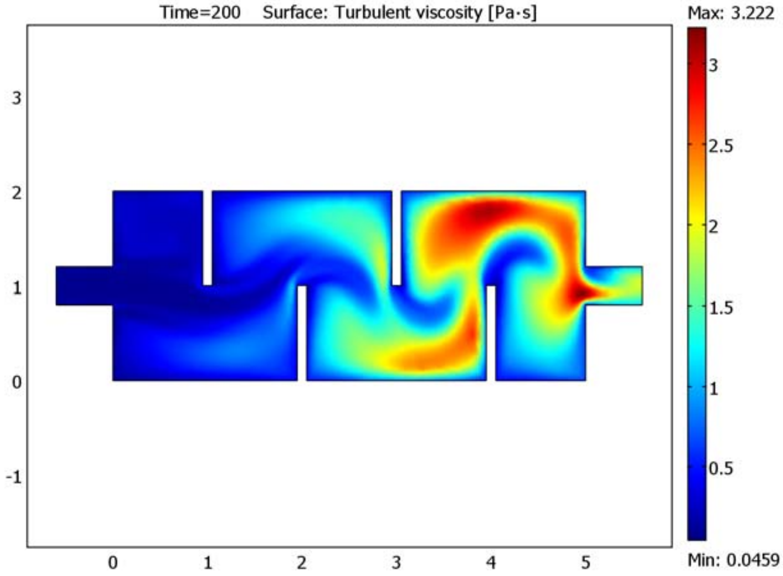


Figure 5-7: Turbulent viscosity.

Figure 5-8 combines snapshots of the concentration field. The figures clearly show that the tracer is kept small in the first third of the reactor. When it enters the second third it dilutes somewhat. In the last section of the reactor, the tracer is strongly diluted due to the large turbulent viscosity in that section. Regions behind the baffles, even in the first chambers, also show a growing amount of tracer species and the mixing effect that recirculation zones have on the reactor.

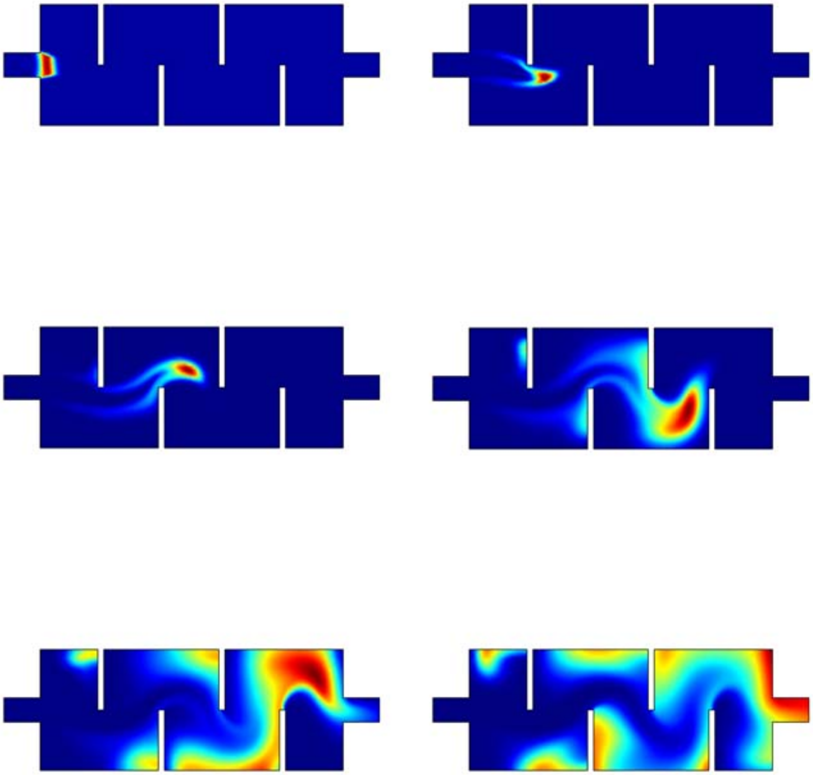


Figure 5-8: Concentration snapshots at t = 10, 20, 30, 45, 65, and 90 s.

By monitoring the integral of the concentration at the outlet you can determine the reactor's residence time. Figure 5-9 shows the integral of the concentration over the outlet. The figure shows that the residence time is roughly 100 s.

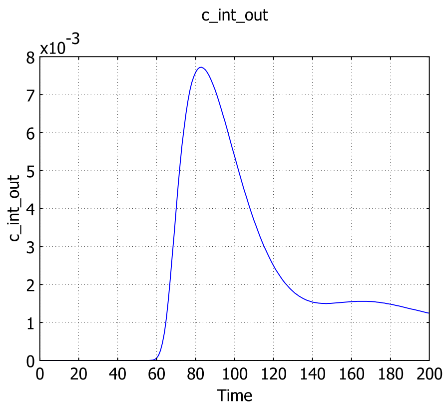


Figure 5-9: Integrated concentration at the outlet.

COMPARISON WITH A 3D REACTOR

A similar reactor modeled in 3D appears in Figure 5-10. The height dimensions are the same as in the 2D reactor, and it includes a depth. Notice that the inlet and outlet are not drawn throughout the entire depth of the model, which leads to the conclusion that dead zones occur toward the front and the back of the reactor.

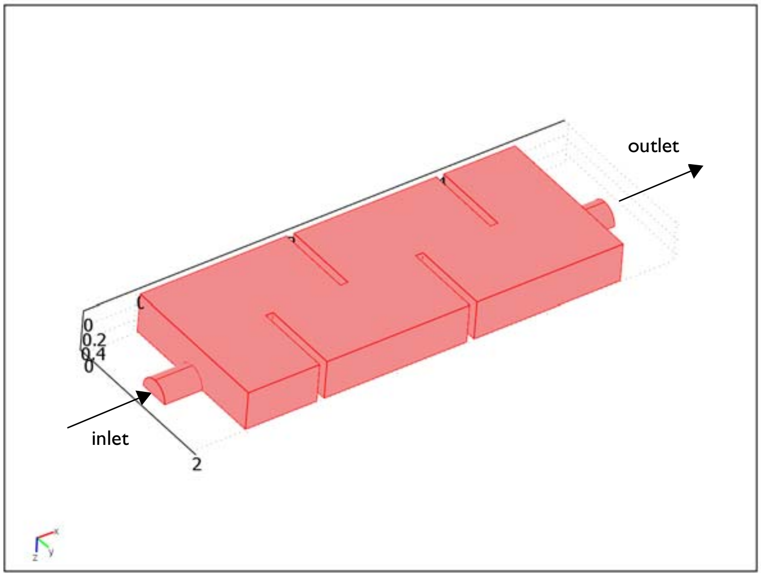


Figure 5-10: 3D reactor geometry.

The velocity field is shown in Figure 5-11:

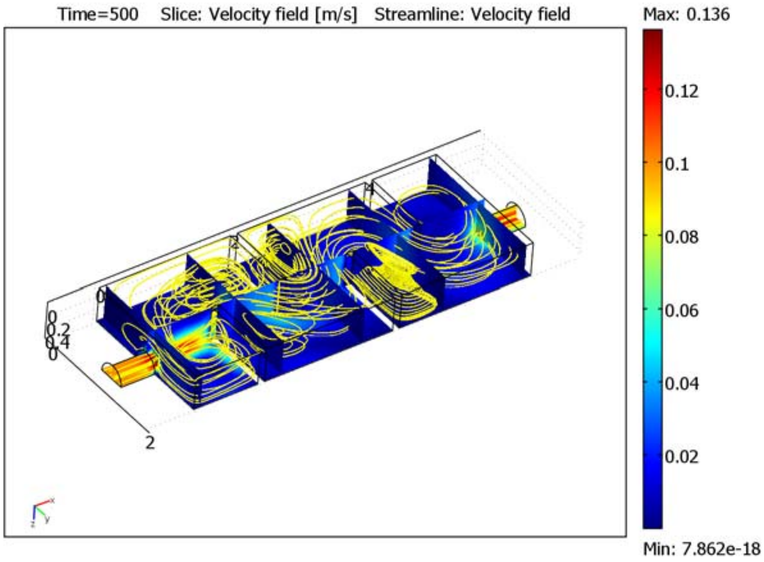


Figure 5-11: Velocity field and streamlines in the 3D reactor.

This case uses identical conditions in the 3D reactor as in the 2D example just described. Figure 5-12 shows the resulting integral of the outlet concentration as a function of time, and it shows that the residence time is greater than in the 2D approximation.

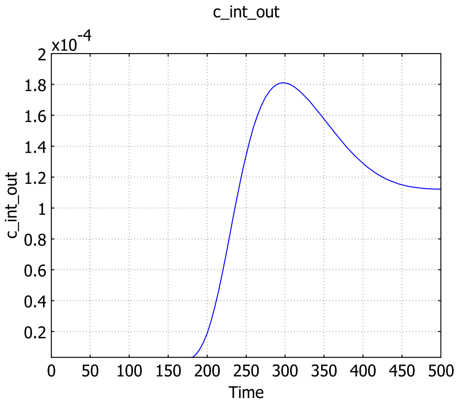


Figure 5-12: Concentration at the outlet.

Reference

1. J. M. Coulson, J. F. Richardson, J. R. Backhurst and J. H. Harker, *Chemical Engineering*, Vol. 1, Fourth ed., Pergamon Press, 1990.

Model Library path: `Chemical_Engineering_Module/Mixers_and_Stirred_Vessels/turbulent_residence_time_2d`

Model Library path: `Chemical_Engineering_Module/Mixers_and_Stirred_Vessels/turbulent_residence_time_3d`

Modeling Using the Graphical User Interface—2D Turbulent Reactor

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator** set the **Space dimension** to **2D**.
3. In the Application Modes tree select **Chemical Engineering Module>Momentum Transport>Turbulent Flow>k-ε Turbulence Model**.
4. Click first the **Multiphysics** button and then the **Add** button to add the selected application mode.
5. Select the application mode **Chemical Engineering Module>Mass Transport>Convection and Diffusion>Transient analysis**, then click **Add**.
6. Click **OK**.

GEOMETRY MODELING

1. Hold the Shift key and click the **Rectangle/Square** button on the Draw toolbar.
2. Enter rectangle properties from this table:

PROPERTY	VALUE
Width	5
Height	2

3 Click **OK**.

4 Click the **Zoom Extents** button on the Main toolbar.

5 Using the procedure just described, draw two more rectangles with these settings:

PROPERTY	R2	R3
Width	`0.6`	`0.1`
Height	`0.4`	1
x-position	`-0.6`	`0.95`
y-position	`0.8`	1

6 Select rectangle R2, then click the **Array** button on the Draw toolbar.

7 Set the **x-displacement** to `5.6` and the **x-Array size** to `2`. Click **OK**.

8 Select rectangle R3, then click the **Array** button.

9 Enter the following array properties, then click **OK**:

PROPERTY	VALUE
x-displacement	1
y-displacement	0
x-Array size	4
y-Array size	1

10 Select the two rectangles R5 and R7 by pressing the Ctrl key and clicking the objects.

11 Click the **Move** button and move the two objects `-1` in the *y* direction, then click **OK**.

12 Select R1, R2, and R4 by pressing the Ctrl key and clicking the objects

13 Click the **Union** button on the Draw toolbar.

14 Select all the geometry objects by pressing Ctrl+A.

15 Click the **Difference** button on the Draw toolbar.

16 Finally, click the **Delete Interior Boundaries** button on the Draw toolbar and the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1000[kg/m^3]`	`Density`
`eta`	`1e-3[Pa*s]`	`Viscosity`
`u_in`	`0.1[m/s]`	`Inlet velocity`
`c0`	`1[mol/m^3]`	`Inlet peak concentration`

3 From the **Options** menu, select **Expressions>Scalar Expressions**.

4 Define the following expression (the description is optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`c_in`	`c0*exp(-(t[1/s]-3)^2)`	`Inlet concentration`

5 From the **Options** menu, select **Integration Coupling Variables>Boundary Variables**.

6 Select Boundary 1.

7 Type `c_int_in` in the first cell of the **Name** column and `c` in the **Expression** column.

8 Select Boundary 28.

9 Type `c_int_out` in the second cell of the **Name** column and `c` in the **Expression** column.

10 Click **OK**.

PHYSICS SETTINGS—k-ε TURBULENCE MODEL

From the **Multiphysics** menu, select **1 k-ε Turbulence model (chns)**.

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1 from the list.

3 Set the **density** to `rho` and the **Dynamic viscosity** to `eta`.

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the following boundary settings (the logarithmic wall function condition is the default and you thus need not set it explicitly); when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 28	ALL OTHERS
Boundary type	Inlet	Outlet	Wall
Boundary condition	Velocity	Pressure, no viscous stress	Logarithmic wall function
u_0	`u_in`	-	-
v_0	0	-	-
L_T	`0.07*0.4`	-	-
p_0	-	0	-

The value of L_T is taken from Table 5-2 in the *Chemical Engineering Module User's Guide*.

PHYSICS SETTINGS—CONVECTION AND DIFFUSION

From the **Multiphysics** menu, select **2 Convection and diffusion (chcd)**.

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1.

3 Enter the following settings; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	`etaT_chns/rho`
R	0
u	u
v	v

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the following boundary conditions (the insulation condition is the default); when done, click **OK**.

SETTING	BOUNDARY 1	BOUNDARY 28	ALL OTHERS
Boundary condition	Concentration	Convective flux	Insulation/ Symmetry
c_0	`c_in`	-	-

MESH GENERATION

To create a mesh that resolves the overall velocity field and the complex flow structure at the convex corners, specify a global maximum element size as well as a local element size for the mesh close to the convex corners:

1. From the **Mesh** menu, select **Free Mesh Parameters**.
2. On the **Global** page, click the **Custom mesh size** button, then set the **Maximum element size** to `0.2`.
3. Click the **Point** tab.
4. In the **Point selection** list, select Points 4, 5, 7, 9, 12, 14, 15, 17, 20, 22, 24, and 25 by pressing the Ctrl key and clicking these entries.
5. Set the **Maximum element size** to `0.05`.
6. Click **Remesh**.
7. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Start by computing the flow field.

1. Click the **Solver Parameters** button on the Main toolbar.
2. Delete segregated group 3 by clicking the **Delete** button for **Group 3**.
3. Click **OK**.
4. Click the **Solver Manager** button on the Main toolbar.
5. On the **Solve For** page, select **k-ε Turbulence Model** from the list.
6. Click the **Solve** button to compute the velocity field.

   Now store the stationary velocity field and compute the transient mass transport problem.
7. On the **Solve For** page, select **Convection and Diffusion** from the list.
8. On the **Initial Value** page in the **Solver Manager** dialog box, click the **Store Solution** button.
9. Set the **Initial value** and **Values of variables not solved for and linearization point** to **Stored solution**.
10. Click **OK**.
11. Click the **Solver Parameters** button on the Main toolbar.
12. From the **Analysis** list, select **Transient**.

13 In the **Time stepping** frame set **Times** to `0:1:200`, the **Relative tolerance** to `0.0001` and the **Absolute tolerance** to `0.00001`.

14 Click **OK**.

15 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 5-6, perform the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Surface** and **Streamline** check boxes in the **Plot type** area.

3 Click the **Surface** tab. From the **Predefined quantities** list on the **Surface Data** page, select **k-ε Turbulence Model (chns)>Velocity field**.

4 Click the **Streamline** tab. From the **Predefined quantities** list on the **Streamline Data** page, select **k-ε Turbulence Model (chns)>Velocity field**.

5 From the **Streamline plot type** list, select **Magnitude controlled**.

6 On the **Line Color** page, click the **Uniform color** option button.

7 Click the **Color** button. Select black, then click **OK**.

8 Click **Apply** to generate the plot.

Proceed to generate Figure 5-7 with the following steps:

9 On the **General** page, clear the **Streamline** check box.

10 On the **Surface** page, select **k-ε Turbulence Model (chns)>Turbulent viscosity** as the **Surface Data**.

11 Click **Apply**.

To generate the plots in Figure 5-8, perform the following steps:

12 On the **Surface** page, set the **Surface Data** to **Convection and Diffusion (chcd)>Concentration, c**.

13 Clear the **Color scale** check box in the **Surface color** area.

14 On the **General** page, select **10** from the **Solution at time** list, then click **Apply**.

15 Repeat the previous step for the times **20**, **30**, **45**, **65**, and **90**.

16 When finished, click **Cancel** to close the **Plot Parameters** dialog box.

To generate the plot in Figure 5-9, perform the following steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2. On the **General** page, click the **Point plot** button.
3. Select all the time steps in the **Solutions to use** list by pressing Ctrl+A.
4. On the **Point** page, select point **28** and type `c_int_out` in the **Expression** edit field in the **y-axis data** area.
5. Click **OK**.

Modeling Using the Graphical User Interface—3D Turbulent Reactor

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, set the **Space dimension** to **3D**.
3. In the Application Modes tree select **Chemical Engineering Module>Momentum Transport>Turbulent Flow>k-ε Turbulence Model**.
4. Click first the **Multiphysics** button and then the **Add** button to add the selected application mode.
5. Select the application mode **Chemical Engineering Module>Mass Transport>Convection and Diffusion>Transient analysis**, then click **Add**.
6. Click **OK**.

GEOMETRY MODELING

1. Select the menu item **File>Import>CAD Data From File**.
2. Browse to the folder `Models>Chemical_Engineering_Module>Mixers_and_Stirred_Vessels`.
3. Select the file `turbulent_residence_time_3d.mphbin`.
4. Click **Import**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Constants**.
2. Define the following constants (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
rho	1000[kg/m^3]	Density
eta	1e-3[Pa*s]	Viscosity

NAME	EXPRESSION	DESCRIPTION
`u_in`	`0.1[m/s]`	`Inlet velocity`
`c0`	`1[mol/m^3]`	`Inlet peak concentration`

3. Click **OK**.
4. Select the menu item **Options>Expressions>Scalar Expressions** and type in the following entry:

NAME	EXPRESSION	DESCRIPTION
`c_in`	`c0*exp(-(t[1/s]-3)^2)`	`Inlet concentration`

5. Click **OK**.
6. Select the menu item **Options>Integration Coupling Variables>Boundary Variables**.
7. From the **Boundary selection** list, select **1**.
8. In the first row of the table, type `c_int_in` in the **Name** column and `c` in the **Expression** column.
9. From the **Boundary selection** list, select **28**.
10. In the second row of the table, type `c_int_out` in the **Name** column and `c` in the **Expression** column.
11. Click **OK**.

PHYSICS SETTINGS—CONVECTION AND DIFFUSION

From the **Multiphysics** menu select **2 Convection and Diffusion (chcd)**.

Subdomain Settings

1. From the **Physics** menu, select **Subdomain Settings**.
2. Select Subdomain 1.
3. Type the following settings into the appropriate edit fields:

PROPERTY	VALUE
D (isotropic)	`etaT_chns/rho`
R	`0`
u	`u`
v	`v`
w	`w`

4. Click **OK**.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.
2 Enter the following boundary settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 28	ALL OTHERS
Boundary condition	Concentration	Convective flux	Insulation/ Symmetry
c_0	`c_in`	-	-

PHYSICS SETTINGS—k-ε TURBULENCE MODEL

From the **Multiphysics** menu, select **1 k-ε Turbulence model (chns)**.

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.
2 Select Subdomain 1.
3 Set the **Density** to `rho` and the **Dynamic viscosity** to `eta`.
4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.
2 Enter the following boundary settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 28	BOUNDARY 3	ALL OTHERS
Boundary type	Inlet	Outlet	Symmetry boundary	Wall
Boundary condition	Velocity	Pressure, no viscous stress		Logarithmic wall function
U_0	`u_in`	-	-	-
L_T	`0.07*0.4`	-	-	-
p_0	-	0	-	-

The value of L_T is taken from Table 5-2 in the *Chemical Engineering Module User's Guide*.

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.
2 On the **Global** page, click the **Custom mesh size** button.
3 Set the **Maximum element size** to `0.2`.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Start by computing the flow field.

1. Click the **Solver Parameters** button on the Main toolbar.
2. Delete segregated group 3 by clicking the **Delete** button for **Group 3**.
3. Click the **Solver Manager** button on the Main toolbar.
4. On the **Solve For** page, select **k-ε Turbulence Model** from the list.
5. Click the **Solve** button to compute the velocity field.

   Now store the stationary velocity field and compute the transient mass transport problem.
6. On the **Solve For** page, select **Convection and Diffusion** from the list.
7. On the **Initial Value** page in the **Solver Manager** dialog box, click the **Store Solution** button.
8. Set the **Initial value** and **Values of variables not solved for and linearization point** to **Stored solution**.
9. Click **OK**.
10. Click the **Solver Parameters** button on the Main toolbar.
11. From the **Analysis** list, select **Transient**.
12. From the **Linear system solver** list, select **Direct (PARDISO)**
13. In the **Time stepping** frame set **Times** to `0:1:500`, the **Relative tolerance** to `0.0001` and the **Absolute tolerance** to `0.00001`.
14. Click **OK**.
15. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create Figure 5-11, perform the following steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, use check boxes to select the plot type **Streamline**.
3. Go to the **Slice** page and type `1` in the **y-levels** edit field.
4. For the **z-levels**, select the **Vector with coordinates** option button, and type `0.49` in the edit field.
5. Go to the **Streamline** page, then click the **Line Color** tab.

6 Select the **Uniform color** option button.

7 Click the **Color** button, select yellow, and click **OK**.

8 Select **Tube** from the **Line type** list.

9 Click the **Tube radius** button, clear the **Auto** check box and type `0.3` in the **Radius scale factor** edit field. Click **OK**.

10 Click the **Advanced** button.

11 In the **Maximum number of integration steps** edit field, type `1000`. Click **OK**.

12 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

13 Click the **Scene Light** button on the Camera toolbar.

To create Figure 5-12, perform the following steps:

1 From the **Postprocessing** menu, open the **Domain Plot Parameters** window.

2 On the **General** page, press Ctrl+A to select all the time steps in the **Solutions to use** list.

3 On the **Point** page, select Point 52 and enter `c_int_out` in the **y-axis data** edit field.

4 Click **OK**.

Note: We recommend a specific set of solver parameters when applying the k-ε Turbulence Model application mode to 3D geometries. These solver parameters are provided as default if you start your modeling by first specifying the k-ε Turbulence Model application mode in the Model Navigator and then move on to draw your 3D geometry. If you do the opposite, that is, first draw your geometry and then add the k-ε Turbulence Model application mode by selecting the menu item **Multiphysics>Model Navigator**, you end up with a default set of solver parameters less suitable for the model.

Swirl Flow Around a Rotating Disk

Introduction

This example models a rotating disk in a tank. The model geometry is shown in Figure 5-13. Because the geometry is rotationally symmetric, it is possible to model it as a 2D cross section. However, the velocities in the angular direction differ from zero, so the model must include all three velocity components, even though the geometry is in 2D.

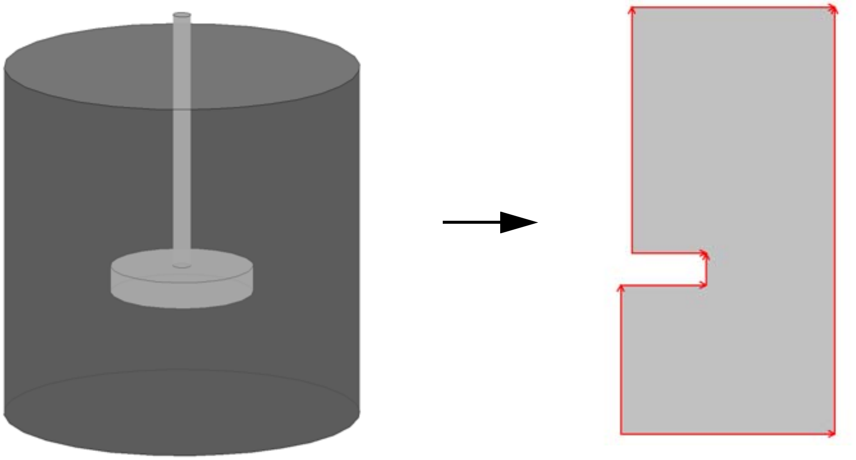


Figure 5-13: The original 3D geometry can be reduced to 2D because the geometry is rotationally symmetric.

Model Definition

DOMAIN EQUATIONS

The flow is described by the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{F} \qquad (5\text{-}9)$$

$$\nabla\cdot\mathbf{u} = 0$$

In these equations, $\mathbf{u}$ denotes the velocity (m/s), ρ the density (kg/m^3), η the dynamic viscosity (Pa·s), and p the pressure (Pa). For a stationary, axisymmetric flow the equations reduce to (Ref. 1):

$$\begin{aligned}
\rho\left(u\frac{\partial u}{\partial r} - \frac{v^2}{r} + w\frac{\partial u}{\partial z}\right) + \frac{\partial p}{\partial r} &= \eta\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2}\right] + F_r \\
\rho\left(u\frac{\partial v}{\partial r} + \frac{uv}{r} + w\frac{\partial v}{\partial z}\right) &= \eta\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v}{\partial r}\right) - \frac{v}{r^2} + \frac{\partial^2 v}{\partial z^2}\right] + F_\varphi \\
\rho\left(u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial z}\right) + \frac{\partial p}{\partial z} &= \eta\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial w}{\partial r}\right) + \frac{\partial^2 w}{\partial z^2}\right] + F_z
\end{aligned} \tag{5-10}$$

Here u is the radial velocity, v the rotational velocity, and w the axial velocity (m/s). In the model you set the volumetric force components F_r, F_φ, and F_z to zero. The swirling flow is 2D even though the model includes all three velocity components.

BOUNDARY CONDITIONS

Figure 5-14 below shows the boundary conditions.

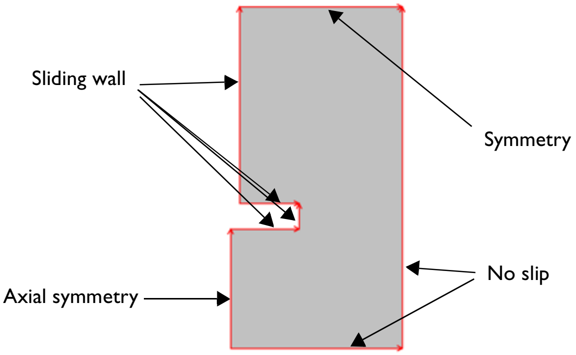


Figure 5-14: Boundary conditions.

On the stirrer, use the Sliding wall boundary condition to specify the velocities. The velocity components in the plane are zero, and that in the angular direction is equal to the angular velocity, ω, times the radius, r:

$$w_{\mathrm{w}} = r\omega \tag{5-11}$$

At the boundaries representing the cylinder surface a No slip condition applies, stating that all velocity components equal zero:

$$\mathbf{u} = (0, 0, 0) \tag{5-12}$$

At the boundary corresponding to the rotation axis, use the Axial symmetry boundary condition allowing flow in the tangential direction of the boundary but not in the normal direction. This is obtained by setting the radial velocity to zero:

$$u = 0 \tag{5-13}$$

On the top boundary, which is a free surface, use the Symmetry condition to allow for flow in the axial and rotational directions only. The boundary condition is mathematically similar to the axial symmetry condition.

POINT SETTINGS

Because there is no outflow boundary in this model, where the pressure would be specified, you need to lock the pressure to some reference pressure in a point. In this model, set the pressure to zero in the top right corner.

Results

The parametric solver provides the solution for four different angular velocities. Figure 5-15 shows the results for the smallest angular velocity, $\omega = 0.25\pi$ rad/s.

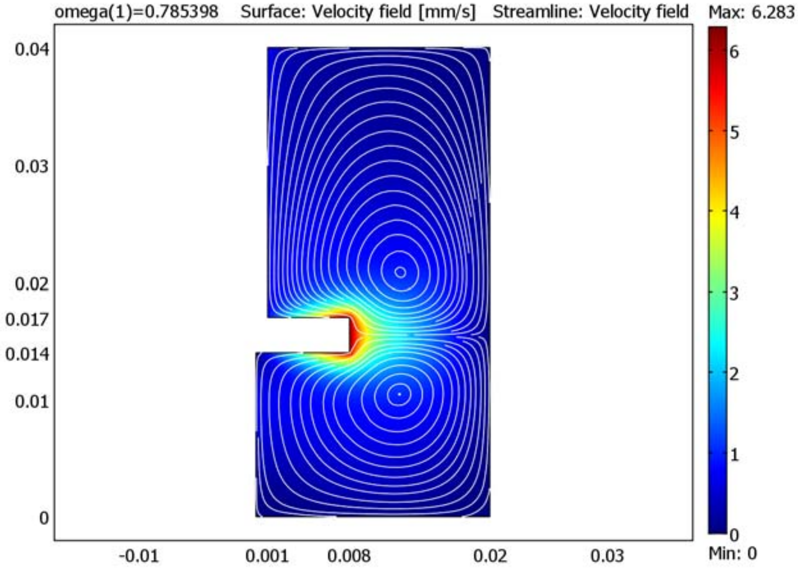


Figure 5-15: Results for angular velocity $\omega = 0.25\pi$ *rad/s. The surface plot shows the magnitude of the velocity field and the white lines are streamlines of the velocity field.*

The shape of the two recirculation zones, which are visualized with streamlines, changes as the angular velocity increases. Figure 5-16 shows the streamlines of the velocity field for higher angular velocities.

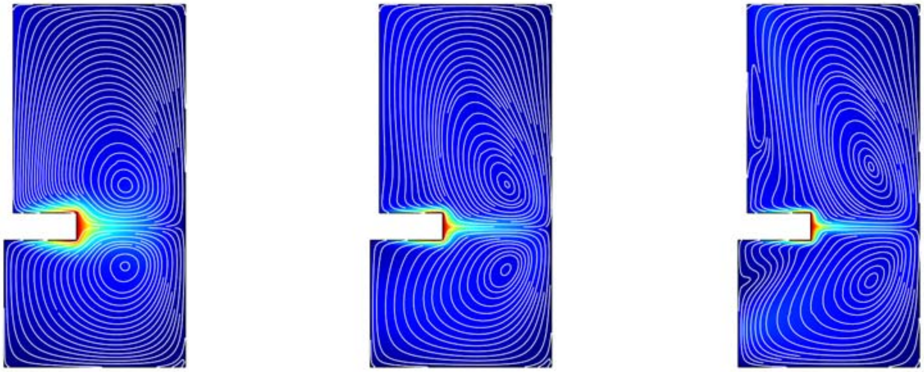


Figure 5-16: Results for angular velocities $\omega = 0.5\pi$, 2π, *and* 4π *rad/s. The surface plot shows the magnitude of the velocity and the white lines are streamlines of the velocity field.*

Figures 5-17 and 5-18 show isocontours of the rotational velocity component together with surface plots of the velocity magnitude for different angular velocities.

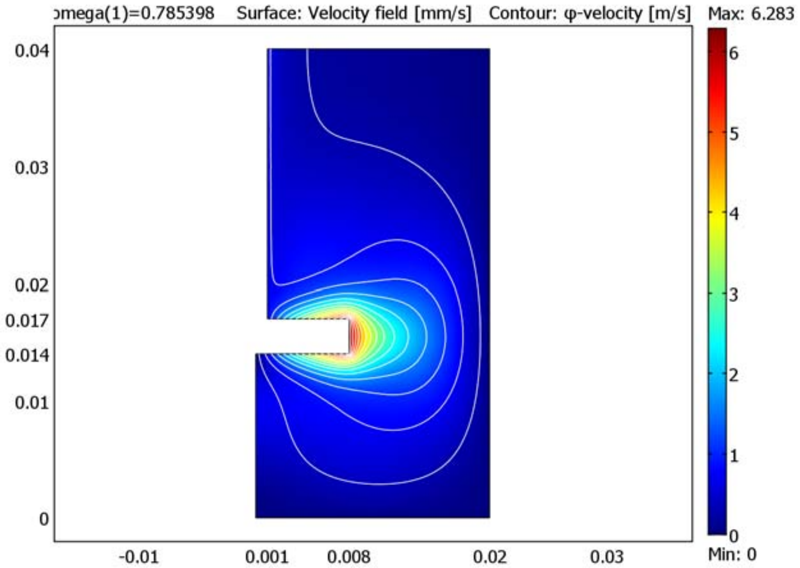


Figure 5-17: Isocontours for the azimuthal velocity component for angular velocity ω = *0.25*π *rad/s. The surface plot shows the magnitude of the velocity.*

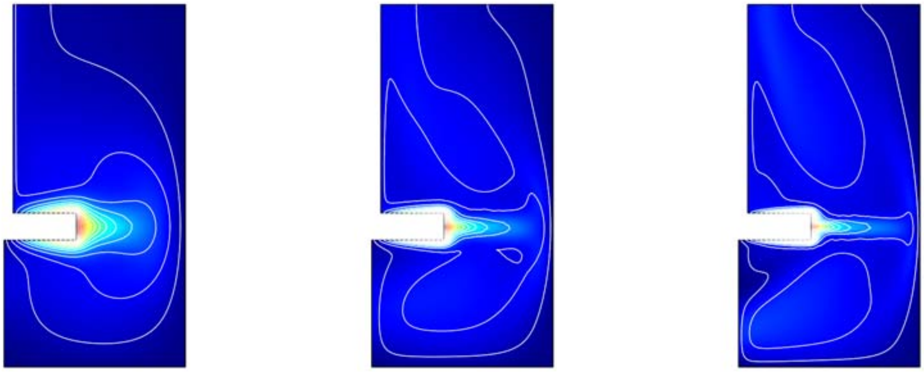


Figure 5-18: Magnitude of the velocity field (surface) and isocontours for the azimuthal velocity component for angular velocities (left to right) ω = *0.5*π*, 2*π*, and 4*π *rad/s.*

In a final modification of the model, set the angular velocity to $\omega = 500\pi$ rad/s, inducing turbulent flow in the mixer volume. Figure 5-19 shows the turbulent viscosity and flow fields under these conditions.

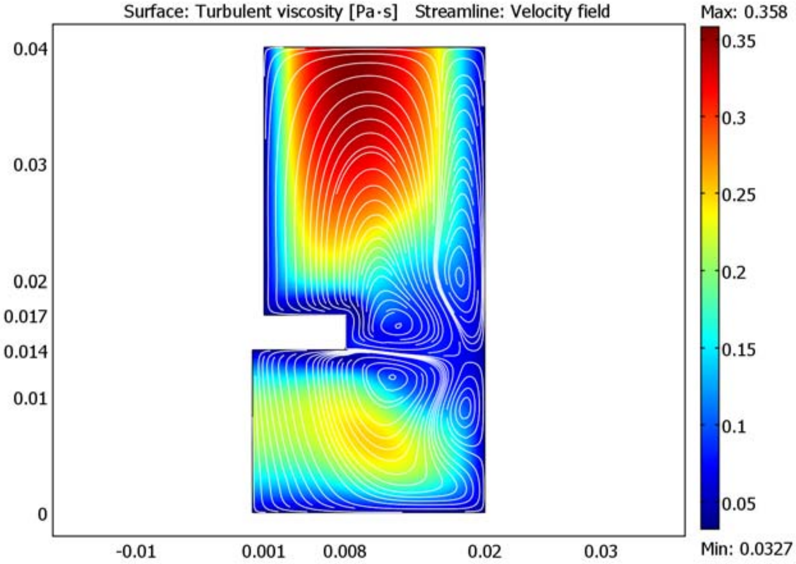


Figure 5-19: Results for angular velocity $\omega = 500\pi$ *rad/s. The surface plot shows the turbulent viscosity and the white lines are streamlines of the velocity field.*

Reference

1. P.M. Gresho and R.L. Sani, *Incompressible Flow and the Finite Element Method*, vol. 2, p. 469, John Wiley and Sons Ltd, 1998.

Model Library path: `Chemical_Engineering_Module/Mixers_and_Stirred_Vessels/rotating_disk`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list.

3 Select **Chemical Engineering Module>Momentum Transport>Laminar Flow >Swirl Flow**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

2 On the **Axis** page, set **r-z limits** according to the following table:

r min	`-0.005`
r max	`0.025`
z min	`-0.005`
z max	`0.045`

3 On the **Grid** page, clear the **Auto** check box.

4 Enter **r-z grid** settings according to the following table:

r spacing	`0.01`
Extra r	`0.001 0.008`
z spacing	`0.01`
Extra z	`0.014 0.017`

5 Click **OK**.

6 From the **Options** menu, open the **Constants** dialog box.

7 Enter constants according to the table below (the descriptions are optional).

NAME	EXPRESSION	DESCRIPTION
`rho`	`1000[kg/m^3]`	`Density`
`eta`	`1e-3[Pa*s]`	`Viscosity`

8 Click **OK**.

GEOMETRY MODELING

Use the line tool to create the geometry.

1. Click the **Line** button in the **Draw** toolbar.
2. Click the following sequence of points. (0, 0), (0.02, 0), (0.02, 0.04), (0.001, 0.04), (0.001, 0.017), (0.008, 0.017), (0.008, 0.014), and (0, 0.014).
3. Close the geometry by right-clicking anywhere in the geometry.
4. Click the **Zoom Extents** button on the Main toolbar.

SUBDOMAIN SETTINGS

From the **Physics** menu, open the **Subdomain Settings** dialog box. Select Subdomain 1, then enter the fluid properties given by the table below. When finished, click **OK**.

QUANTITY	VALUE/EXPRESSION
ρ	`rho`
η	`eta`

BOUNDARY CONDITIONS

From the **Physics** menu, open the **Boundary Settings** dialog box. Enter the boundary conditions in the table below (the default condition is Wall/No slip). When finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 8	BOUNDARIES 3–5, 7	BOUNDARY 6
Boundary type	Symmetry boundary	Wall	Wall	Symmetry boundary
Boundary condition	Axial symmetry	No slip	Sliding wall	Symmetry
U_w			`0`	
w_w			`omega*r`	

POINT SETTINGS

1. From the **Physics** menu, open the **Point Settings** dialog box.
2. From the **Point selection** list, select Point 8.
3. Select the **Point constraint** check box.
4. Click **OK**.

MESH GENERATION

1. From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 Click the **Custom mesh size** button.

3 Set the **Maximum element size** to `2e-3`.

4 Click the **Boundary** tab, then select all entries in the **Boundary selection** list by clicking in the list and then pressing Ctrl+A.

5 Set the **Maximum element size** to `5e-4`.

6 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Solver** list, select **Parametric**.

3 In the **Parameter name** edit field, type `omega`.

4 In the **Parameter values** edit field, type `0.25*pi 0.5*pi 2*pi 4*pi`.

5 Click **OK**.

6 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create Figure 5-15 do the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Surface**, **Streamline**, and **Geometry edges** check boxes to enable those plot types.

3 From the **Parameter value** list in the **Solution to use** area, select **0.785398** (which is approximately equal to 0.25π).

4 On the **Surface** page, verify that **Swirl Flow (chns)>Velocity field** is selected from the **Predefined quantities** list on the **Surface Data** page. From the **Unit** list, select **mm/s**.

5 On the **Streamline** page, select **Uniform density** from the **Streamline plot type** list.

6 In the **Separating distance** edit field, type `0.02`.

7 Click the **Line Color** tab.

8 Click the **Uniform color** button, then click the **Color** button.

9 Select the white swatch, then click **OK**.

10 Click the **Contour** tab.

11 In the **Number of levels** edit field, type `15`.

12 Click **Apply** in the **Plot Parameters** dialog box to generate the plot.

13 To generate the plots in Figure 5-16, return to the **General** page and select, in turn, the solutions for the parameter values 0.5π, 2π, and 4π from the **Parameter value** list, clicking **Apply** in between.

To generate the plot in Figure 5-17, proceed as follows:

14 In the **Plot type** area, select the **Surface**, **Contour**, and **Geometry edges** check boxes and clear all other **Plot type** check boxes.

15 From the **Parameter value** list, select **0.785398**.

16 Click the **Contour** tab.

17 From the **Predefined quantities** list, select **Swirl Flow (chns)>φ -velocity**.

18 In the **Contour color** area, click first the **Uniform color** button and then the **Color** button.

19 Select the white swatch, then click **OK**.

20 Click **Apply** in the **Plot Parameters** dialog box.

21 Return to the **General** page.

22 Select, in turn the solutions for the parameter values 0.5π, 2π, and 4π from the **Parameter value** list, clicking **Apply** in between to generate the corresponding plots in Figure 5-18.

23 When done, click **Cancel** or **OK** to close the dialog box.

Now, modify the model to simulate turbulent swirl flow.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Constants** dialog box.

2 Add the following constant to the list.

NAME	EXPRESSION	DESCRIPTION
`omega`	`500*pi[rad/s]`	`Angular velocity`

3 Click **OK**.

PHYSICS SETTINGS

1 From the **Physics** menu, select **Properties**.

2 Select **k-ε** from the **Turbulence model** list, then click **OK**.

BOUNDARY CONDITIONS

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Enter the boundary conditions given in the table below. For the boundaries that are not listed, the conditions you specified for the laminar case still apply.

SETTINGS	BOUNDARIES 2, 8	BOUNDARIES 3–5, 7
Type	Wall	Wall
Condition	Logarithmic wall function	Sliding wall
U_w		0
w_w		`omega*r`
δ_w^+	100	100

You can ignore the unexpected base unit warning for $\mathbf{w_w}$. It appears because the constant `omega` is the current solver parameter.

3 Click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Solver** list, select **Stationary segregated**.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 5-19 execute the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Surface**, **Streamline**, and **Geometry edges** check boxes and clear all other **Plot type** check boxes.

3 Click the **Streamline** tab.

4 From the **Predefined quantities** list, select **Swirl Flow (chns)>Velocity field**.

5 Click the **Surface** tab.

6 From the **Predefined quantities** list, select **Swirl Flow (chns)>Turbulent viscosity**.

7 Click **OK** to generate the plot and close the dialog box.

Modeling of Rotating Parts

Introduction

This exercise exemplifies the use of the rotating machinery feature in the Chemical Engineering Module. The Rotating Machinery predefined multiphysics coupling allows you to model moving rotating parts in, for example, stirred tanks, mixers, and pumps.

This combination of application modes formulates the Navier-Stokes equations in a rotating coordinate system. Parts that are not rotated are expressed in the fixed coordinate system. The predefined coupling then takes care of the necessary administration to join the parts of the model that use a rotating coordinate system with the parts that are fixed.

You can use the rotating machinery predefined multiphysics coupling in cases where it is possible to divide the modeled device into rotationally invariant geometries. The desired operation can be, for example, to rotate an impeller in a baffled tank. This is exemplified in Figure 5-20, where the impeller rotates from position 1 to 2. The first step is to divide the geometry into two parts that are both rotationally invariant, as shown in Step 1a. The second step is to specify the parts to model using a rotating frame and the ones to model using a fixed frame (Step 1b). The predefined coupling then automatically does the coordinate transformation and the joining of the fixed and moving parts (Step 2a).

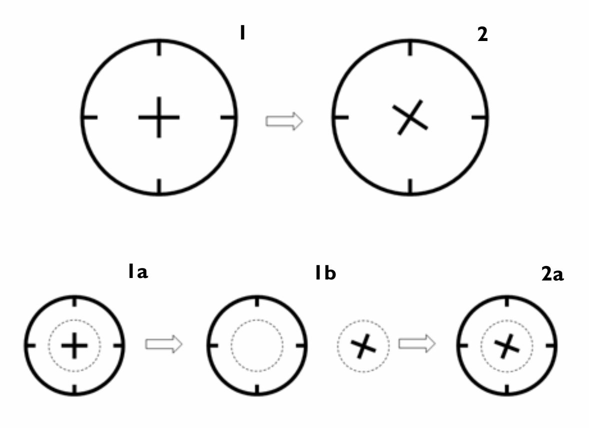


Figure 5-20: The modeling procedure in the rotating machinery application mode in the Chemical Engineering Module.

Model Definition

The model you treat in this example is that of a pump. Despite the model being somewhat schematic, the example contains all the components needed to describe more realistic geometries. Figure 5-21 shows the modeled geometry. The impeller rotates clockwise at a speed of 10 RPM.

The model equations are the Navier-Stokes equations formulated in a rotating frame in the inner subdomain and in fixed coordinates in the outer one.

At the pump's fixed wall no-slip boundary conditions apply. The boundary conditions for the impeller blades are no-slip clockwise rotation conditions. At the pump inlet and outlet, you set the normal stress to zero.

The implementation, using the Rotating Navier-Stokes predefined multiphysics coupling, is quite straightforward. First you draw the geometry using two separate subdomains for the fixed and rotating parts. Then you activate the assembly feature, which makes it possible to treat the two subdomains as separate parts in an assembly. You then specify which part uses a rotating frame. Once you have done this, you can proceed to the usual steps of setting the fluid properties and the boundary conditions, and finally to meshing and solving the problem.

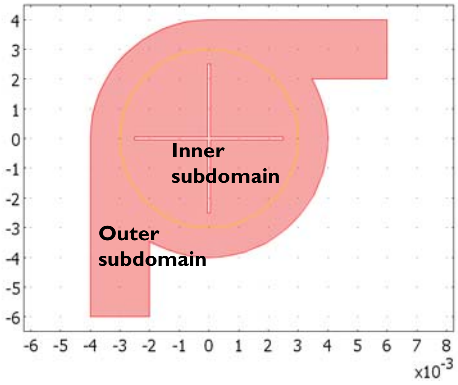


Figure 5-21: Geometry of the schematic pump. The inner subdomain is described in a rotating frame and the outer one in a fixed frame.

Results

Figure 5-22 below shows the flow field as the modulus of the velocity vector and as equidistant streamlines.

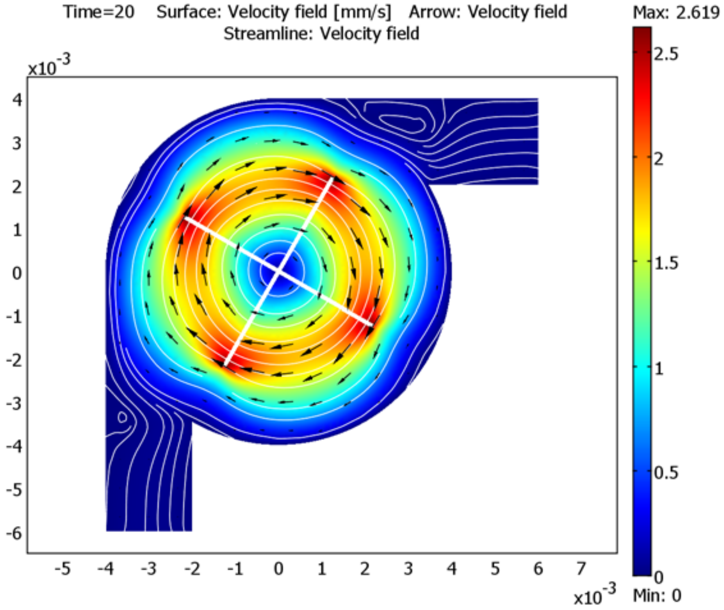


Figure 5-22: The flow field after 20 seconds. The plot shows that two small eddies are formed when the blades enters the inlet and outlet sections.

In Figure 5-22, you can clearly see that two eddies are created as the blades of the pump pass inlet and outlet sections. These eddies reduce the efficiency of the pump. In addition, the streamlines show that a large part of the fluid rotates around the blade without leaving the pump.

By decreasing the cross section of the recirculation area in the pump, it is possible to increase the performance of the pump as a function of the rotating speed of the blades. Figure 5-23 shows the velocity field for such a pump geometry. The net flow through the pump compared to the case shown in Figure 5-22 is increased by almost a factor of 5 without increasing the rotational speed of the pump.

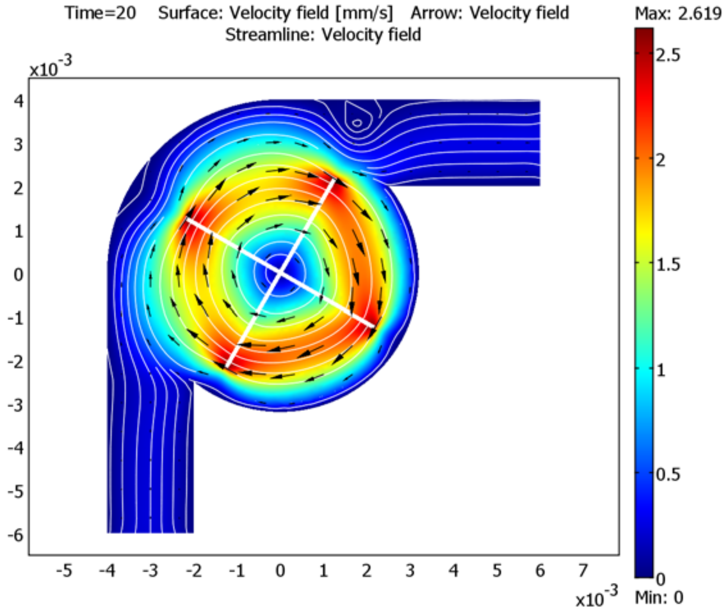


Figure 5-23: Velocity field for an improved geometry, where parts of the recirculation section has been removed.

Model Library path: `Chemical_Engineering_Module/`
`Mixers_and_Stirred_Vessels/schematic_pump_1`

Model Library path: `Chemical_Engineering_Module/`
`Mixers_and_Stirred_Vessels/schematic_pump_2`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **2D** from the **Space dimension** list.

3 From the list of application modes, select **Chemical Engineering Module>Rotating Machinery>Rotating Navier-Stokes**.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Enter the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1e3[kg/m^3]	Density
eta	1e-2[Pa*s]	Viscosity
rpm	10[1/min]	Rotation speed

Note that in this example you specify the rotation speed in revolutions per minute.

GEOMETRY MODELING

1 Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar. Draw a circle of radius `4e-3` centered at the point (`0`, `0`).

2 Click the **Zoom Extents** button in the Main toolbar.

3 Shift-click the **Rectangle/Square** button on the Draw toolbar. Specify a rectangle with the following settings; when finished, click **OK**.

OBJECT	WIDTH	HEIGHT	BASE X	BASE Y
R1	2e-3	6e-3	-4e-3	-6e-3

4 Press Ctrl+A to select both objects.

5 Click the **Create Composite Object** button on the Draw toolbar. Clear the **Keep interior boundaries** check box. Click **OK**.

6 Create a second rectangle with the following properties; when finished, click **OK**.

OBJECT	WIDTH	HEIGHT	BASE X	BASE Y
R1	6e-3	2e-3	0	2e-3

7 Again, press Ctrl+A to select both objects.

8 Click the **Create Composite Object** button, then click **OK**.

9 Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar. Draw a circle of radius `3e-3` centered at the point (`0`, `0`).

10 Press Ctrl+A to select both objects.

11 Click the **Create Composite Object** button on the Draw toolbar. Activate the **Keep interior boundaries** check box. Click **OK**.

12 Click the **Split Object** button on the **Draw** toolbar.

13 Shift-click the **Rectangle/Square** button on the Draw toolbar. In the **Width** field type `5e-3`, and in the **Height** field type `1e-4`. Set **Base** to **Center**, then click **OK**.

14 Press Ctrl+C to make a copy of the rectangle.

15 Press Ctrl+V and click **OK**.

16 Click the **Rotate** button on the Draw toolbar.

17 Set the **Rotation angle** to `90` degrees, then click **OK**.

18 Shift-click to select both rectangles. Click the **Create Composite Object** button on the Draw toolbar. Clear the **Keep interior boundaries** check box, then click **OK**.

19 Shift-click again to select the cross and the inner circle. Click the **Difference** button on the Draw toolbar.

20 Press Ctrl+A.

21 In the **Draw** menu, activate the **Use Assembly** option.

22 From the **Draw** menu, select **Create Pairs**. Click **OK**.

23 Click the **Zoom Extents** button in the main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select the **Moving Mesh (ALE) (ale)** application mode.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 2.

4 In the **Subdomain selection** area, set the **Group** selection to **rotate_CW**.

5 Click **OK**.

6 From the **Multiphysics** menu, select **Incompressible Navier-Stokes (chns)**.

7 From the **Physics** menu, select **Subdomain Settings**.

8 For both subdomains, set the **Density** to `rho` and the **Dynamic viscosity** to `eta`.

9 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select boundary 15–26 (the twelve boundaries on the impeller surface).

3 In the **Boundary selection** area, set the **Group** selection to **no_slip_CW**.

4 Select Boundaries 2 and 6. Choose the **Boundary type Open Boundary** and select **Normal stress** from the **Boundary condition** list. Leave f_0 at zero.

5 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Fine**.

3 Click **OK** to close the **Free Mesh Parameters** dialog box.

4 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Time stepping** area on the **General** page, set **Times** to `0:0.5:20`, **Relative tolerance** to `1e-4`, and **Absolute tolerance** to `1e-5`.

3 Click **OK** to close the dialog box, then click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default plot shows the magnitude of the velocity field. To reproduce the plot in Figure 5-22, follow these instructions:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 On the **Surface** page, verify that **Velocity field** is selected in the **Predefined quantities** list on the **Surface Data** page. From the **Unit** list, select **mm/s**.

3 On the **Arrow** page, select the **Arrow plot** check box.

4 Verify that **Velocity field** is selected in the **Predefined quantities** list on the **Subdomain Data** page.

5 In the **Arrow parameters** area, select **3D arrow** from the **Arrow type** list.

6 Click the **Color** button. In the **Arrow Color** dialog box, select black. Click **OK**.

7 On the **Streamline** page, select the **Streamline plot** check box.

8 Verify that **Velocity field** is selected in the **Predefined quantities** list on the **Streamline Data** page.

9 From the **Streamline plot type** list, select **Uniform density**. On the **Density** page, set the **Separating distance** to `0.02`.

10. On the **Line Color** page, click the **Color** button. In the **Streamline Color** dialog box, select white. Click **OK**.
11. On the **General** page, clear the **Geometry edges** check box in the **Plot type** area.
12. Verify that the selection in the **Solution at time** list is **20**.
13. Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

6

Multiphase Flow

This chapter contains examples of multiphase fluid flow.

The first four models—Rigid Body Motion, Rising Bubble, Boiling Flow, and Droplet Breakup of a T-Junction—use physical descriptions where the phase boundary is tracked in detail. These models account for the effect of gravity, surface tension, and phase change; tracking the phase boundary with a level set method.

For many industrial applications, the macroscopic motion of flow is of more importance than the detailed dynamics of each phase interface. The examples in this section include the flow within a bubble column reactor, the separation of solid particles from water during wastewater treatment, and the dynamics of a dense suspension.

Rigid Body Motion

Introduction

This is a simple tutorial model that demonstrates how to use the Level Set application mode to track a moving interface. The example shows how to set up the model and how the choice of the level set parameters effects the solution.

Model Definition

In this example you use the Level Set application mode to model a circle that rotates around the origin. The velocity field is given by

$$\mathbf{u} = (-\omega y, \omega x)$$

where ω is the angular frequency (rad/s). Figure 6-1 shows the computational domain together with the initial position of the interface.

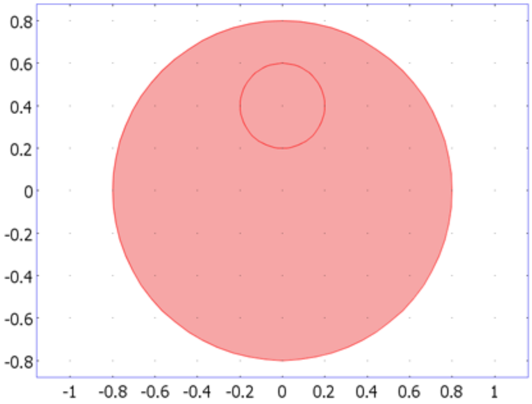


Figure 6-1: Computational domain (large circle) and initial position of the interface (small circle).

The corresponding level set equation is given by

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{6-1}$$

The interface, in this case the smaller circle, is defined by the $\phi = 0.5$ contour.

After setting up the problem using the Level Set application mode, the example explains how to choose the level set parameters ε and γ for optimal results.

Results

To get accurate results, it is important that you give suitable values for the parameters γ and ε. Most important is γ, while the default value on ε usually gives satisfying results. Figure 6-2 shows the initial interface and the position of the interface 1 s, for $\gamma = 1$ and $\gamma = 0.01$. The result using $\gamma = 0.01$ is significantly better for this problem, because less artificial stabilization is added. However, if γ is chosen smaller still, numerical instabilities lead to oscillations.

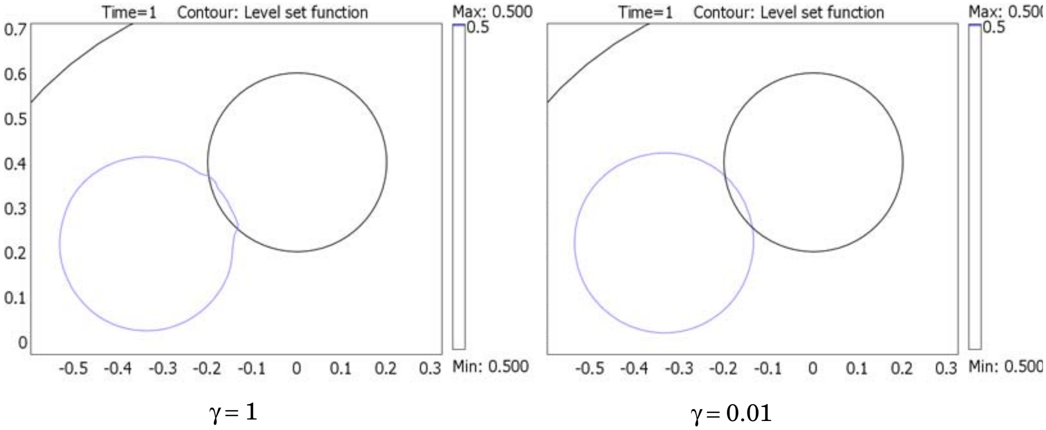


Figure 6-2: Initial interface and interface after 1 s for γ = 1 (left) and γ = 0.01 (right).

By using a constant value for ε on the entire computational domain, the solution is even more accurate. Figure 6-3 shows the result for $\gamma = 0.01$ and $\varepsilon = 0.06$. Because ε is constant within the entire computational domain, the thickness of the interface is constant.

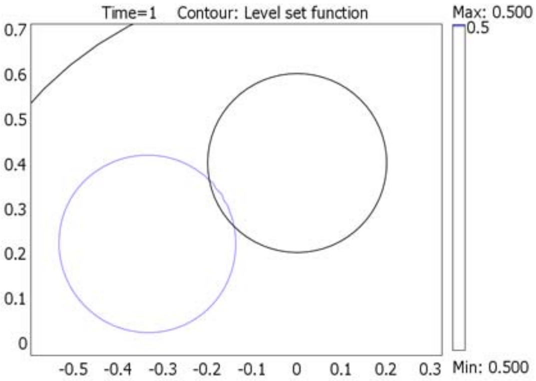


Figure 6-3: Solution at t = 1 s for $\gamma = 0.01$ *and* $\varepsilon = 0.06$.

Model Library path:

`Chemical_Engineering_Module/Multiphase_Flow/rigid_body_motion`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** from the **Space dimension** list.
2. From the list of application modes, select **Chemical Engineering Module> Momentum Transport>Multiphase Flow>Level Set**.
3. Click **OK**.

GEOMETRY MODELING

1. On the Draw toolbar, click the **Ellipse/Circle (Centered)** button. Click the point (0, 0) and drag the pointer to draw a circle with radius 0.8. Click again to create the circle. Click the **Ellipse/Circle (Centered)** button once more and create another circle centered at (0, 0.4) with radius 0.2.
2. Click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constant (the description is optional):

NAME	EXPRESSION	DESCRIPTION
`omega`	`1[rad/s]`	`Angular frequency`

3 Click **OK**.

4 From the **Options** menu, select **Expressions>Scalar Expressions**.

5 Define the following two variables:

NAME	EXPRESSION	DESCRIPTION
`u`	`-y*omega`	`x-component of velocity`
`v`	`x*omega`	`y-component of velocity`

6 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Ctrl-click to select both Subdomain 1 and Subdomain 2.

3 Type `u` in the **x-velocity** edit field and `v` in the **y-velocity** field.

4 Click the **Init** tab.

5 Select Subdomain 1 and type `0` in the edit field for the initial condition.

6 Select Subdomain 2 and type `1` in the edit field for the initial condition.

7 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundaries 3, 4, 6, and 7, then select the **Interior boundaries** check box.

3 From the **Boundary condition** list, select **Initial interface**.

4 Click **OK**.

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar.

2 In general, a relatively fine mesh is required to get accurate results for this kind of problem. Therefore, click the **Refine Mesh** button on the Main toolbar to create a finer grid.

COMPUTING THE SOLUTION—INITIALIZATION

1 From the **Solve** menu, select **Get Initial Value**.

2 Click the **Plot Parameters** button on the Main toolbar.

3 Click the **Surface** tab. On the **Surface Data** page, type `5*epsilon_mmls/gamma_mmls` in the **Expression** edit field. Click **OK**.

The maximum of $5\varepsilon/\gamma$ is a suitable time for initialization, in this case 0.3 s.

4 Click the **Solver Parameters** button on the Main toolbar. Type `0.3` in the **Times** edit field. Click **OK**.

5 Click the **Solve** button on the Main toolbar to solve for the initial level set function.

6 Click the **Solver Manager** button on the Main toolbar.

7 Click the **Store Solution** button.

8 From the **Solution at time** list, select **0.3**, then click **OK**.

9 In the **Initial value** area, select **Stored solution** and select **0.3** from the **Solution at time** list.

10 Click **OK**.

COMPUTING THE SOLUTION AND POSTPROCESSING

1 Click the **Solver Parameters** button on the Main toolbar. Type `0:0.1:1` in the **Times** edit field. Click **OK**.

2 In the Model Tree, right-click **Level Set (mmls)** and select **Properties**.

3 Select **Transient** from the **Analysis type** list, then click **OK**.

4 Click the **Solve** button on the Main toolbar.

5 Click the **Plot Parameters** button on the Main toolbar.

6 On the **General** page, clear the **Surface** check box and select the **Contour** check box.

7 Click the **Contour** tab.

8 Click the **Vector with isolevels** option button, then type `0.5` in the corresponding edit field.

9 Click **OK**.

10 Click the **Zoom Window** button on the Main toolbar if you want to inspect the position of the interface in more detail. Then click the **Zoom Extents** button to view the entire computational domain.

The resulting solution is quite poor. The reason is that the reinitialization parameter γ is too large. Therefore, change the value of γ and compute a new solution:

1. In the Model Tree, double-click **Level Set (mmls)>Subdomain Settings**.
2. Click the **Physics** tab.
3. Select both subdomains, then type `0.01` in the γ edit field. Click **OK**.
4. Click the **Solve** button on the Main toolbar.

The solution can be improved further if ε is constant in all domains the interface passes.

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **Surface** page, select the **Surface plot** check box.
3. On the **Surface Data** page, type `epsilon_mmls` in the **Expression** edit field (`epsilon_mmls` is the name of the variable for ε).
4. Click **OK** to create the plot in Figure 6-4.

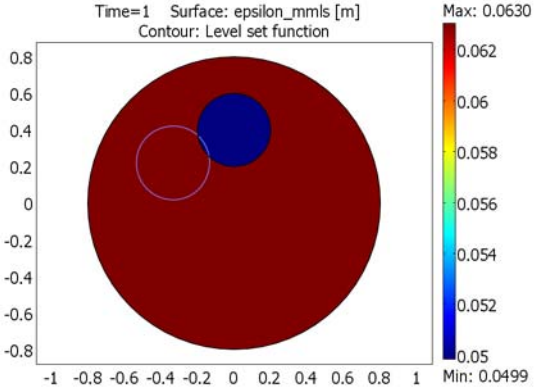


Figure 6-4: Surface plot of the parameter ε*.*

As you can see, ε is constant within each of the two subdomains but differs between the two domains. The maximum value is about 0.06. To further improve the results, let ε be constant in the whole domain.

5. In the Model Tree, double-click **Level Set (mmls)>Subdomain Settings**.
6. Click the **Physics** tab.

7 Select both subdomains and type `0.06` in the ε edit field. Click **OK**.

8 In the **Model Tree**, right-click **Level Set (mmls)** and select **Properties**.

9 Select **Transient initialization** from the **Analysis type** list, then click **OK**.

10 Click the **Solver Parameters** button on the Main toolbar. Type `30` in the **Times** edit field. Click **OK**.

Note that because γ now is only 0.01, a suitable time for initialization is 30 s instead of 0.3 s.

11 Click the **Solver Manager** button on the Main toolbar.

12 In the **Initial value** area, click the **Initial value expression** option button.

13 Click the **Solve** button. When the solver has finished, click the **Store Solution** button.

14 From the **Solution at time** list, select **30**, then click **OK**.

15 In the **Initial value** area, click the **Stored solution** option button and select **30** from the **Solution at time** list. Click **OK**.

16 In the Model Tree, right-click **Level Set (mmls)** and select **Properties**.

17 Select **Transient** from the **Analysis type** list, then click **OK**.

18 Click the **Solver Parameters** button on the Main toolbar. Type `0:0.1:1` in the **Times** edit field. Click **OK**.

19 Click the **Solve** button on the Main toolbar.

20 Click the **Plot Parameters** button on the Main toolbar.

21 Clear the **Surface plot** check box, then click **OK** to generate the plot in Figure 6-3.

If you solve for a longer time, the accuracy of the solution decreases with time. To further improve the accuracy, you can reduce the error tolerances. You specify the tolerances in the **Solver Parameters** dialog box on **General** page. There, you can for instance set the **Relative tolerance** to `0.001` and the **Absolute tolerance** to `0.0001`.

Rising Bubble Modeled with the Level Set Method

Introduction

This example shows a model of two immiscible fluids using a level set method. The level set method is well suited for problems with moving boundaries in which the geometry's topology changes with time. A bubble of oil that travels up through water and finally merges with oil at the top causes this kind of topology change. For problems where the topology is unchanged as a function of time, as in free surface movement in a tank (no splashing) and impeller stirring, it is also possible to use the ALE (arbitrary Lagrangian-Eulerian) method.

Three different regions exist initially: the oil bubble, the oil at the top of the container, and the water surrounding the bubble (see Figure 6-5). The Level Set Two-Phase Flow application mode makes it easy to set up the model.

This model treats an oil bubble traveling through water to finally merge with oil already residing at the top of the container. The container is cylindrical with a diameter of $1 \cdot 10^{-2}$ m and a height of $1.5 \cdot 10^{-2}$ m. Figure 6-5 depicts the initial position of the two fluids. Both geometry and initial data are axisymmetric.

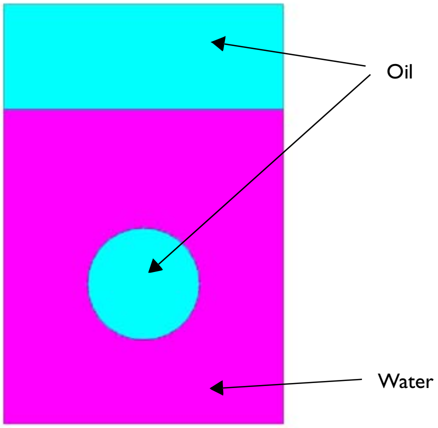


Figure 6-5: Initial bubble position.

The oil studied in this example has viscosity 0.0168 Pa·s and density 880 kg/m^3. For water viscosity is $1.04 \cdot 10^{-3}$ Pa·s and density 997 kg/m^3. The driving force for the bubble's movement is the difference in density between oil and water. The oil is lighter than water and the bubble therefore starts to rise due to gravitation.

A level set method is used to track the interface. This means that the interface is represented by a certain level set or contour of the globally defined level set function, ϕ. The level set application modes in COMSOL Multiphysics use a smooth step function with the interface defined by the contour $\phi = 0.5$ as level set function. The water is located in the domain where $0 \le \phi \le 0.5$, while the oil occupies the domain where $0.5 \le \phi \le 1$. The function is continuously reinitialized so that it keeps the correct shape across the interface.

Model Definition

The momentum and mass transport are governed by the Navier-Stokes equations:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - \nabla \cdot [\eta(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \nabla p = \sigma\kappa\mathbf{n}\delta + \rho\mathbf{g} \tag{6-2}$$

$$\nabla \cdot \mathbf{u} = 0\,. \tag{6-3}$$

In the above equations, ρ (kg/m^3) denotes the density, $\mathbf{u}$ is the velocity (m/s), t equals time (s), η represents the viscosity (Pa·s), p equals the pressure (Pa), σ is the surface tension coefficient, $\mathbf{n}$ is the unit normal to the interface, $\kappa = -\nabla \cdot \mathbf{n}$ is the curvature of the fluid interface, δ is a delta function concentrated at the interface between the fluids, and $\mathbf{g}$ is the gravity vector.

In Equation 6-2, the term $\sigma\kappa\mathbf{n}\delta$ defines the surface tension forces and $\rho\mathbf{g}$ is the gravity force. Equation 6-3 is the continuity equation, which follows from mass conservation and incompressibility of the fluids.

The level set method models the fluid interface by tracing the isolines of the level set function, ϕ. The level set or isocontour $\phi = 0.5$ determines the position of the interface. ϕ is transported and reinitialized by the equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = \gamma\nabla \cdot \left(-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|} + \varepsilon\nabla\phi\right), \tag{6-4}$$

where $\mathbf{u}$ is the fluid velocity, and γ and ε are reinitialization parameters. The parameter ε determines the thickness of the layer around the interface where ϕ goes from zero to one.

Because the level set function is a smooth step function, it is used to determine the density and dynamic viscosity globally by

$$\rho = \rho_w + (\rho_o - \rho_w)\phi$$

and

$$\mu = \mu_w + (\mu_o - \mu_w)\phi,$$

where ρ_w, μ_w, ρ_o, and μ_o denote the constant density and viscosity of water and oil, respectively.

The application mode also uses ϕ to calculate a smooth δ-function,

$$\delta = 6|\phi(1-\phi)||\nabla\phi|,$$

and to calculate the interface normal from the expression

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0.5} . \qquad (6\text{-}5)$$

INITIAL CONDITION

At $t = 0$, the velocity and pressure are both zero. The initial ϕ is given in Figure 6-6.

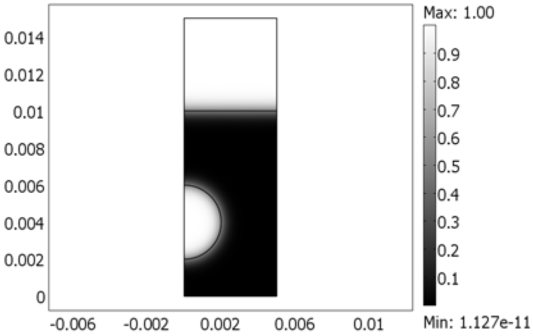


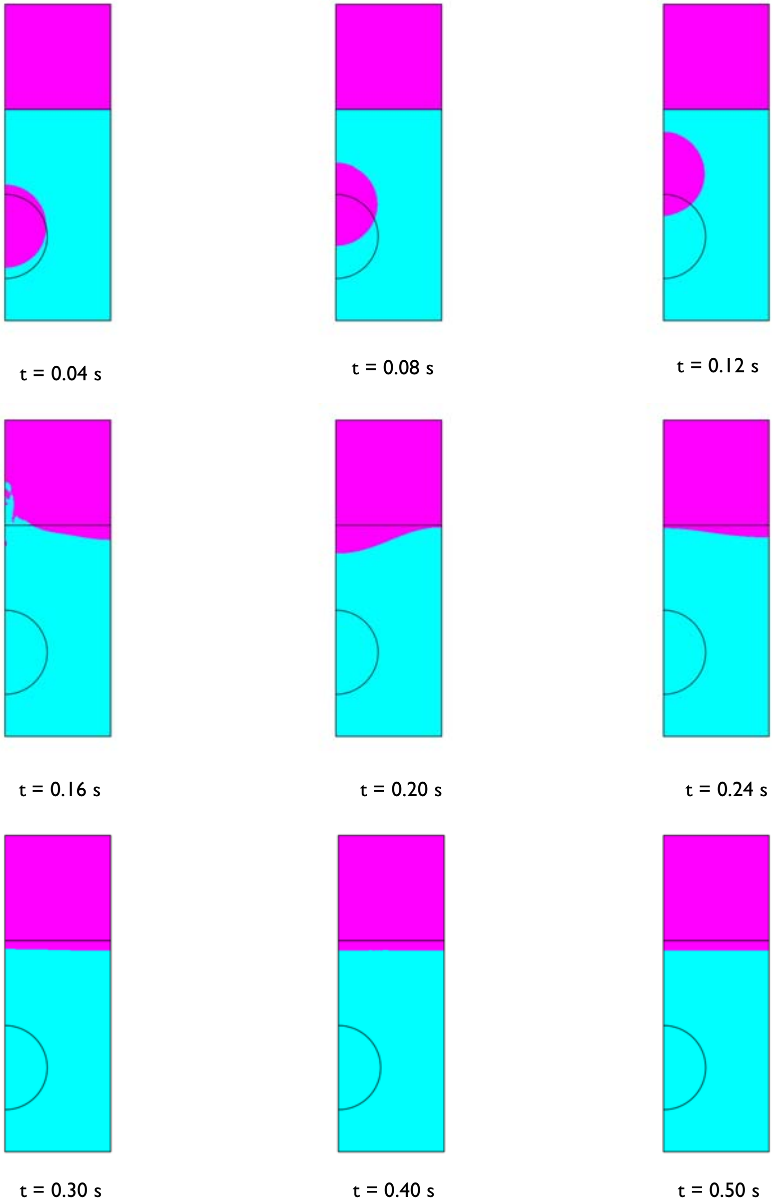
Figure 6-6: A surface and contour plot of the initial level set function.

BOUNDARY SETTINGS

No-slip conditions, $\mathbf{u} = 0$, are used at the top and bottom of the cylinder. Slip conditions are used at the vertical walls in order to allow the fluid interface to move along these walls.

Results and Discussion

Figure 6-7 contains snapshots of the fluid interface. The snapshots show how the bubble travels up through the water and merges with the oil above. As the bubble rises, its shape remains spherical because the viscosity of the oil is large and because of the surface tension. As the droplet hits the water surface, it splashes and creates waves on the surface.



t = 0.04 s

t = 0.08 s

t = 0.12 s

t = 0.16 s

t = 0.20 s

t = 0.24 s

t = 0.30 s

t = 0.40 s

t = 0.50 s

Figure 6-7: The initial interface position together with snapshot images showing the fluid interface at different times.

One way to investigate the quality of the numerical results is to check the conservation of mass. Because there are no reactions and no flow through the boundaries, the total mass of each fluid should be constant in time. Figure 6-8 shows the total mass of oil as a function of time. During the simulation, there is a mass loss of about 0.05%, which shows that mass is very well conserved by the model. The reason for the small mass loss is that the divergence-free condition on the velocity is not exactly fulfilled for the P_2P_1 elements used for the velocity and pressure. See the section "The Level Set Method for Two-Phase Flow" on page 165 of the *Chemical Engineering Module User's Guide* for information on how you can obtain exact mass conservation by using the application mode property Conservative level set.

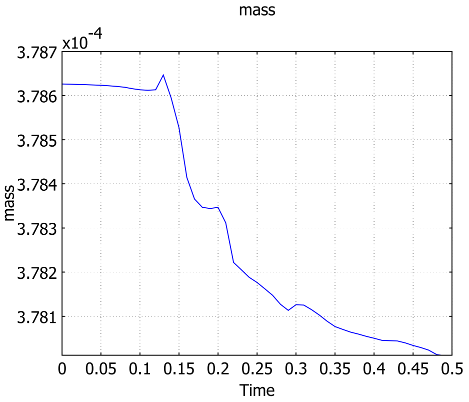


Figure 6-8: Total mass of oil as a function of time. The total mass loss during the simulation is small, about 0.05%.

Modeling in COMSOL Multiphysics

It is straightforward to set up the model with the Level Set Two-Phase Flow application mode available in the Chemical Engineering Module. You first initialize the level set function, then store the solution, change to the Transient analysis type, and start the fluid flow calculation.

Model Library path: `Chemical_Engineering_Module/Multiphase_Flow/rising_bubble`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator** select **Axial symmetry (2D)** from the **Space dimension** list.

2 From the list of application modes select **Chemical Engineering Module> Momentum Transport>Multiphase Flow>Level Set Two-Phase Flow, Laminar**.

3 Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar.

2 Specify the rectangle with these settings:

PROPERTY	EXPRESSION
Width	`5e-3`
Height	`1.5e-2`
Position, r	0
Position, z	0

3 Click **OK** and then click the **Zoom Extents** button on the Main toolbar.

4 Click the **2nd Degree Bézier Curve** on the Draw toolbar to draw a circular arc. Click the points (0, 6e-3), (2e-3, 6e-3), (2e-3, 4e-3), (2e-3, 2e-3), (0, 2e-3). The coordinates of the pointer appear in the lower left corner of the graphical user interface. Right-click to finalize the curve.

5 Click the **Line** button, also on the Draw toolbar. Click the points (0, 0.01) and (6e-3,0.01). Right-click to create the line, then double-click the line you just drew. Select **1** from the **Curve selection** list. Replace the number on the second row of the **r** column by `0.005` and click **OK**.

OPTIONS AND SETTINGS

1 Select **Constants** from the **Options** menu and enter the following constant names and expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`etaW`	`1.04e-3[Pa*s]`	`Viscosity of water`
`etaO`	`0.0168[Pa*s]`	`Viscosity of oil`
`rhoW`	`997[kg/m^3]`	`Density of water`
`rhoO`	`880[kg/m^3]`	`Density of oil`

NAME	EXPRESSION	DESCRIPTION
`gz`	`-9.81[m/s^2]`	`Gravity constant`
`sigma`	`0.073[N/m]`	`Surface tension coefficient`

2 Click **Options>Integration Coupling Variables>Subdomain Variables**, and select all three subdomains by selecting one and then clicking Ctrl+A. Enter the following variable in the dialog box; when done, click **OK**.

NAME	EXPRESSION
`mass`	`2*pi*r*rho0*phi`

PHYSICS SETTINGS

Subdomain Settings

1 Open the **Subdomain Settings** dialog box from the **Physics** menu and select all subdomains.

2 Enter fluid properties according to the following table:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ_1	`rhoW`	Density, fluid 1
η_1	`etaW`	Dynamic viscosity, fluid 1
ρ_2	`rho0`	Density, fluid 2
η_2	`eta0`	Dynamic viscosity, fluid 2

3 On the **Sources/Sinks** page, type `sigma` in the **Surface tension coefficient** edit field and `gz` in the **Gravitation, z component** edit field.

4 On the **Level Set** page, type `0.1` in the γ edit field.

5 Click the **Init** tab. Select Subdomains 2 and 3, then click the option button **Fluid 2**.

6 Click **OK**.

Boundary Conditions

1 Open the **Boundary Settings** dialog box from the **Physics** menu.

2 Select Boundaries 1, 3, 4, and 5, then set the **Boundary type** to **Symmetry boundary** and the **Boundary condition** to **Axial symmetry**.

3 Select Boundaries 8 and 9, then set the type to **Symmetry boundary** and the condition to **Symmetry**.

4 Select Boundaries 6, 10, and 11, then select the **Interior boundaries** check box. Set **Initial fluid interface** as boundary condition.

For the other boundaries, the default condition (**Wall, No slip**) applies.

5 Click **OK**.

Point Settings

1 Open the **Point Settings** dialog box from the **Physics** menu.

2 Select Point 7 from the **Point selection** list (the lower right corner).

3 Select the **Point constraint** check box and leave **p_0** at zero. Click **OK**.

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar.

2 Click the **Refine Mesh** button twice to obtain a sufficient mesh resolution.

The resulting mesh should consist of about 6400 elements.

COMPUTING THE SOLUTION

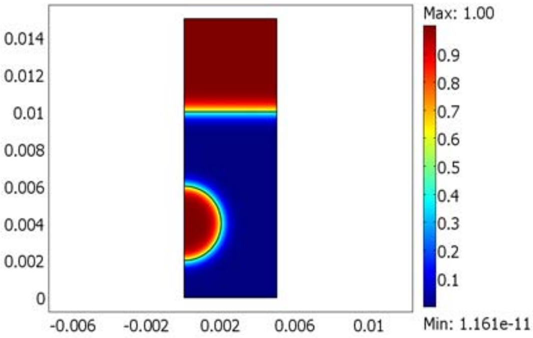
You first have to calculate the initial level set function.

1 Open the **Solver Parameters** dialog box by selecting **Solve>Solver Parameters**.

2 In the **Time stepping** area, type `1e-2` in the **Times** edit field, `0.1` in the **Relative tolerance** edit field, and `0.01` in the **Absolute tolerance** edit field. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

The following figure shows the plot you should obtain.



Initial level set function.

Use the obtained solution as initial condition for the motion of the rising bubble:

4 Click the **Solver Manager** button on the Main toolbar.

5 On the **Initial Value** page, click the **Store Solution** button. Select **0.01**, then click **OK**.

6 In the **Initial value** area, click the **Stored solution** option button. Select **0.01** from the **Solution at time** list.

7 Click **OK**.

8 From the **Physics** menu, select **Properties**. Change the **Analysis type** to **Transient**. Click **OK**.

9 Open the **Solver Parameters** dialog box.

10 In the **Time stepping** area, type `0:1e-2:0.5` in the **Times** edit field. Click **OK**.

11 Click the **Solve** button on the Main toolbar to compute the solution.

The solution takes 30–60 minutes to calculate.

POSTPROCESSING AND VISUALIZATION

First plot the distribution of oil and water as in Figure 6-7:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Clear the **Surface plot** check box.

3 On the **Contour** page, select the **Contour plot** check box. From the **Predefined quantities** list, select **Volume fraction of fluid 2**. Select the **Filled** check box.

4 Click the **Vector with isolevels** option button and type `0.5` in the corresponding edit field.

5 Click the **General** tab and select a time from the **Solution at time** list. Click **Apply**.

6 Repeat Step 5 above to plot the solution at other times.

7 Click **OK**.

To create the 3D images of the fluid interface, do the following steps:

1 From the **Draw** menu, choose **Revolve**.

2 Select **R1**, **CO1**, and **B1** from the **Objects to revolve** list and click **OK**.

3 In the **Model Tree**, click **Geom1** to return to the two-dimensional model.

4 Choose **Options>Extrusion Coupling Variables>Subdomain Variables**.

5 Select all subdomains.

6 Type `phi3d` in the **Name** edit field and `phi` in the **Expression** edit field.

7 Select **General transformation**.

8 Click the **Destination** tab.

9 In the **Geometry** list, select **Geom2**.

10 In the **Level** list, select **Subdomain**.

11 Select all three subdomains.

12 Select the **Use selected subdomains as destination** check box.

13 Type `sqrt(x^2+z^2)` in the **x** edit field, then click **OK**.

14 From the **Solve** menu, choose **Update Model**.

15 Click the **Plot Parameters** button on the Main toolbar.

16 Click the **General** tab. Clear the **Geometry edges** and **Slice** check boxes and select the **Isosurface** check box.

17 Clear the **Element refinement Auto** check box and type `4` in the edit field.

18 Click the **Isosurface** tab.

19 Type `phi3d` in the **Expression** field. Select **Vector with isolevels** and type `0.5` in the corresponding edit field.

20 Select **Uniform Color** and click the **Color** button. Choose a blue color to plot the fluid interface. Click **OK**.

21 Click the **General** tab. In the **Solution at time** list, select **0**. Click **OK**.

22 Click the **Scene Light** button on the Camera toolbar.

23 Click the **Camera Parameters** button on the Camera toolbar to open the **Camera Parameters** dialog box. Click the **Y** option button in the **Camera constraint** area and the **Vertical** option button in the **Mouse constraint** area. Click in the drawing area and hold the mouse button down as you move the mouse pointer to rotate the object to obtain the plot in Figure 6-9.

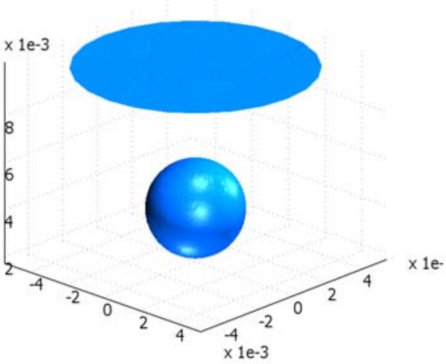


Figure 6-9: 3D plot of the initial position of the fluid interfaces.

24 To plot the solution at other times, click the **Plot Parameters** button and select other values in the **Solution at time** list. Click **Apply** to plot the solution at the corresponding time.

25 To create an animation of the evolving interface, click the **Animate** button.

Perform the following steps to plot the mass of oil as a function of time:

1 From the **Postprocessing** menu, select **Global Variables Plot**.

2 In the **Expression** edit field type `mass`, then click the **Add Entered Expression** button (the button marked **>**).

3 Click **OK** to generate the plot in Figure 6-8.

Boiling Flow

This example shows how you can make a detailed fluid flow calculation of a boiling fluid, using a level set approach to track the liquid-vapor interface in detail. To model boiling flows, you need to account for mass transfer across the phase boundary as well as the absorption of latent heat as the liquid evaporates. From the results, you can investigate flow field, the temperature evolution, as well as the transient position of the phase boundary.

The model is based on results presented in Ref. 1 and Ref. 2, with some modifications.

Model Definition

A liquid is initially at rest above a thin layer of vapor, where the temperature in both phases is that of the saturation temperature. A heat flux is applied at the bottom surface of the domain and, as the vapor-liquid interface heats up, liquid starts to evaporate causing the positions of the two phases and the interface to change. Figure 6-10 shows the axisymmetric model's geometry, the boundary conditions, and the initial position of the two phases.

To model boiling flow, you have to couple a thermal transport with a momentum and a mass transport using a level set method to represent the phase boundary. In COMSOL Multiphysics, it is possible to set up such a model by coupling the Level Set Two-Phase Flow application mode with the Convection and Conduction application mode, which can be done directly in the graphical user interface.

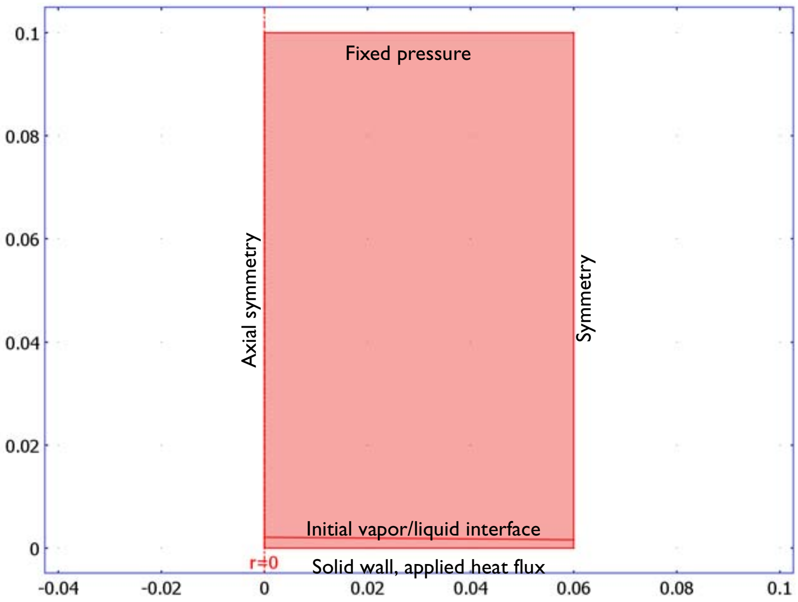


Figure 6-10: Model geometry. Liquid is initially present in the upper domain, while the lower domain is filled with vapor. The bottom boundary is heated, and the pressure is fixed at the upper boundary.

The thermal transport in the fluids is described by the following equation for the temperature

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = -mL\delta - \rho C_p \mathbf{u} \cdot \nabla T$$

where ρ denotes density (kg/m^3), C_p heat capacity (J/(kg·K)), k thermal conductivity (W/(m·K)), T temperature (K), and $\mathbf{u}$ fluid velocity (m/s). The first term on the right-hand side of the equation is a source term that accounts for latent heat liberation or absorption due to phase change; L denotes latent heat (J/kg), while m is the interfacial mass flux (kg/(m^2·s)), and δ is a Dirac delta function that is nonzero at the phase interface only.

The interface moves as a function of the fluid flow and motion due to phase change:

$$\mathbf{u}_{\text{interface}} = \mathbf{u} + \frac{m}{\rho}\mathbf{n}$$

where **n** denotes the unit normal to the interface, directed toward the liquid phase.

The interface is defined by the level set variable ϕ, which is a smooth step function that takes the value 0 in the gas and 1 in the liquid, with a smooth transition between these values across the interface. The 0.5 contour represents the interface. With this representation, it is possible to describe the interface by solving the following equation for ϕ:

$$\frac{\partial\phi}{\partial t} + \nabla\phi \cdot \mathbf{u}_{\mathrm{interface}} = \gamma\nabla \cdot \left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

The term on the right-hand side of the equation is required to stabilize the equation and to preserve the same smooth profile of ϕ across the interface. Suitable values for the parameters ε and γ are the size of the mesh elements and the speed of the interface, respectively.

Because the interface normal, **n**, is given by

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$$

the level set equation can be expressed as

$$\frac{\partial\phi}{\partial t} + \nabla\phi \cdot \mathbf{u} + \frac{m}{\rho}|\nabla\phi| = \gamma\nabla \cdot \left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

A momentum balance gives

$$\rho\frac{\partial\mathbf{u}}{\partial t} - \nabla \cdot \left[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2\eta}{3}(\nabla \cdot \mathbf{u})\mathbf{I}\right] + \rho\mathbf{u} \cdot \nabla\mathbf{u} + \nabla p = \sigma\kappa\delta\mathbf{n} + \rho\mathbf{g}$$

while the conservation of mass requires that

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0 \tag{6-6}$$

Note that even though there is mass transfer between the two phases, the total mass of gas and liquid must be conserved.

The material parameters ρ, η, C_p, and k are all approximately constant within each phase. To smooth out the discontinuities, the Level Set Two-Phase Flow application mode uses the relations

$$\rho = \rho_g + (\rho_l - \rho_g)\phi \tag{6-7}$$

$$\eta = \eta_g + (\eta_l - \eta_g)\phi \tag{6-8}$$

$$\delta = 6\phi(1-\phi)|\nabla\phi| \tag{6-9}$$

In the heat equation, you can use the same approach for the specific heat and the conductivity:

$$C_p = C_{pg} + (C_{pl} - C_{pg})\phi$$

$$k = k_g + (k_l - k_g)\phi$$

where the subscripts "g" and "l" denote the gas and liquid phases, respectively. For numerical calculations, it can be helpful to reformulate the mass conservation equation using Equation 6-7 and the level set equation, neglecting the stabilizing terms. The resulting form of the mass conservation equation is then

$$(\rho_l - \rho_g)\frac{m}{\rho}|\nabla\phi| - \rho(\nabla\cdot\mathbf{u}) = 0 \tag{6-10}$$

Finally, you must specify an expression for the interfacial mass flux. As discussed in Ref. 1, it is not yet clear how the mass flux relates to the interface temperature. In this example, use the expression

$$m = C\rho\frac{(T - T_{\mathrm{sat}})}{T_{\mathrm{sat}}} \tag{6-11}$$

The result is a mass flux from liquid to vapor when the temperature at the interface is larger than T_{sat}. The constant, C (m/s), relates to the mobility of the interface. The larger C is, the more rapidly the boundary is allowed to move due to phase change, and the more rapidly the temperature approaches the saturation temperature at the interface. Note that you can use any expression of the modeled variables to describe the mass flux and that you can enter such an expression directly in the graphical user interface. For example, it is straightforward to let the saturation temperature depend on, for instance, pressure. It is also possible to use any of the more complex expressions discussed in Ref. 1.

PHYSICAL PARAMETERS

As in Ref. 2, the liquid and vapor have the following physical properties:

QUANTITY	VALUE, GAS PHASE	VALUE, LIQUID PHASE
Density (kg/m^3)	5	200
Dynamic viscosity (Pa·s)	0.005	0.1
Conductivity (W/(m·K))	1	40
Heat capacity (J/(kg·K))	200	400

The surface tension coefficient is 0.1 N/m, the gravity vector $(0, -9.82)$ m/s^2, the latent heat 1000 J/kg, and the saturation temperature 273 K.

LEVEL SET PARAMETERS

In addition to the physical parameters, you need to assign appropriate values for the two level set parameters ε and γ. A suitable value for ε is the maximum mesh element size. The parameter γ should be approximately as large as the maximum speed of the interface. In this case, the speed of the interface varies significantly with time. Therefore, it is suitable to choose γ such that it varies with time and is equal to three times the average speed of the interface. To calculate the average speed of the interface, you can use the following expression

$$\frac{\int |\mathbf{u}_{\mathrm{interface}}| \delta d\Omega}{\int \delta d\Omega}$$

BOUNDARY CONDITIONS

At the bottom boundary, the velocity is zero and the inward heat flux is 100 W/m^2. At the upper wall, pressure and diffusive heat flux are both zero. Symmetry conditions hold on the outer cylindrical boundary.

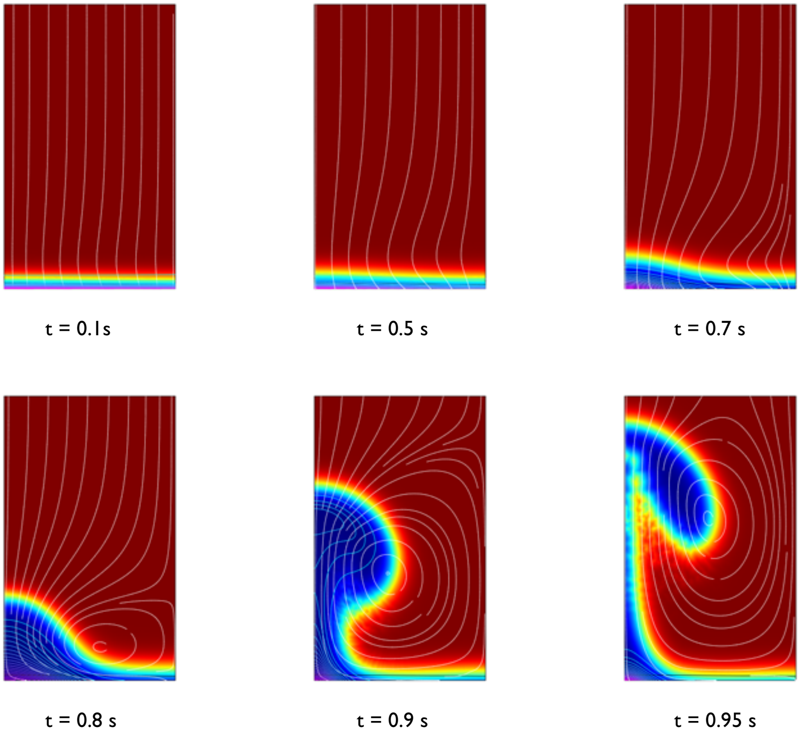
INITIAL CONDITIONS

Initially, a layer of vapor covers the bottom surface. The temperature equals 273 K, the saturation temperature while the velocity is zero.

Results and Discussion

Snapshots of the velocity field (streamlines), the temperature (contour lines) and the fluid interface at different times, ranging from $t = 0.1$ s to $t = 0.95$ s are seen in Figure 6-11. The results show how a mushroom-shaped bubble forms, with a narrow stream of vapor beneath it, qualitatively similar to the result obtained in Ref. 2. Note that it is not possible to strictly compare the results with the results in the reference, since the authors of Ref. 2 use a planar 2D coordinate system while an axisymmetric system is used here. Other differences are the initial shape of the interface, the initial temperature, and the boundary conditions for the temperature.

The temperature in the liquid phase remains close to the saturation temperature, which justifies the choice of the interfacial mass flux according to Equation 6-11.



t = 0.1s

t = 0.5 s

t = 0.7 s

t = 0.8 s

t = 0.9 s

t = 0.95 s

Figure 6-11: White velocity streamlines, temperature (contour lines) and the phase boundary (surface plot of the level set function) at different times.

Modeling in COMSOL Multiphysics

In order to set up the model in COMSOL Multiphysics, you need two application modes: The Level Set Two-Phase Flow, Laminar application mode, and the Convection and Conduction application mode. For the Level Set Two-Phase Flow, Laminar application mode, you must switch on the property Weakly compressible flow.

You also have to add a term in the level set equation and a source term in the heat transfer equation to account for phase change and release/absorption of latent heat, respectively. To simplify the numerical calculations, you can reformulate the continuity equation according to Equation 6-10.

If the velocity field varies significantly across the interface, the interface may become unsmooth, causing the time dependent solver to run into problems. In such cases, it can be useful to stop the calculation, recalculating the level set variable according to

$$\phi_{\text{new}} = 3\phi_{\text{old}}^2 - 2\phi_{\text{old}}^3 \tag{6-12}$$

and then continue the calculation. ϕ_{new} makes a sharper transition across the interface, but has the same 0.5 contour as ϕ_{old}. Use the reinitialization, according to Equation 6-12, only when necessary because it results in a small mass loss.

References

1. D. Juric and G. Tryggvason, "Computations of Boiling Flows," *Int. J. Multiphase Flow*, vol. 24, no. 3, pp. 387–410, 1998.

2. F. Gibou, L. Chen, D. Nguyen, and S. Banerjee, "A Level Set Based Sharp Interface Method for the Multiphase Incompressible Navier-Stokes Equations with Phase Change," *J. Comput. Phys.*, vol. 222, pp. 536–555, 2007.

Model Library path:
`Chemical_Engineering_Module/Multiphase_Flow/boiling_flow`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator** select **Axial symmetry (2D)** from the **Space dimension** list.
2. Click the **Multiphysics** button.
3. From the list of application modes select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Level Set Two-Phase Flow, Laminar**. Click **Add**.
4. Select **COMSOL Multiphysics>Heat Transfer>Convection and Conduction>Transient analysis**. Click **Add**.

5 Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1 Press shift and click the **Rectangle/Square** button on the Draw toolbar.

2 Type `0.06` in the **Width** edit field and `0.1` in the **Height** edit field. Click **OK**.

3 From the **Draw** menu, select **Specify Objects>Line**.

4 In the **r** edit field, type `0 0.06`.

5 In the **z** edit field, type `0.002 0.0015`.

6 Click **OK**.

7 Click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, choose **Constants**.

2 Enter constants according to the following table. The units and the descriptions are optional.

NAME	EXPRESSION	DESCRIPTION
L	1000[J/kg]	Latent heat of evaporation
Cp_l	400[J/(kg*K)]	Heat capacity, liquid
Cp_g	200[J/(kg*K)]	Heat capacity, gas
T_sat	273[K]	Saturation temperature
k_l	40[W/(m*K)]	Thermal conductivity, liquid
k_g	1[W/(m*K)]	Thermal conductivity, gas
q	100[W/m^2]	Inward heat flux, bottom boundary
C	200[m/s]	Scaling constant in mass-flux expression

3 Click **OK**.

4 From the **Options** menu, select **Expressions>Scalar Expressions**.

5 Add the following expressions:

NAME	EXPRESSION	DESCRIPTION
m	C*rho_chns*(T-T_sat)/T_sat	Interfacial mass flux due to evaporation
phi_source	-r*gradphi_chns*m/rho_chns	Source term in the level set equation

NAME	EXPRESSION	DESCRIPTION
`v_int`	`sqrt((u+normr_chns*m/rho_chns)^2+(v+normz_chns*m/rho_chns)^2)`	`Interface speed`
`gamma`	`3*nojac(I1/I2)`	`The level set parameter gamma`

In these expressions, `rho_chns` and `gradphi_chns` are internal variables defined by the Level Set Two-Phase Flow application mode: `rho_chns` is the density and `gradphi_chns` is the magnitude of the gradient of ϕ. Moreover, the factor `r` in the source term, representing the the radial coordinate *r*, is required to achieve the correct equations for the axisymmetric geometry.

6 Click **OK**.

7 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**.

8 Select both subdomains, then specify two integration coupling variables according to the following table:

NAME	EXPRESSION
`I1`	`v_int*delta_chns`
`I2`	`delta_chns`

9 Click **OK**.

PHYSICS SETTINGS

Application Mode Properties

1 Open the **Application Mode Properties** dialog box for the **Level Set Two-Phase Flow, Laminar (chns)** application mode.

You can open the dialog box in two different ways. Either, you first select **Level Set Two-Phase Flow, Laminar (chns)** from the **Multiphysics** menu, and then select **Properties** from the **Physics** menu. Alternatively, go to the **Model Tree** window, right-click **Level Set Two-Phase Flow, Laminar (chns)**, and select **Properties**.

2 Set the property **Weakly compressible flow** to **On**.

3 Click **OK**.

Subdomain Settings—Fluid Flow

1 Open the **Subdomain Settings** dialog box for the **Level Set Two-Phase Flow, Laminar (chns)** application mode, either from the **Physics** menu, or using the **Model Tree**.

2 Select both subdomains by selecting one subdomain and then press Ctrl and A.

3 Enter the following values in the different edit fields.

QUANTITY	VALUE/EXPRESSION
ρ_1	`5`
η_1	`0.005`
ρ_2	`200`
η_2	`0.1`

4 Click the **Sources/Sinks** tab. Type `0.1` in the σ edit field and `-9.82` in the $\mathbf{g_z}$ edit field.

5 Click the **Artificial Diffusion** button.

6 Select the **Streamline diffusion** check box and select **Anisotropic Diffusion** from the list.

7 Click **OK**.

8 Click the **Level Set** tab. Set ε to `hmax2_chns` (the largest element size in Subdomain 2).

9 Click the **Init** tab and select Subdomain 2 only. As **Initial fluid in this domain**, select **Fluid 2**.

10 Click **OK** to close the dialog box.

Boundary Conditions—Fluid Flow

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundary 4 and select the **Interior boundaries** check box. From the **Boundary condition** list, select **Initial fluid interface**.

3 Set conditions on the other boundaries according to the following table:

SETTINGS	BOUNDARIES 1,3	BOUNDARY 2	BOUNDARY 5	BOUNDARIES 6, 7
Boundary type	Symmetry boundary	Wall	Outlet	Symmetry boundary
Boundary condition	Axial symmetry	No slip	Pressure	Symmetry

4 Click **OK**.

Subdomain Settings—Heat Transfer

1 Open the **Subdomain Settings - Convection and Conduction (cc)** dialog box, either using the **Model Tree** or by selecting first **Multiphysics>2 Convection and Conduction (cc)** and then **Physics>Subdomain Settings**.

2 Select both subdomains.

3 On the **Physics** page, enter subdomain settings according to the following table:

QUANTITY	VALUE/EXPRESSION
k (isotropic)	`k_g+phi*(k_l-k_g)`
ρ	`rho_chns`
C_p	`Cp_g+phi*(Cp_l-Cp_g)`
Q	`-m*L*delta_chns`

4 Type `u` and `v` in the **Velocity field** edit fields.

5 Click the **Init** tab. Type `T_sat` in the **T(t_0)** edit field, then click **OK**.

Boundary Conditions—Heat Transfer

1 Open the **Boundary Settings** dialog box for the **Convection and Conduction (cc)** application mode.

2 Set boundary conditions as in the following table:

SETTINGS	BOUNDARIES 1, 3	BOUNDARY 2	BOUNDARY 5	BOUNDARIES 6, 7
Boundary condition	Axial symmetry	Heat flux	Convective flux	Thermal insulation

3 Select Boundary 2 and type `q` in the **q_0** edit field.

4 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Subdomain** tab and select both subdomains. In the **Element growth rate** edit field, type `1.005`.

3 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

First, you must initialize the level set function. To do this, make a transient calculation for the level set variable only. The appropriate time for initialization is the thickness of the interface (about 5ε) divided by the value of the level set parameter γ. In this case, the thickness is about 0.005 and γ is 1. A suitable initialization time is therefore 0.005.

1 Click the **Solver Parameters** button on the Main toolbar.

2 Type `0.005` in the **Times** edit field.

3 In the **Relative tolerance** edit field, type `0.005` and in the **Absolute tolerance** edit field, type `0.0005`. By lowering the tolerances you increase the accuracy and improve the stability.

4 Click the **Time Stepping** tab and type `1` in the **Maximum BDF order** edit field for increased stability.

5 Click **OK**.

6 Click the **Solver Manager** button on the Main toolbar.

7 Go to the **Solve For** page and select only **phi**.

8 Click **OK**.

9 Click the **Solve** button to start the initial calculation.

10 When the calculation has finished, click the **Solver Manager** button again.

11 On the **Initial Value** page, click the **Store Solution** button. Select the time **0.005** from the list, then click **OK**.

12 In the **Initial value** area, click the **Stored solution** option button and select **0.005** from the **Solution at time** list.

13 Click the **Solve For** tab. Select both application modes by clicking **Geom1 (2D)**.

14 Click **OK**.

15 In the **Model Tree**, right click **Level Set Two-Phase Flow, Laminar (chns)** and select **Properties**.

16 From the **Analysis type** list, select **Transient**. Click **OK**.

Now you have initialized the level set function. Before you can start the fluid flow calculation, you must modify the level set equation to account for the phase change. You also need to rewrite the continuity equation according to Equation 6-10 to simplify the numerical solution of the equations.

1 From the **Physics** menu, select **Equation System>Subdomain Settings**.

2 Select both subdomains and click the **f** tab.

3 The expression on the third row represents the continuity equation. Replace the expression by `-r*(rho2_chns-rho1_chns)*m/rho_chns*sqrt(gradphiz_chns^2+gradphir_chns^2+eps)+r*rho_chns*div U_chns`.

4 The expression on the fourth row corresponds to the source term in the level set equation. Add the term `phi_source` to the expression. The expression should now read `-r*u*gradphir_chns-r*v*gradphiz_chns+phi_source`.

5 Click the **Differentiate** button.

6 Click **OK**.

You also want to change the value of the level set parameter γ, so that it relates to the speed of the interface.

7 Open the **Subdomain Settings** dialog box for the **Level Set Two-Phase Flow, Laminar (chns)** application mode.

8 Go to the **Level Set** page, select both subdomains, and type `gamma` in the γ edit field.

9 Click **OK**.

10 Click the **Solver Parameters** button on the Main toolbar.

11 On the **General** page, type `[0:0.1:0.7]` in the **Times** edit field.

12 Click the **Time Stepping** tab. From the **Time steps taken by solver** list, select **Intermediate**. The **Intermediate** option ensures that the solver takes at least one time step within each of the specified time intervals.

13 Click **OK**.

14 Click the **Solve** button on the Main toolbar to start the calculation.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 Go to the **Streamline** page and select the **Streamline plot** check box.

3 From the **Predefined quantities** list, select **Level Set Two-Phase Flow, Laminar (chns)>Velocity field**. From the **Streamline plot type** list, select **Uniform density**.

4 On the **Contour** page, select the **Contour plot** check box.

5 From the **Predefined quantities** list, select **Convection and Conduction (cc)>Temperature**.

6 Click **Apply**.

7 On the **General** page, select the time you want to visualize the solution at from the **Solution at time** list.

8 Click **OK**.

9 To create a movie, click the **Animate** button on the Plot toolbar.

If the velocity field varies significantly across the interface, the time dependent solver sometimes becomes slow. This typically occurs if the reinitialization does not manage to keep the transition of the level set function across the interface sharp enough. A solution is to stop the solver, and manually reinitialize the level set function such that it becomes sharper. If the solver starts to take smaller time steps, stop the solver. Define the initial value for the level set variable, ϕ_{init}, from the solution at the last time, ϕ_{stored}, as

$$\phi_{\mathrm{init}} = 3\phi_{\mathrm{stored}}^2 - 2\phi_{\mathrm{stored}}^3 \tag{6-13}$$

ϕ_{init}, has the same 0.5 contour as ϕ_{stored}, but a sharper transition from zero to one. Use the reinitialization, according to Equation 6-13, only when necessary because it results in a small mass loss.

1 From the **Physics** menu, select **Equation System>Subdomain Settings**.

2 Click the **Init** tab. For both subdomains, specify the following initial values:

VARIABLE	EXPRESSION
u(t0)	u
v(t0)	v
p(t0)	p
phi(t0)	`3*phi^2-2*phi^3`
T(t0)	T

3 Click **OK**.

4 Click the **Solver Manager** button and go to the **Initial Value** page.

5 In the **Initial value** area, select **Initial value expression evaluated using current solution**.

6 Select **0.7** from the **Solution at time** list.

7 Click **OK**.

8 Click the **Solver Parameters** button. Type `0:0.01:0.1` in the **Times** edit field.

9 Click **OK**.

10 Click the **Solve** button on the Main toolbar.

11 While the software is solving the problem, click the **Log** tab to inspect how the solver proceeds. If the solver starts to take very small time steps (second column, `Time`) at the same time as the numbers in any of the two right most columns (number of time-discretization failures, `Tfail`, and nonlinear failures, `NLfail`) start to increase you might want to stop the calculation. In that case, go to the **Progress** page and click the **Stop** buttons and wait until the solver has stopped.

12 Open the **Solver Manager** again.

13 From the **Solution at time** list, select the time you want to restart the calculation from. Click **OK**.

14 Repeat Steps 10–13 until you have calculated as many time steps as you desire.

Droplet Breakup in a T-Junction

Introduction

Emulsions consist of small liquid droplets immersed in another liquid and are widely used, for instance in the production of food, cosmetics, and pharmaceutical products. The quality of the products typically depends on the size of these droplets. This model studies in detail how droplets in an emulsion can be created.

The model is easily set up using the Level Set Two-Phase Flow application mode. The model uses the predefined wetted wall boundary condition at the solid walls, with a contact angle of 135°. From the results, you can determine the size of the created droplets and the rate with which they are produced. The results compare well with those presented in Ref. 1.

Model Definition

Figure 6-12 shows the geometry of the T-shaped microchannel. The fluid to be dispersed into small droplets, Fluid 2, enters through the vertical channel. The other fluid, Fluid 1, flows from the right to left through the horizontal channel.

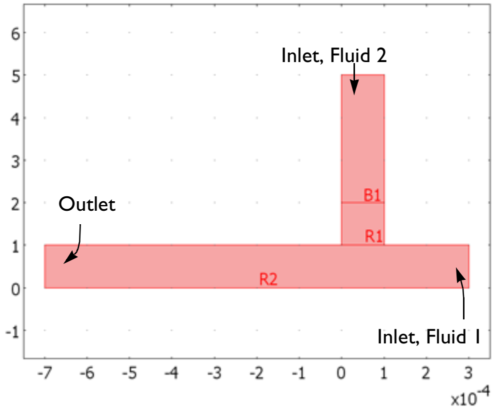


Figure 6-12: The geometry of the T-junction.

You can easily set up the problem with the Level Set Two-Phase Flow application mode. The application mode sets up a momentum transport equation, a continuity equation, and a level set equation for the level set variable. The fluid interface is defined by the 0.5 contour of the level set function.

The application mode uses the following equations

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - \nabla \cdot [\eta(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \nabla p = \mathbf{F}_{\mathrm{st}} \tag{6-14}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{6-15}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(-\phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} + \varepsilon \nabla \phi\right) \tag{6-16}$$

In the equations above, ρ denotes density (kg/m^3), $\mathbf{u}$ velocity (m/s), t time (s), η dynamic viscosity (Pa·s), p pressure (Pa) and $\mathbf{F}_{\mathrm{st}}$ the surface tension force. ϕ is the level set function and γ and ε are numerical stabilization parameters. The density and viscosity are calculated from

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

$$\eta = \eta_1 + (\eta_2 - \eta_1)\phi$$

where ρ_1, ρ_2, η_1, and η_2 are the densities and viscosities of Fluid 1 and Fluid 2.

PHYSICAL PARAMETERS

The two liquids have the following physical properties:

QUANTITY	VALUE, FLUID 1	VALUE, FLUID 2
Density (kg/m^3)	1000	1000
Dynamic viscosity (Pa·s)	0.00195	0.00671

The surface tension coefficient is $5 \cdot 10^{-3}$ N/m.

BOUNDARY CONDITIONS

Parabolic velocity profiles are specified at both inlets, while at the outflow boundary you specify the pressure. The Wetted wall boundary condition applies to all solid boundaries with the contact angle specified as 135° and a slip length equal to the mesh size h. The contact angle is the angle between the fluid interface and the solid wall at points where the fluid interface attaches to the wall. The slip length is the distance to the position outside the wall where the extrapolated tangential velocity component is zero (Figure 6-13).

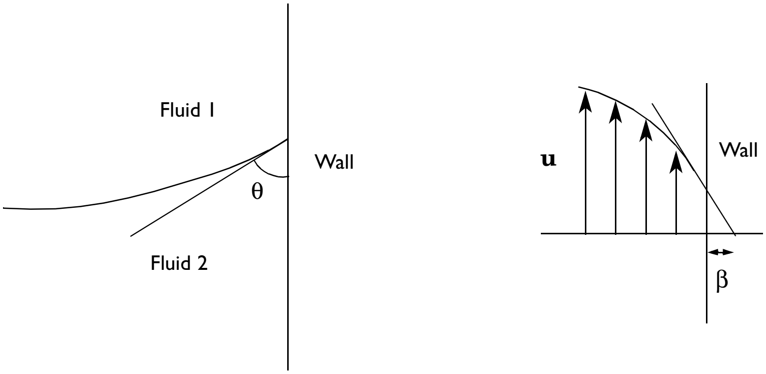


Figure 6-13: The contact angle, θ*, and the slip length,* β.

Results and Discussion

Figure 6-14 shows the fluid interface (the level set function) and the velocity streamlines at various times. After 0.08 s the first droplet is formed.

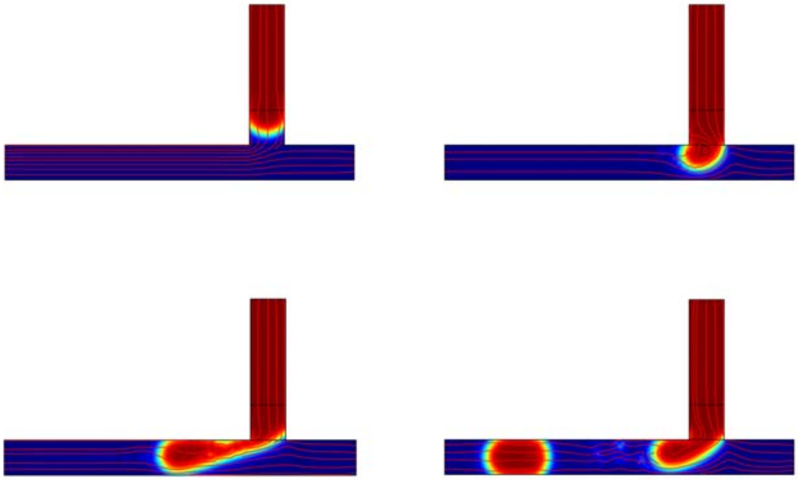


Figure 6-14: Velocity streamlines and the phase boundary at t = 0.02 s, 0.04 s, 0.06 s, and 0.08 s.

The diameter of the produced droplet at $t = 0.08$ s can be calculated from

$$d = 2\sqrt{\frac{\int_{\Omega} (\phi > 0.5)d\Omega}{\pi}}$$

where Ω is the leftmost part of the horizontal channel, where $x < -3\cdot10^{-4}$ m. In this case, the results show that $d = 1.45\cdot10^{-4}$ m.

Reference

1. Graaf and others, “Lattice Boltzmann Simulations of Droplet Formation in a T-Shaped Microchannel,” *Langmuir*, vol. 22, pp. 4144–4152, 2006.

Model Library path: `Chemical_Engineering_Module/Multiphase_Flow/droplet_breakup`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator** select **Chemical Engineering Module> Momentum Transport>Multiphase Flow>Level Set Two-Phase Flow, Laminar**.

2 Click **OK**.

GEOMETRY MODELING

1 Press Shift and click the **Rectangle/Square** button on the Draw toolbar.

2 Type in the following values:

WIDTH	HEIGHT	BASE, X	BASE, Y
1e-4	4e-4	0	1e-4

3 Click **OK**.

4 Click the **Zoom Extents** button on the Main toolbar.

5 In the same way, create another rectangle with the following settings:

WIDTH	HEIGHT	BASE, X	BASE, Y
1e-3	1e-4	-7e-4	0

6 From the **Draw** menu, select **Specify Objects>Line**.

7 In the **x** edit field, type `0 1e-4`.

8 In the **y** edit field, type `2e-4 2e-4`.

9 Click **OK**.

10 Click the **Zoom Extents** button.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define constants according to the following table. The units and the descriptions are optional.

NAME	EXPRESSION	DESCRIPTION
rho1	1e3[kg/m^3]	Density, Fluid 1
eta1	1.95e-3[Pa*s]	Viscosity, Fluid 1
rho2	1e3[kg/m^3]	Density, Fluid 2
eta2	6.71e-3[Pa*s]	Viscosity, Fluid 2
vmax1	2*vmax2	Maximum inlet speed, Fluid 1
vmax2	0.0083[m/s]	Maximum inlet speed, Fluid 2
sigma	5e-3[N/m]	Surface tension coefficient

3 Click **OK**.

4 From the **Options** menu, select **Expressions>Global Expressions**.

5 Add the following three expressions:

NAME	EXPRESSION	DESCRIPTION
ramp	flc1hs(t[1/s]-1e-2,1e-2)	Smooth step function
uin1	-vmax1*4*s*(1-s)*ramp	Velocity profile, inlet 1
vin2	-vmax2*4*s*(1-s)*ramp	Velocity profile, inlet 2

6 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 Open the **Subdomain Settings** dialog box for the **Level Set Two-Phase Flow, Laminar** application mode, either from the **Physics** menu, or using the **Model Tree**.

2 Select all subdomains by selecting one subdomain and then pressing Ctrl+A.

3 Enter the following values in the different edit fields:

QUANTITY	VALUE/EXPRESSION
ρ_1	`rho1`
η_1	`eta1`
ρ_2	`rho2`
η_2	`eta2`

4 Click the **Sources/Sinks** tab. In the σ edit field, type `sigma`.

5 Click the **Init** tab. Select Subdomain 3 only. As **Initial fluid in this domain**, select **Fluid 2**.

6 Click **OK** to close the dialog box.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundary 7 and select the **Interior boundaries** check box. From the **Boundary condition** list, select **Initial fluid interface**.

3 Set the conditions on the other boundaries according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARIES 2–4, 6, 9–11	BOUNDARY 8	BOUNDARY 12
Boundary type	Outlet	Wall	Inlet	Inlet
Boundary condition	Normal stress	Wetted wall	Velocity	Velocity
f_0	0			
ϕ_0			1	0
u_0			0	`uin1`
v_0			`vin2`	0
p_0				
θ		`3*pi/4`		
β		`h`		

4 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Mapped Mesh Parameters**. Click the **Boundary** tab.

2 While pressing Ctrl, select the Boundaries 1, 4, and 5. Select the **Constrained edge element distribution** check box and type `10` in the **Number of edge elements** edit field.

3. Select Boundary 2. Select the **Constrained edge element distribution** check box and type `100` in the **Number of edge elements** edit field.
4. Finally, select Boundary 6. Select the **Constrained edge element distribution** check box and type `30` in the **Number of edge elements** edit field.
5. Click the **Remesh** button. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

First, you must determine the time suitable for initialization, which is given by the expression $5\varepsilon/\gamma$:

1. From the **Solve** menu, select **Get Initial Value**.
2. Click the **Plot Parameters** button on the Main toolbar.
3. Click the **Surface** tab. On the **Surface Data** page, type `5*epsilon_chns/gamma_chns` in the **Expression** edit field.
4. Click **OK**.

The plot shows that a suitable time for initialization is $5 \cdot 10^{-5}$ s.

1. Click the **Solver Parameters** button on the Main toolbar.
2. In the **Times** edit field, type `5e-5`, then click **OK**.
3. Click the **Solve** button on the Main toolbar.
4. Click the **Plot Parameters** button. Type `phi` in the **Expression** edit field, then click **OK**.

The plot shows your initialized level set function. Now continue with the fluid flow calculation.

1. From the **Physics** menu, select **Properties**.
2. From the **Analysis type** list, select **Transient**. Click **OK**.
3. Click the **Solver Manager** button on the Main toolbar.
4. Click the **Store Solution** button. Select only **5e-5** in the dialog box that appears, then click **OK**.
5. In the **Initial value** area, click the **Stored solution** button and select **5e-5** from the **Solution at time** list.
6. Click **OK**.
7. Click the **Solver Parameters** button on the Main toolbar.
8. In the **Times** edit field, type `0:0.5e-2:0.08`, then click **OK**.
9. Click the **Solve** button on the Main toolbar.

10 In the **Progress-Solve Problem** window, click the **Log** tab. When the solver reaches $t = 0.025$ s it starts to take small time steps. This is an indication that the level set parameter γ has not been assigned a suitable value. Therefore, click the **Progress** tab, then click both **Stop** buttons. Click **Close**.

11 Click the **Plot Parameters** button on the Main toolbar.

12 On the **Surface** page, select **Velocity field** from the **Predefined quantities** list.

13 Click the **General** tab. From the **Solution at time** list, select **0.025**. Click **OK**.

The maximal velocity is a suitable value for the level set parameter γ. The plot shows a maximal velocity of about 0.028 m/s, which is significantly lower than γ. By default, γ is 1 m/s.

1 Open the **Subdomain Settings** dialog box. Select all subdomains, then click the **Level Set** tab. In the γ edit field, type `0.03`, then click **OK**.

2 Click the **Solve** button on the Main toolbar.

The solver now runs better, but eventually starts to become slow. Click the **Stop** button when this occurs (after 0.04 s). As you can see, the maximum velocity now exceeds 0.03 m/s, and your value for γ is too low. Therefore, change γ to 0.1. Also, add artificial diffusion to the momentum equation for increased stability.

1 From the **Physics** menu, select **Subdomain Settings**.

2 In the γ edit field, type `0.1`.

3 On the **Sources/Sinks** page, click the **Artificial Diffusion** button.

4 Select the **Streamline diffusion** check box, then select **Anisotropic Diffusion** from the list. Click **OK** to close the **Artificial Diffusion** dialog box.

5 Click **OK** to close the **Subdomain Settings** dialog box.

6 Click the **Solve** button on the Main toolbar. The solver needs approximately half an hour to calculate the solution until the final time.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Surface** page, select **Volume fraction of fluid 2** from the **Predefined quantities** list.

3 On the **Streamline** page, select the **Streamline plot** check box. Select **Velocity field** from the **Predefined quantities** list.

4 From the **Streamline plot type** list, select **Uniform density**. In the **Separating distance** edit field, type `0.02`.

5 On the **Animate** page, click the **Start Animation** button.

6 Click **OK** to close the **Plot Parameters** dialog box.

Finally, calculate the radius of the droplet:

1 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**.

2 Select all subdomains and specify an integration coupling variable with the **Name** `area` and the **Expression** `(phi>0.5)*(x<-3e-4)`. Click **OK**.

3 From the **Solve** menu, select **Update Model**.

4 From the **Postprocessing** menu, select **Global Variables Plot**.

5 Type `2*sqrt(area/pi)` in the **Expression** edit field. Click the **Add Entered Expression** (**>**) button, then click **OK**.

The plot shows that the diameter of the droplet is approximately $1.45 \cdot 10^{-4}$ m.

Bubble Column Reactor

Introduction

This example illustrates multiphase flow modeling in a bubble column reactor. The reactor is filled with water and gas bubbles are injected from the bottom. Due to buoyancy, the bubbles rise, inducing a circulating motion of the liquid. Furthermore, as the bubbles rise through the water, gas dissolves from the bubbles into the liquid.

The Bubbly Flow application mode tracks the averaged phase concentration rather than each bubble in detail, and is therefore well suited to model the flow. You can easily couple the multiphase flow with a mass transport equation to model the transport of gas dissolved in the liquid.

Model Definition

This example treats a bubble column reactor of height 2.1 m and a diameter of 0.2 m. A cylindrical wall of diameter 0.1 m is placed within the tank to prevent gas from moving to the outer parts of the tank. Figure 6-15 and Figure 6-16 depict the geometry with boundary conditions for the corresponding axisymmetric model. Note that the scales of the r- and z-axes are different in the figures.

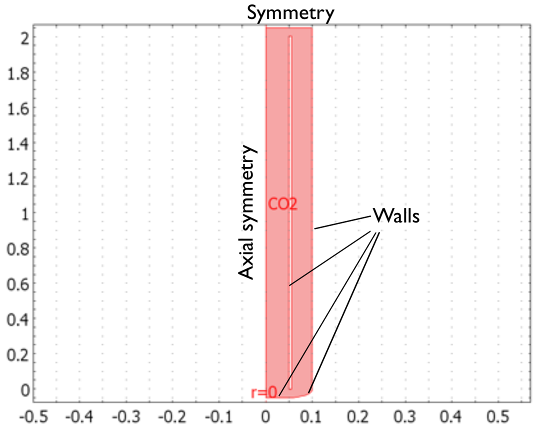


Figure 6-15: Geometry and boundary conditions, liquid phase.

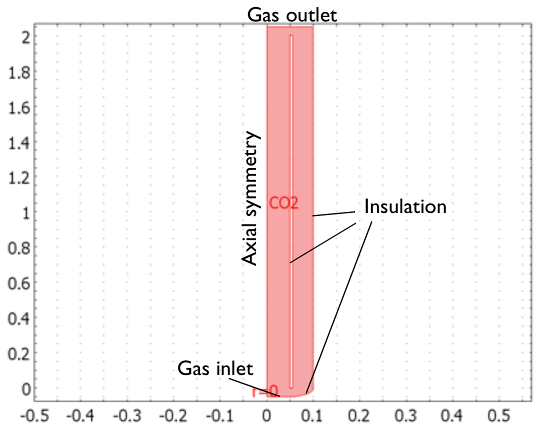


Figure 6-16: Boundary conditions, gas phase.

The Bubbly Flow application mode makes it easy to set up a multiphase flow model for gas bubbles rising through a liquid. It solves for the liquid velocity, the pressure, and the volume fraction of the gas phase. The momentum transport equation for the mixture is

$$\phi_l\rho_l\frac{\partial \mathbf{u}_l}{\partial t} + \phi_l\rho_l\mathbf{u}_l \cdot \nabla\mathbf{u}_l = -\nabla p + \nabla \cdot [\phi_l\eta_l(\nabla\mathbf{u}_l + \nabla\mathbf{u}_l{}^T)] + \phi_l\rho_l\mathbf{g} \qquad (6\text{-}17)$$

where ϕ_l denotes the volume fraction of the liquid phase (m^3/m^3), ρ_l the liquid's density (kg/m^3), $\mathbf{u}_l$ the liquid phase velocity (m/s), p pressure (Pa), η_l the liquid's dynamic viscosity (Pa·s) and $\mathbf{g}$ the gravity vector (m/s^2).

For low gas concentrations, the application mode approximates the mass conservation equation by

$$\nabla \cdot \mathbf{u}_l = 0$$

For the gas phase transport, the application mode solves the equation

$$\frac{\partial \rho_g\phi_g}{\partial t} + \nabla \cdot (\phi_g\rho_g\mathbf{u}_g) = -m_{gl}$$

where $\mathbf{u}_g$ is the gas phase velocity (m/s), ρ_g is the gas density (kg/m^3), ϕ_g gives the volume fraction of gas, and m_{gl} refers to the mass transfer rate from gas to liquid ($kg/(m^3 \cdot s)$). The gas density is calculated from the ideal gas law:

$$\rho_g = \frac{(p + p_{ref})M}{RT}$$

where M is the molecular weight of the gas (kg/mol), R denotes the ideal gas constant (8.31 J/(mol·K)), p_{ref} is a reference pressure ($1 \cdot 10^5$ Pa), and T the temperature (K). The liquid volume fraction is calculated from

$$\phi_l = 1 - \phi_g$$

and the gas velocity from

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip}$$

where $\mathbf{u}_{slip}$ is the relative velocity between gas and liquid.

For bubbles rising through a liquid, due to buoyancy, it is valid to assume that the pressure forces approximately balance the viscous drag forces on a gas bubble. The relative velocity between the two phases can then be determined from the relation

$$\frac{3}{4}\frac{C_d}{d_b}\rho_l|\mathbf{u}_{slip}|\mathbf{u}_{slip} = -\nabla p \tag{6-18}$$

where C_d is the drag coefficient (dimensionless) and d_b bubble diameter (m). For large ($d_b > 2$ mm) gas bubbles in water, an empirical expression for the drag coefficient is

$$C_d = \frac{0.622}{\frac{1}{\text{Eö}} + 0.235} \tag{6-19}$$

$$\text{Eö} = \frac{g\rho_l d_b^2}{\sigma} \tag{6-20}$$

Here, g denotes the magnitude of the gravity vector (m/s^2) and σ the surface tension coefficient (N/m). The slip model defined by Equation 6-18, Equation 6-19, and Equation 6-20 is available as one of the predefined slip models in the application mode. You only need to give values for the physical parameters of gravity, density, bubble diameter and the surface tension coefficient. From these values, the application mode automatically calculates the slip velocity.

TURBULENCE MODELING

For turbulent flows, you can use the k-ε turbulence model and solve for the averaged velocity field. The turbulence model relevant for bubbly flows is similar to the single-phase k-ε turbulence model. However, there are additional source terms in order to account for the extra production of turbulence due to the relative motion between the gas bubbles and the liquid.

When you use the k-ε turbulence model, COMSOL Multiphysics adds a turbulent viscosity to the physical viscosity in the momentum transport equation. The turbulent viscosity is modeled by

$$\eta_T = \rho_l C_\mu \frac{k^2}{\varepsilon} \tag{6-21}$$

where C_μ is a model constant.

The transport equation for the turbulent kinetic energy k is

$$\rho_l \frac{\partial k}{\partial t} - \nabla \cdot \left[\left(\eta + \frac{\eta_T}{\sigma_k}\right)\nabla k\right] + \rho_l \mathbf{u}_l \cdot \nabla k = \frac{1}{2}\eta_T(\nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T)^2 - \rho_l \varepsilon + S_k \tag{6-22}$$

and the evolution of the turbulent energy's dissipation rate ε is governed by

$$\begin{aligned} \rho_l \frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left[\left(\eta + \frac{\eta_T}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + \rho_l \mathbf{u}_l \cdot \nabla \varepsilon &= \\ = \frac{1}{2}C_{\varepsilon 1}\frac{\varepsilon}{k}\eta_T(\nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T)^2 - \rho_l C_{\varepsilon 2}\frac{\varepsilon^2}{k} + \frac{\varepsilon}{k}C_\varepsilon S_k & \end{aligned} \tag{6-23}$$

The term S_k accounts for the bubble induced turbulence and is given by

$$S_k = -C_k \phi_g \nabla p \cdot \mathbf{u}_{\mathrm{slip}}$$

For the gas phase's velocity field, a drift velocity is added:

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{\mathrm{slip}} + \mathbf{u}_{\mathrm{drift}}$$

where

$$\mathbf{u}_{\mathrm{drift}} = -\frac{\eta_T}{\rho_l}\frac{\nabla \phi_g}{\phi_g}$$

In the Bubbly Flow application mode, you can easily switch on and off the k-ε turbulence model, either with or without the bubble induced turbulence term S_k.

DISSOLUTION OF GAS

You can use the two-film theory to account for the dissolution of gas. The application mode then calculates the mass transfer rate according to

$$m_{\mathrm{gl}} = k\left(\frac{p + p_{\mathrm{ref}}}{H} - c\right)\mathrm{Ma}$$

$$a = (4n\pi)^{1/3}(3\phi_{\mathrm{g}})^{2/3}$$

In the equations, k represents the mass transfer coefficient (m/s), H represents Henrys constant (Pa·m^3/mol), c the concentration of gas dissolved in liquid (mol/m^3), M the molecular weight (kg/mol), and a the interfacial area per volume (m^2/m^3). The interfacial area per volume depends on the volume fraction of gas but also on the number of bubbles per volume, n (1/m^3). If you select the two-film theory model, the application mode automatically also solves for n. It assumes that bubbles cannot split or merge, while the size of each bubble can vary:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}_{\mathrm{g}}) = 0$$

The transport equation for dissolved gas is

$$\frac{\partial c}{\partial t} + \nabla c \cdot \mathbf{u}_{\mathrm{l}} = \nabla \cdot (D\nabla c) + \frac{m_{\mathrm{gl}}}{M} \qquad (6\text{-}24)$$

where D is the diffusion coefficient (m^2/s). When you use a turbulence model for the flow field, the diffusion coefficient is

$$D = \frac{\eta_T}{\rho_{\mathrm{l}}}$$

In this example, you make the approximation that the flow field and the bubble number density, n, are not affected by the dissolution of gas. Therefore, you can first solve for the flow without inclusion of the dissolution of gas. Then you solve for the volume fraction of gas and the concentration of the dissolved gas, accounting for the mass transfer. The transport equation for the dissolved gas (Equation 6-24) is not included in the Bubbly Flow application mode, but you can easily set up the equation using a Convection and Diffusion application mode.

Results and Discussion

In this example, you first make a time-dependent simulation with no turbulence and without taking into account the dissolution of gas. You then continue with a turbulent, stationary calculation to obtain the time-averaged velocity field and volume fractions, both with and without the inclusion of bubble induced turbulence. Note that having the laminar solution as an initial guess to the turbulent problem makes it much easier for the solver to converge in this case. Finally, you can account for the dissolution of gas.

Figure 6-17 shows results of the transient simulation, with no mass transfer from gas to liquid and without any turbulence modeling.The figures show the gas volume fraction and the velocity of the liquid phase.

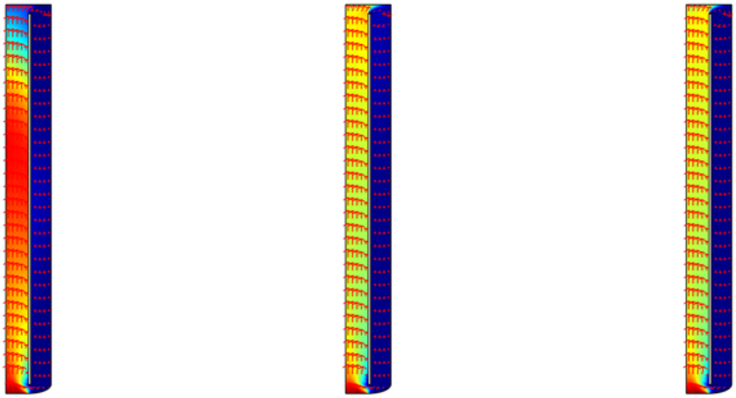


Figure 6-17: Results of a time dependent simulation with no turbulence at t = 5 s, 10 s, and 20 s. The surface plot shows the gas volume fraction and the arrows the liquid velocity.

By using a turbulence model, it is possible to calculate the time-averaged velocity and gas concentration. The standard k-ε turbulence model for single phase flow can also be used for multiphase flows. In this case, you would then completely neglect the fact that bubbles produce turbulence as they rise through the liquid. The k-ε turbulence model can also be modified so that it does account for the effect of bubble-induced turbulence. Figure 6-18 and Figure 6-19 show results using the k-ε turbulence model with and without bubble-induced turbulence. The turbulent viscosity differs significantly for the two models, but the flow with respect to the speed of the liquid and the gas concentration is similar for both cases.

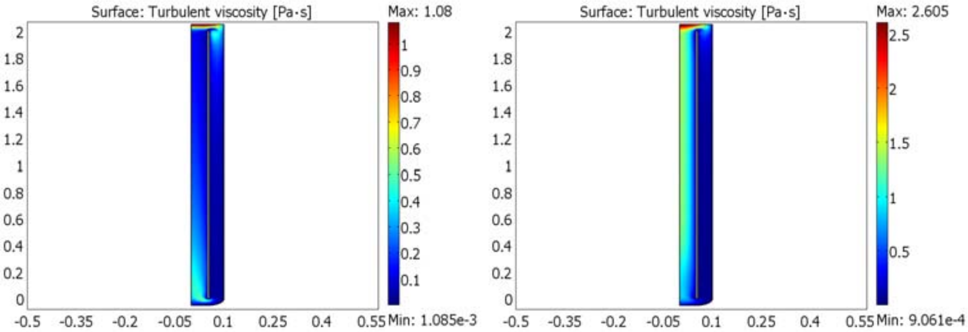


Figure 6-18: Turbulent viscosity when bubble induced turbulence is not (left) and is (right) accounted for. The bubble induced turbulence results in significantly more turbulent viscosity at the center of the bubble column.

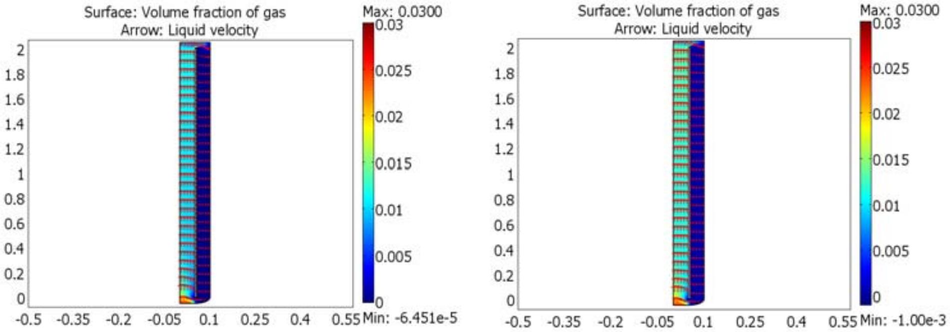


Figure 6-19: Liquid velocity and volume fraction of gas using single phase k-ε (left) and k-ε with bubble induced turbulence (right). Even though the turbulent viscosity differs significantly for the two turbulence models, the gas concentration and velocities are similar for both models.

If gas dissolves into the liquid, the gas volume fraction decreases, which Figure 6-20 clearly shows. Finally, Figure 6-21 shows snapshots of the concentration of dissolved gas at t = 0 s, 10 s, and 20 s. Because the liquid circulates in the tank, the dissolved species is rapidly distributed within the entire tank.

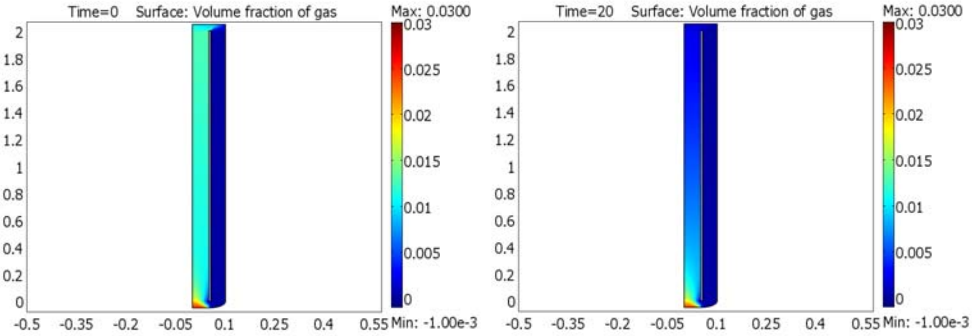


Figure 6-20: The volume fraction of gas initially (left) and after 20 s (right), accounting for the dissolution of gas.

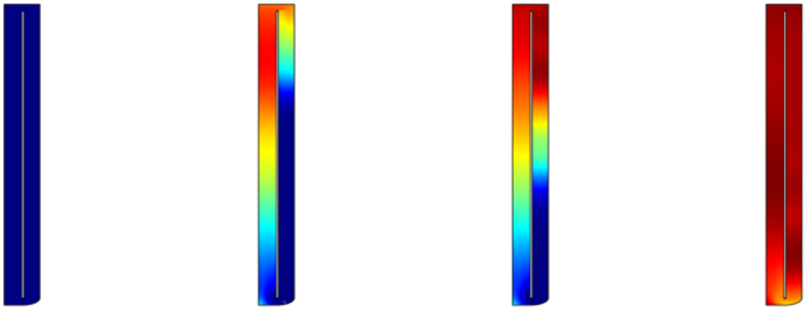


Figure 6-21: Snapshots showing the concentration of gas dissolved in liquid at t = 0 s, 5 s, 10 s, and 20 s. The four figures all use the same color scale with a maximum value of 0.83 mol/m^3.

Modeling in COMSOL Multiphysics

To model the two-phase fluid flow, use the Bubbly Flow application mode. In order to account for gas dissolution, you need to add a Convection and Diffusion application mode. It is easy to switch from a laminar to a turbulent fluid flow model by selecting the turbulence model in the **Application Mode Properties** dialog box.

Model Library path: `Chemical_Engineering_Module/Multiphase_Flow/bubble_column`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 From the **Space dimension** list, select **Axial symmetry (2D)**.

2 Select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Bubbly Flow, Laminar>Transient analysis**.

3 Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu, select **Specify Objects>Rectangle**.

2 Enter values according to the following table:

WIDTH	HEIGHT	BASE	r	z
0.005	2	Corner	0.05	0

3 Click **OK**.

4 Click the **Zoom Extents** button on the Main toolbar.

5 From the **Options** menu, select **Axes/Grid Settings**.

6 Go to the **Grid** tab and clear the **Auto** check box.

7 Type `0.05` in the **r spacing** as well as the **z spacing** edit fields.

8 Click **OK**.

9 On the Draw toolbar, click the **Line** button. Click once at each of the following coordinates: (0.1, 0), (0.1, 2.05), (0, 2.05), (0, –0.05), and (0.05, –0.05). The coordinates are displayed in the lower left corner of the graphical user interface.

10 Click **2nd Degree Bézier Curve**, also on the Draw toolbar. Click the coordinates (0.05, –0.05), (0.1, –0.05), and (0.1, 0).

11 Right-click anywhere to create a geometry of the drawn lines and curves.

12 From the **Draw** menu, select **Specify Objects>Circle**. Enter settings according to the following table:

RADIUS	r	z
`0.0025`	`0.0525`	`2`

13 Click **OK**.

14 From the **Edit** menu, select **Copy**. Alternatively, press Ctrl+C.

15 Also from the **Edit** menu, select **Paste**, or press Ctrl+V.

16 Type `-2` in the **z** edit field in the dialog box that appears. Click **OK**.

17 On the Draw toolbar, click the **Create Composite Object** button. In the **Set formula** edit field, type `CO1-R1-C1-C2`.

18 Click **OK**.

19 In order to view the geometry with different scales on the r- and z-axes, double-click **EQUAL** in the status bar at the bottom of the user interface, then click the **Zoom Window** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1. Type `28e-3` in the **Molecular weight of gas** edit field and `-9.81` in the z-component edit field for **Gravity** (the one to the right).

3 Click the **Artificial Diffusion** button.

4 On the **Momentum Transport** page, select the **Isotropic diffusion** check box and type `0.05` in the corresponding edit field.

5 Click **OK**.

6 On the **Slip Model** page, select **Pressure/drag balance**.

7 Select **Large bubbles** from the list. Type `2e-3` in the **Bubble diameter** edit field.

8 Click **OK**.

Point Settings

1 From the **Physics** menu, select **Point Settings**.

2 Select Point 11 and select the **Point constraint** check box. Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundary 1. From the **Boundary type** list, select **Symmetry boundary**, and from the **Boundary condition** list, select **Axial symmetry**.

3 Select Boundary 3. From the **Boundary type** list, select **Symmetry boundary**, and from the **Boundary condition** list, select **Symmetry**.

4 Click the **Gas Phase** tab.

5 For Boundary 1, set the boundary condition **Axial symmetry**.

6 Select Boundary 2 and select the boundary condition **Gas flux**. In the $\mathbf{N}_\rho$ edit field, type `0.01`.

7 Set the boundary condition for Boundary 3 to **Gas Outlet**.

8 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 On the **Subdomain** page, set the **Maximum element size** to `0.02`.

3 On the **Boundary** page, select Boundary 7. Set the **Maximum element size** to `0.005`.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Times** edit field, type `0:1:20`.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar to start the calculation.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 Go to the **Arrow** tab and select the **Arrow plot** check box. In the **r points** edit field, type `10`, and in the **z points** edit field, type `30`.

3 Click **OK** to plot the right most plot of Figure 6-17.

Proceed with a turbulent-flow simulation.

PHYSICS SETTINGS

1 From the **Physics** menu, select **Properties**.

2 From the **Analysis type** list, select **Stationary**.

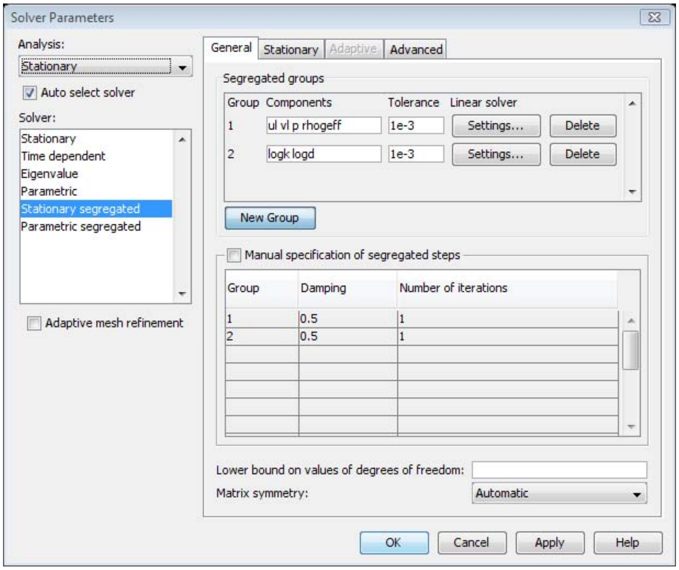
3 From the **Turbulence model** list, select **k-ε without bubble induced turbulence**.

4 Click **OK**.

COMPUTING THE SOLUTION

When solving stationary problems consisting of several variables, you can use the segregated solver to reduce the memory resources used by the software and to more easily obtain convergence. For the segregated solver, you need to divide the dependent variables into different groups. The velocity and pressure variables must always belong to the same group, and usually it is optimal to define a separate group for the turbulence variables.

1. Click the **Solver Manager** button on the Main toolbar.
2. In the **Initial value** area on the **Initial Value** page, select **Current solution**. From the corresponding **Solution at time** list, select **20**.
3. Click **OK**.
4. Click the **Solver Parameters** button.
5. From the **Solver** list, select **Stationary segregated**.
6. Click the **New Group** button. There should now be two groups, one containing the variables `ul vl p rhogeff` and one with `logk logd`.



Analysis: Stationary

☑ Auto select solver

Solver:
- Stationary
- Time dependent
- Eigenvalue
- Parametric
- Stationary segregated
- Parametric segregated

☐ Adaptive mesh refinement

Segregated groups

Group	Components	Tolerance	Linear solver
1	ul vl p rhogeff	1e-3	Settings...
2	logk logd	1e-3	Settings...

☐ Manual specification of segregated steps

Group	Damping	Number of iterations
1	0.5	1
2	0.5	1

Lower bound on values of degrees of freedom:

Matrix symmetry: Automatic

7. Click **OK**.
8. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Surface** page, click the **Range** button.

3 Clear the **Auto** check box and type `0.03` in the **Max** edit field. Click **OK**.

4 Click **Apply** to view the left plot in Figure 6-19.

5 From the list of **Predefined quantities,** select **Bubbly Flow>Turbulent viscosity**.

6 Click the **Range** button, select the **Auto** check box, and click **OK**.

7 On the **Arrow** page, clear the **Arrow plot** check box.

8 Click **OK** to create the left plot of Figure 6-18.

Next, account for additional turbulence induced by the bubbles.

PHYSICS SETTINGS

1 From the **Physics** menu, select **Properties**.

2 From the **Turbulence model** list, select **k-ε with bubble induced turbulence**.

3 Click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

You should now obtain the right plot of Figure 6-18. To create the right plot of Figure 6-19, perform the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Surface** page, select **Bubbly Flow>Volume fraction of gas** from the **Predefined quantities** list.

3 Click the **Range** button. Clear the **Auto** check box and type `0.03` in the **Max** edit field and `-0.001` in the **Min** edit field. Click **OK**.

4 On the **Arrow** page, select the **Arrow plot** check box.

5 Click **OK**.

Finally, account for dissolution of gas into the liquid phase.

PHYSICS SETTING

1 Open the **Subdomain Settings** dialog box.

2 Select Subdomain 1, then go to the **Mass Transfer** page. Select **Two-film theory model** from the list.

3 In the **H** edit field, type `2.9e3`, in the **k** edit field, type `0.001`, and in the **c** edit field, type `c`.

4 Click **Apply**.

5 Go to the **Physics** tab and click the **Artificial Diffusion** button.

6 On the **Gas Transport** tab, type `10000` in the **Scale, bubble density** edit field.

7 Click **OK**.

8 Click **OK**.

9 From the **Physics** menu, select **Boundary Settings**.

10 Go to the **Gas Phase** tab, select Boundary 2, and type `10000` in the $\mathbf{N_n}$ edit field. Click **OK**.

11 From the **Multiphysics** menu, select **Model Navigator**.

12 Select **Chemical Engineering Module>Mass Transport>Convection and Diffusion**.

13 Click **Add** and then **OK**.

14 Open the **Subdomain Settings** dialog box for the **Convection and Diffusion** application mode, either from the **Physics** menu or from the **Model Tree**.

15 Type the following expressions in the edit fields:

D (ISOTROPIC)	R	U	V
`etaT_chbf/rhol_chbf`	`masstrans_chbf/M_chbf`	`ul`	`vl`

16 Click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Manager** button on the Main toolbar.

2 In the **Initial value** area on the **Initial Value** page, select **Initial value expression**.

3 In the **Values of variables not solved for and linearization point** area, select **Current solution**.

4 On the **Solve For** page, select **nbub** only. Click **OK**.

5 Click the **Solver Parameters** button. Select **Stationary segregated** from the **Solver** list.

6 Click the **Delete** button for Group 2 and 3. Replace the expression in the **Components** edit field for Group 1 by `nbub`.

7 Click **OK**.

8 Click the **Solve** button.

9 In the **Model Tree**, right-click **Bubbly flow (chbf)** and select **Properties**.

10 From the **Analysis type**, select **Transient**. Click **OK**.

11 Right-click **Convection and Diffusion (chcd)** in the **Model Tree** and select **Properties**.

12 From the **Analysis type** list, select **Transient**. Click **OK**.

13 Click the **Solver Manager** button.

14 On the **Solve For** page, Ctrl-click to select both **rhogeff** and **c**.

15 Click the **Initial Value** tab.

16 In the **Initial value** area, select **Current solution**.

17 Click **OK**.

18 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Perform the following steps to create animations corresponding to the snapshots shown in Figure 6-20 and Figure 6-21.

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, clear the **Arrow plot** check box in the **Plot type** area.

3 Click the **Animate** page.

4 Select the **Use camera settings from main window** check box. Click the **Start Animation** button to see how the gas volume fraction changes with time due to dissolution of gas.

5 Click the **Surface** tab. From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

6 Click the **Range** button. Select the **Auto** check box and click **OK**.

7 Return to the **Animate** page and click the **Start Animation** button to create a movie showing how the concentration of the dissolved gas evolves in time.

Contaminant-Removal from Wastewater in a Secondary Clarifier

Introduction

Wastewater treatment is a several-step process for removing contaminants. First, large, solid particles are removed through sedimentation, flotation, and filtration. In a second step, biological treatment causes the smaller particles to aggregate, forming so called flocs. These flocs can more easily be removed, for instance by sedimentation. The present example studies the separation of flocs from water in a circular secondary clarifier. To model the turbulent multiphase flow in the tank, the Mixture Model application mode is used.

Model Definition

In a circular secondary clarifier, flocs are removed from water by sedimentation. Gravity causes the flocs to fall toward the tank bottom. However, the turbulent flow in the tank tends to mix the phases together, and thus has a negative effect on the separation. The object of this example is to study the complex turbulent multiphase flow within a circular secondary clarifier.

Figure 6-22 shows the geometry of the clarifier. The incoming sludge, consisting of a mixture of solid flocs and water, enters through the inlet in the middle of the tank. The tank contains two outlets. One is located at the center of the tank bottom. The purpose of the outlet is to remove the sedimented flocs from the tank. There is also a peripheral outlet for the purified water as shown in the figure. Figure 6-23 shows the corresponding axisymmetric 2D model. For simplicity, you can model the flocs as circular solid particles of equal size.

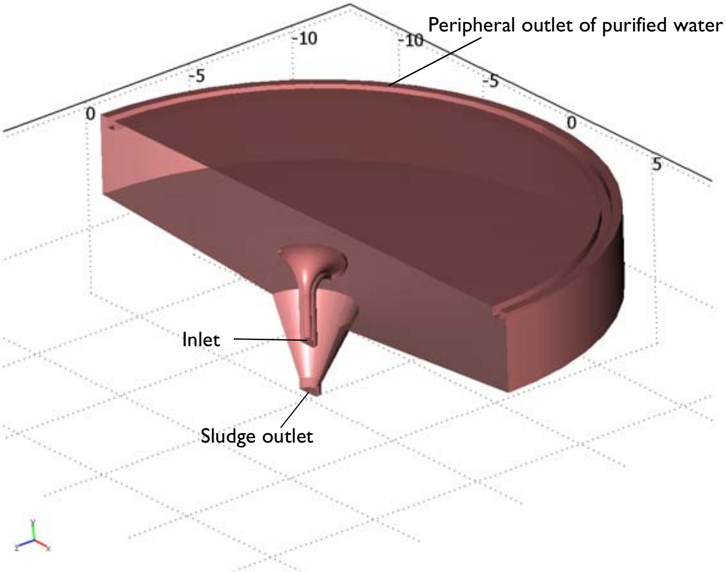


Figure 6-22: Cross section of the circular clarifier.

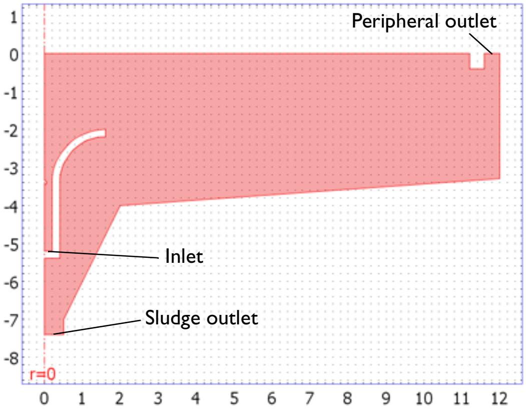


Figure 6-23: Axisymmetric representation of the clarifier geometry.

To solve for the mixture velocity, pressure and the phase volume fractions, you can use the Mixture Model application mode. The mixture model is a multiphase flow model, particularly well suited for suspensions, that is, mixtures of solid particles and liquid. Based on momentum balance and mass conservation of each phase, the mixture model uses the following equations:

$$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p - \nabla\cdot(\rho c_d(1-c_d)\mathbf{u}_{\mathrm{slip}}\mathbf{u}_{\mathrm{slip}}) + \nabla\cdot\tau_{\mathrm{Gm}} + \rho\mathbf{g}$$

$$(\rho_c - \rho_d)[\nabla\cdot(\phi_d(1-c_d)\mathbf{u}_{\mathrm{slip}} - D_{md}\nabla\phi_d)] + \rho_c(\nabla\cdot\mathbf{u}) = 0$$

$$\frac{\partial}{\partial t}(\phi_d\rho_d) + \nabla\cdot(\phi_d\rho_d\mathbf{u}_d) = 0$$

Here $\mathbf{u}$ denotes mixture velocity (m/s), ρ mixture density (kg/m^3), p pressure (Pa), c_d mass fraction of the solid phase (kg/kg). Furthermore, $\mathbf{u}_{\mathrm{slip}}$ is the relative velocity between the two phases (m/s), τ_{Gm} the sum of viscous and turbulent stress (kg/(m·s^2)), and $\mathbf{g}$ the gravity vector (m/s^2). The mixture velocity (m/s) is defined as

$$\mathbf{u} = \frac{\phi_c\rho_c\mathbf{u}_c + \phi_d\rho_d\mathbf{u}_d}{\rho}$$

where ϕ_c and ϕ_d denote the volume fractions of the liquid (continuous) phase and the solid (dispersed) phase (m^3/m^3), respectively, $\mathbf{u}_c$ the liquid-phase velocity (m/s), $\mathbf{u}_d$ the solid-phase velocity (m/s), ρ_c the liquid-phase density (kg/m^3), ρ_d the solid-phase density (kg/m^3), and ρ the mixture density (kg/m^3). The relation between the velocities of the two phases is defined by

$$\mathbf{u}_d - \mathbf{u}_c = \mathbf{u}_{cd} = \mathbf{u}_{\mathrm{slip}} - \frac{D_{md}}{(1-c_d)\phi_d}\nabla\phi_d$$

For the slip velocity, you can use the Hadamard-Rybczynski drag law for solid particles. In the Mixture Model application mode, the Hadamard-Rybczynski drag is available as a predefined model for the slip velocity. The application mode then calculates the slip velocity according to

$$\mathbf{u}_{\mathrm{slip}} = -\frac{(\rho-\rho_d)d_d^2}{18\rho\eta}\nabla p$$

where d_d denotes the diameter of the solid particles (m). For the mixture density and viscosity, you use the following predefined expressions

$$\eta = \eta_c\left(1 - \frac{\phi_d}{\phi_{\max}}\right)^{-2.5\phi_{\max}}$$

$$\rho = \phi_c\rho_c + \phi_d\rho_d$$

To determine the turbulent viscosity, use the k-ε turbulence model. The application mode then calculates the particle dispersion coefficient D_{md} ($\mathrm{m^2/s}$) from

$$D_{md} = \frac{\eta_T}{\rho\sigma_T}$$

where η_T is the turbulent viscosity (Pa·s) and σ_T is the (dimensionless) turbulent Schmidt number, in this example 0.35.

Note that the Mixture Model application mode automatically sets up all the modeling equations. You only need to provide the physical properties of the two phases according to the following table:

QUANTITY	VALUE	DESCRIPTION
ρ_c	1000 kg/m^3	Liquid phase density
η_c	$1\cdot10^{-3}$ Pa·s	Liquid phase viscosity
ρ_d	1100 kg/m^3	Solid phase density
d_d	$2\cdot10^{-4}$ m	Diameter of solid particles
g_z	-9.82 m/s^2	z-component of gravity vector
ϕ_{max}	0.62	Solid phase maximum packing concentration
v_{in}	1.25 m/s	Inlet velocity
v_{out}	-0.05 m/s	Outlet velocity
ϕ_{din}	0.003	Volume fraction of solid phase of incoming sludge

BOUNDARY CONDITIONS

At the sludge inlet, the velocity is fixed to 1.25 m/s and the solid phase concentration is 0.003. The velocity is also fixed at the bottom outlet, while a constant pressure is set on the peripheral outlet. Symmetry conditions apply at the water surface and at the axial symmetry line. Logarithmic wall functions with insulation of the solid phase hold for all solid walls.

INITIAL CONDITIONS

Initially, the velocity as well as the solid phase volume fraction is zero in the entire clarifier.

Results and Discussion

Figure 6-24 shows streamlines of the mixture velocity and the solid phase concentration, measured in kg/m^3, after 24 hours. At this point, the flow has reached a steady state. Because turbulence modeling is used, you can interpret the velocity as the time-averaged mixture velocity. As expected, the solid particles fall toward the bottom. However, the turbulent fluctuations results in diffusion of the solid phase that has a negative effect on the separation.

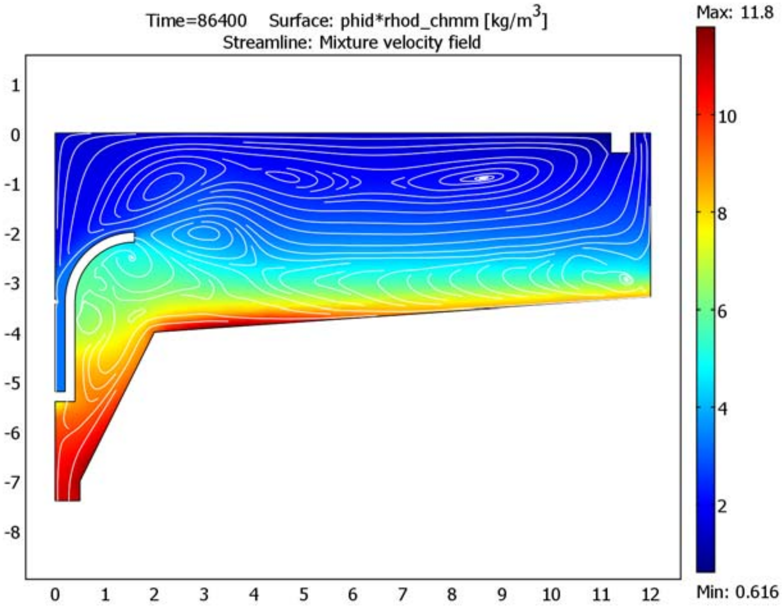


Figure 6-24: Velocity streamlines and solid phase concentration after 24 hours, when the flow has reached a steady state solution.

Figure 6-25 shows the solid phase volume fraction at three points, namely close to the inlet and close to the two outlets. The figure clearly shows that the solid phase volume fraction is about three times lower at the purified water outlet, compared to the incoming mixture.

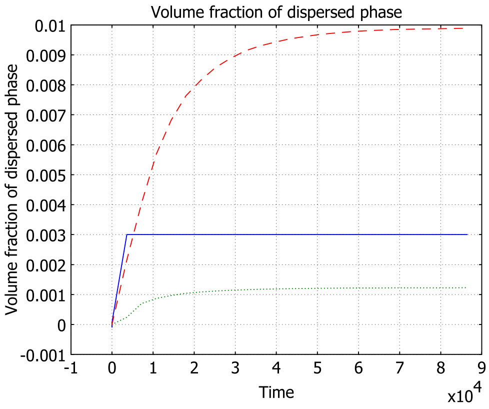


Figure 6-25: Comparison of the solid phase volume fraction close to the inlet (solid line), the sludge outlet (dashed line), and the peripheral outlet (dotted line).

The mass flux of the solid phase through the inlet is given by

$$M_{\text{in}} = \int_{\text{inlet}} |v_{\text{in}}|\phi_{\text{din}}\rho_d dS$$

and correspondingly for the outflow through the peripheral outlet

$$M_{\text{out}} = \int_{\text{outlet}} |v_{\text{out}}|\phi_{\text{dout}}\rho_d dS$$

The clarifier thus removes solid particles at a rate of $M_{\text{in}} - M_{\text{out}}$. Computing the removal rate from the results shows that the clarifier removes $0.518 - 0.151 = 0.367$ kg solid particles per second.

To further examine the performance of the clarifier, you can easily modify the model in several ways. You can, for instance, modify the geometry by adding baffles, changing the inlet and outlet velocities, increasing the solid phase volume fraction of the incoming sludge, or change the density and size of the solid particles.

Modeling in COMSOL Multiphysics

It is straightforward to set up a multiphase flow model with the Mixture Model application mode. To simplify the startup of the transient calculation, you can gradually increase the inlet and outlet velocity and the solid phase volume fraction at the inlet from zero to their constant values. For this purpose, use the built-in smooth step function `flc1hs(t,dt)`, which gradually increases from zero to one as `t` varies from `-dt` to `dt`.

Model Library path: `Chemical_Engineering_Module/Multiphase_Flow/sedimentation`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 From the **Space dimension** list, select **Axial symmetry (2D)**.

2 Select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Mixture Model, k-ε Turbulence Model>Transient analysis**.

3 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Expressions>Scalar Expressions**. Enter the following variables (the units and descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
`v_in`	`1.25*flc1hs(t[1/s],0.1)[m/s]`	`Inlet velocity`
`v_out`	`-0.05*flc1hs(t[1/s],0.1)[m/s]`	`Outlet velocity`
`phid_in`	`0.003*flc1hs(t[1/s],0.1)`	`Inlet solid phase volume fraction`

2 Click **OK**.

GEOMETRY MODELING

1 From the **Options** menu, select **Axes/Grid Settings**.

2 Type in the following values in the edit fields.

r MIN	*r* MAX	*z* MIN	*z* MAX
-1	13	-8	1

3 Go to the **Grid** tab and clear the **Auto** check box.

4 In both the **r spacing** and the **z spacing** edit fields, type `0.2`. Click **OK**.

5 On the Draw toolbar, click the **Line** button while pressing the Shift button on the keyboard. Enter the following settings in the dialog box that appears.

r	z	STYLE
`0 12 12 2 0.5 0.5 0`	`0 0 -3.3 -4 -7 -7.4 -7.4`	Closed polyline (solid)

6 Click **OK**.

7 Click the **Line** button once more, this time *without* pressing Shift.

8 Click at the following three coordinates in turn. Note that the coordinates are displayed in the lower left corner of the graphical interface.

COORDINATE 1	COORDINATE 2	COORDINATE 3
(0, -5.4)	(0.4, -5.4)	(0.4, -3.4)

9 On the Draw toolbar, click the **2nd Degree Bézier Curve**, then click the points with the following coordinates:

COORDINATE 1	COORDINATE 2
(0.4, -2.2)	(1.6, -2.2)

10 Click the **Line** button, and click on the point with coordinates (1.6, –2).

11 Click the **2nd Degree Bézier Curve**, the click the following coordinates:

COORDINATE 1	COORDINATE 2
(0.2, -2)	(0.2, -3.4)

12 Click the **Line** button and click on the coordinates:

COORDINATE 1	COORDINATE 2
(0.2, -5.2)	(0, -5.2)

13 Right-click anywhere in the drawing area to create a solid object.

14 Shift-click the **Ellipse/Circle (Centered)** button. Type in the following settings:

RADIUS	BASE	R	Z
`0.05`	Center	0	`-3.4`

15 Click **OK**.

16 Click the **Rectangle/Square** button and click on the two points (11.2, 0) and (11.6, –0.4) to draw a square. When you click the second point, the status bar should show **w=0.4, h=0.4**.

17 Click the **Create Composite Object** button on the Draw toolbar.

18 In the **Set formula** edit field, type `CO1-CO2-C1-R1`. Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1. In the **Dispersed phase** area, type `1100` in the ρ_d edit field.

3 Click the **Physics** tab. Type `2e-4` in the $\mathbf{d_d}$ edit field and `-9.82` in the $\mathbf{g_z}$ edit field.

4 Click the **Mixture Model** tab. From the **Slip model** list, select **Hadamard-Rybczynski, solid particles**.

5 Click the **Init** tab. Type `-8` in both the **logk(t_0)** and the **logd(t_0)** edit fields.

6 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 On the **Mixture** tab, apply the following boundary conditions:

SETTINGS	BOUNDARIES 1, 4, 6	BOUNDARY 5	BOUNDARY 2	BOUNDARY 17	BOUNDARY 7	ALL OTHERS
Boundary type	Symmetry boundary	Inlet	Outlet	Outlet	Wall	Wall
Boundary condition	Axial symmetry	Velocity	Velocity	Pressure	Slip	Logarithmic wall function
v		`v_in`	`v_out`			
L_T		`0.4*0.07`				
p				0		

The value for the turbulent length scale, 0.4·0.07, is based on the suggested value for turbulent flow through a pipe given in Table 5-2 in the *Chemical Engineering Module User's Guide*.

3 On the **Dispersed Phase** page, apply the following conditions; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 4, 6	BOUNDARY 5	BOUNDARIES 2, 17	ALL OTHERS
Boundary condition	Axial symmetry	Dispersed phase concentration	Dispersed phase outlet	Insulation/ Symmetry
ϕ_d^0		`phid_in`		

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Go to the **Subdomain** page and type `1.1` in the **Element growth rate** edit field.

3 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu, select **Solver Parameters**.

2 In the **Times** edit field, type `[-0.1:0.01:-0.01 0:3600:3600*24]`.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar to start the calculation.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Surface** page, type `phid*rhod_chmm` in the **Expression** edit field.

3 On the **Streamline** page, select the **Streamline plot** check box. Make sure **Mixture velocity field** is selected in the **Predefined quantities** list.

4 From the **Streamline plot type** list, select **Uniform density**. On the **Density** page, type `0.02` in the **Separating distance** edit field. Click the **Line Color** tab, select **Uniform Color** and click the **Color** button. Select the white color and click **OK**.

5 Click **OK** to produce the plot in Figure 6-24.

6 Click the **Animate** button on the Postprocessing toolbar to create a movie from the result. As you can see, a steady state solution has been reached.

7 Click the **Draw Points for Cross-Section Point Plot**, also on the Postprocessing toolbar. Double-click on **SNAP** in the status bar at the bottom of the user interface to disable the snap function. Click on a point close to the inlet, and two more points close to the two outlets. All points should lie within the computational domain.

8 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

9 On the **Point** page, verify that **Volume fraction of dispersed phase** is selected from the **Predefined quantities** list.

10 Click the **Line Settings** button. From the **Line style** list, select **Cycle**. Select the **Legend** check box, then click **OK**.

11 Click **OK**. In the plot that appears you can compare the solid phase volume fraction at the three different points (Figure 6-25).

Finally, calculate the inflow and outflow rates of the solid phase.

1. From the **Postprocessing** menu, choose **Boundary Integration**.
2. Select Boundary 5 (the inlet) and type `v*phid*rhod_chmm` in the **Expression** edit field. Select the **Compute surface integral (for axisymmetric modes)** check box.
3. Click **Apply**.

   The value of the integral, which gives the solid-particle inflow rate, is displayed in the message log below the drawing area (approximately 0.518 kg/s).
4. Return to the **Boundary Integration** dialog box and select Boundary 17 (the peripheral outlet). Click **OK** to get the solid-phase mass flux through the outlet (approximately 0.151 kg/s).

Two-Phase Flow Modeling of a Dense Suspension

Introduction

Liquid-solid mixtures (suspensions) are important in a variety of industrial fields, such as oil and gas refinement, paper manufacturing, food processing, slurry transport, and wastewater treatment. Several different modeling approaches have been developed, ranging from discrete, particle-based methods to macroscopic, semi-empirical two-phase descriptions. Particle-based methods are suitable when there is a limited number of solid particles. When, on the other hand, there are many particles, it is better to use a macroscopic, or averaged, model that tracks the volume fractions of the phases.

The following example illustrates how you can set up a macroscopic two-phase flow model in COMSOL Multiphysics using the Mixture Model application mode. The model is based on the “diffusive flux” model described in Refs. 1, 2, and 3, suitable for liquid-solid mixtures with high concentrations of solid particles. It accounts for not only buoyancy effects but also shear-induced migration; that is, the tendency of particles to migrate toward regions of lower shear rates.

The model simulates the flow of a dense suspension consisting of light, solid particles in a liquid placed between two concentric cylinders. The inner cylinder rotates while the outer is fixed.

Model Definition

A suspension is a mixture of solid particles and a liquid. The dynamics of a suspension can be modeled by a momentum transport equation for the mixture, a continuity equation, and a transport equation for the solid phase volume fraction. The Mixture Model application mode automatically sets up these equations. It uses the following equation to model the momentum transport:

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p-\nabla\cdot(\rho c_s(1-c_s)\mathbf{u}_{\mathrm{slip}}\mathbf{u}_{\mathrm{slip}})+\nabla\cdot[\eta(\nabla\mathbf{u}+\nabla\mathbf{u}^T)]+\rho\mathbf{g}$$

where $\mathbf{u}$ is the mass averaged mixture velocity (m/s), p denotes the pressure (Pa), $\mathbf{g}$ refers to the gravity vector (m/s^2), c_s is the dimensionless particle mass fraction, and

$\mathbf{u}_{\mathrm{slip}}$ gives the relative velocity between the solid and the liquid phases (m/s). Further, $\rho = (1-\phi_s)\rho_f + \phi_s\rho_s$ is the mixture density, where ρ_f and ρ_s are the pure-phase densities (kg/m^3) of liquid and solids, respectively, and ϕ_s is the solid-phase volume fraction (m^3/m^3). Finally, η represents the mixture viscosity (Ns/m^2) according to the Krieger-type expression

$$\eta = \eta_f\left(1-\frac{\phi_s}{\phi_{\max}}\right)^{-2.5\phi_{\max}} \qquad (6\text{-}25)$$

where η_f is the dynamic viscosity of the pure fluid and $\phi_{\max}$ is the maximum packing concentration.

The mixture model uses the following form of the continuity equation

$$(\rho_f-\rho_s)[\nabla\cdot(\phi_s(1-c_s)\mathbf{u}_{\mathrm{slip}})]+\rho_f(\nabla\cdot\mathbf{u}) = 0 \qquad (6\text{-}26)$$

The transport equation for the solid-phase volume fraction is

$$\frac{\partial\phi_s}{\partial t}+\nabla\cdot(\phi_s\mathbf{u}_s) = 0 \qquad (6\text{-}27)$$

The solid-phase velocity, $\mathbf{u}_s$, is given by $\mathbf{u}_s = \mathbf{u} + (1-c_s)\,\mathbf{u}_{\mathrm{slip}}$. Consequently, Equation 6-27 is equivalent to

$$\frac{\partial\phi_s}{\partial t}+\nabla\cdot(\phi_s\mathbf{u}+\phi_s(1-c_s)\mathbf{u}_{\mathrm{slip}}) = 0 \qquad (6\text{-}28)$$

Rao and others (Ref. 2) formulate the continuity equation and the particle transport in a slightly different way. Instead of the slip velocity, $\mathbf{u}_{\mathrm{slip}}$, they define a particle flux, $\mathbf{J}_s$ (kg /(m^2·s)), and write the continuity equation as

$$\nabla\cdot\mathbf{u} = \frac{\rho_s-\rho_f}{\rho_s\rho_f}(\nabla\cdot\mathbf{J}_s) \qquad (6\text{-}29)$$

and the solid phase transport according to

$$\frac{\partial\phi_s}{\partial t}+\nabla\cdot(\phi_s\mathbf{u}) = -\frac{\nabla\cdot\mathbf{J}_s}{\rho_s} \qquad (6\text{-}30)$$

By comparing Equation 6-29 and Equation 6-30 with Equation 6-26 and Equation 6-28, it is clear that they are equivalent if

$$\mathbf{u}_{\text{slip}} = \frac{\mathbf{J}_{\text{s}}}{\phi_{\text{s}}\rho_{\text{s}}(1-c_{\text{s}})}$$

In this example you use the model for the particle flux, $\mathbf{J}_{\text{s}}$, as suggested by Subia and others (Ref. 3) and Rao and others (Ref. 2), but the open and editable format of COMSOL Multiphysics makes it possible to specify the expression arbitrarily.

Following Rao and others, the particle flux is

$$\frac{\mathbf{J}_{\text{s}}}{\rho_{\text{s}}} = -[\phi \text{D}_{\phi}\nabla(\dot{\gamma}\phi) + \phi^2\dot{\gamma}\text{D}_{\mu}\nabla(\ln\mu)] + f_{\text{h}}\mathbf{u}_{\text{st}}\phi$$

Here, $\mathbf{u}_{\text{st}}$ is the settling velocity (m/s) of a single particle surrounded by fluid and D_{ϕ} and D_{μ} are empirically fitted parameters (m^2) given by

$$\text{D}_{\phi} = 0.41a^2$$

$$\text{D}_{\mu} = 0.62a^2$$

where a is the particle radius (m).

The shear rate tensor, $\dot{\underset{\sim}{\gamma}}$ (1/s), is given by

$$\dot{\underset{\sim}{\gamma}} = \nabla\mathbf{u} + (\nabla\mathbf{u})^T$$

and its magnitude by

$$\dot{\gamma} = \sqrt{\frac{1}{2}(\dot{\underset{\sim}{\gamma}}:\dot{\underset{\sim}{\gamma}})}$$

which for a 2-dimensional problem is

$$\dot{\gamma} = \sqrt{\frac{1}{2}(4u_x^2 + 2(u_y + v_x)^2 + 4v_y^2)}$$

The settling velocity, $\mathbf{u}_{\text{st}}$, for a single spherical particle surrounded by pure fluid is given by

$$\mathbf{u}_{\text{st}} = \frac{2}{9}\frac{a^2(\rho_{\text{s}} - \rho_{\text{f}})}{\eta_0}\mathbf{g}$$

For several particles in a fluid, the settling velocity is lower. To account for the surrounding particles, the settling velocity for a single particle is multiplied by the hindering function, f_{h}, defined as

$$f_{\mathrm{h}} = \frac{\eta_{\mathrm{f}}(1-\phi_{\mathrm{av}})}{\eta}$$

where ϕ_{av} is the average solid phase volume fraction in the suspension, η_{f} is the dynamic viscosity of the pure fluid ($\mathrm{Ns/m^2}$), and η is the mixture viscosity (Equation 6-25).

The following table gives the physical properties of the solid and the liquid phases.

NAME	VALUE	DESCRIPTION
ρ_{s}	1180 $\mathrm{kg/m^3}$	Density of particles
ρ_{f}	1250 $\mathrm{kg/m^3}$	Density of pure fluid
a	678 µm	Particle radius
η_{f}	0.589 Pa·s	Viscosity of pure fluid

BOUNDARY CONDITIONS

The suspension is placed in a Couette device, that is, between two concentric cylinders. The inner cylinder rotates while the outer one is fixed. The radii of the two cylinders are 0.64 cm and 2.54 cm, respectively. The inner cylinder rotates at a steady rate of 55 rpm. With the cylinder centered at (0,0), this corresponds to a velocity of

$$(u, v) = \frac{110\pi}{60}(y, -x)$$

The fluid and particle motion is small along the direction of the cylinder axes. You can therefore use a 2-dimensional model. Figure 6-26 shows the corresponding geometry.

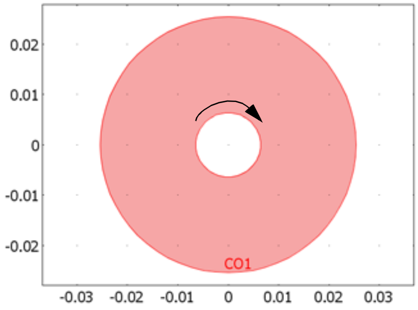


Figure 6-26: Geometry of the Couette device. The inner cylinder rotates, the outer one is fixed.

There is no particle flux through the boundaries, and the suspension velocity satisfies no-slip conditions at all walls.

INITIAL CONDITIONS

There are two different initial particle distributions. In the first example, the particles are evenly distributed within the device. In the second example, the particles are initially gathered at the top of the device.

Results

CASE 1—INITIALLY EVENLY DISTRIBUTED PARTICLES

A suspension with particles lighter than the fluid is placed in a concentric Couette device. Initially, the particles are evenly distributed with a constant volume fraction of 0.35. The shear rate in the device varies radially across the gap and thus it is expected that particles will migrate (shear-induced migration) from regions of high shear to regions of low shear (toward the outer wall). Because the particles are lighter than the fluid, they also rise.

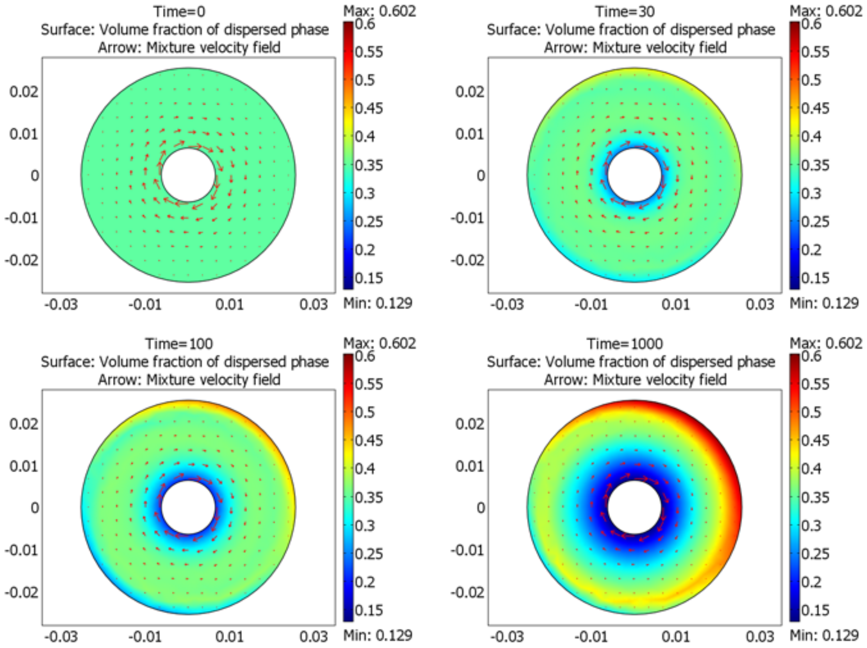


Figure 6-27: The particle concentration ϕ_s at different times. The particles move to regions with lower shear rate and rise because of buoyancy.

Figure 6-27 shows the particle concentration ϕ_s in the device at $t = 0$ s, $t = 30$ s, $t = 100$ s and $t = 1000$ s. The migration of the particles toward the outer wall is apparent. As a result of the shear induced migration and gravity, the solid phase volume fraction approaches the value for maximum packing close to the upper right outer wall. The suspension viscosity thus becomes high in this region. The results compare well with those presented in Ref. 2.

CASE 2—PARTICLES INITIALLY GATHERED AT THE TOP OF THE DEVICE

In this case the particles are initially gathered at the top of the device. The particle volume fraction is initially zero in the lower part, while it is 0.59 at the top.

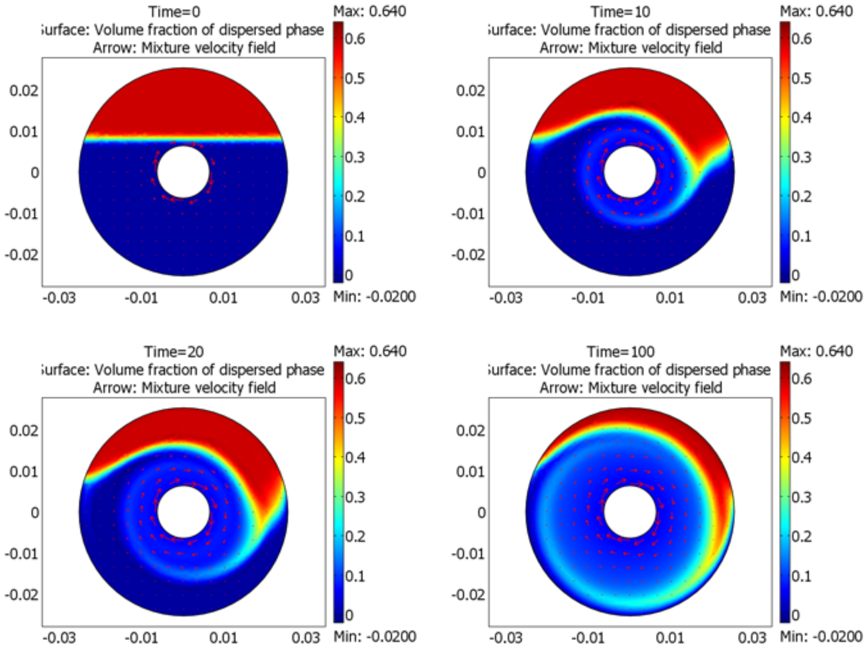


Figure 6-28: Particle concentrations for t = 0 s, 10 s, 20 s, and100 s with particles initially at the top. Note that the same color range values are used in each of the plots.

Figure 6-28 shows the numerically predicted particle concentration at times 0 s, 10 s, 20 s, and 100 s. Initially, the particle motion is dominated by inertia and the effect of the shear-induced migration is not visible. At later times, shear-induced migration causes the particles to move toward the outer boundary. In this case also, the results agree well with the results in Ref. 2.

References

1. R.J. Phillips, R.C. Armstrong, R.A. Brown, A.L. Graham, and J.R. Abbot, “A constitutive equation for concentrated suspensions that accounts for shear-induced particle migration,” *Phys. Fluids A,* vol. 4, pp. 30–40, 1992.

2. R. Rao, L. Mondy, A. Sun, and S. Altobelli, “A numerical and experimental study of batch sedimentation and viscous resuspension,” *Int. J. Num. Methods in Fluids*, vol. 39, pp. 465–483, 2002.

3. S.R. Subia, M.S. Ingber, L.A. Mondy, S.A. Altobelli, and A.L. Graham, “Modelling of concentrated suspensions using a continuum constitutive equation,” *J. Fluid Mech.*, vol. 373, pp. 193–219, 1998.

Modeling in COMSOL Multiphysics

To set up the model with COMSOL Multiphysics, you will use the Mixture Model application mode. The shear rate is discretized as an additional equation to improve accuracy because the particle flux contains derivatives of this quantity, which in turn depend on the derivatives of the velocity.

Model Library path: `Chemical_Engineering_Module/Multiphase_Flow/dense_suspension`

Modeling Using the Graphical User Interface—Case 1

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** from the **Space dimension** list. Click the **Multiphysics** button.
2. From the **Application Modes** tree, select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Mixture Model, Laminar>Transient analysis**. Click **Add**.
3. Select **COMSOL Multiphysics>PDE Modes>PDE, General Form>Time-dependent analysis**. Type `gamma` in the **Dependent variables** edit field. Click **Add**.
4. Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1. Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar.
2. Type `0.0064` in the **Radius** edit field and click **OK**.
3. Click the **Zoom Extents** button on the Main toolbar.
4. Shift-click the **Ellipse/Circle (Centered)** button once more to create a second circle.

5 Type `0.0254` in the **Radius** edit field and click **OK**.

6 Click the **Zoom Extents** button.

7 Click the **Create Composite Object** button on the Draw toolbar.

8 In the **Set formula** edit field, type `C2-C1` to cut out the smaller circle from the larger one. Click **OK**.

OPTIONS AND SETTINGS

1 Select **Constants** from the **Options** menu and enter the following constant names and expressions:

NAME	EXPRESSION	DESCRIPTION
rho_s	1180[kg/m^3]	Density of solid particles
rho_f	1253[kg/m^3]	Density of pure fluid
eta_f	0.5889[Pa*s]	Viscosity of pure fluid
phi_max	0.64	Maximum packing
g	-9.82[m/s^2]	Gravity constant
phi0	0.35	Average concentration
R	3.97e-4[m]	Particle radius
rpm	55[1/min]	Revolutions per minute
c_vel	2*pi*rpm	Scaling of velocity
u_st	(2/9)*g*R^2*(rho_s-rho_f)/eta_f	Settling velocity
D1	0.41*R^2	Model parameter D_phi
D2	0.62*R^2	Model parameter D_mu

2 Click **OK**.

3 From the **Options** menu, select **Expressions>Scalar Expressions**. Enter variables and expressions in the following table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
eta_phi	diff(eta_chmm,phid)	Derivative of viscosity with respect to concentration
J1	-rho_s*(phid*D1*(phid*gammax+phidx*gamma)+phid*phid*gamma*D2*eta_phi*phidx/eta_chmm)	Particle flux, x direction

NAME	EXPRESSION	DESCRIPTION
`J2`	`-rho_s*(phid*D1*(phid*gammay+phidy*gamma)+phid*phid*gamma*D2*eta_phi*phidy/eta_chmm)+rho_s*f_hinder*phid*u_st`	`Particle flux, y direction`
`f_hinder`	`eta_f*(1-phi0)/eta_chmm`	`Hindering function`

Note: `eta_chmm` is the internal name for the mixture viscosity variable. To see names and descriptions for other internal variables, select **Physics>Equation System>Subdomain Settings**, select a subdomain, and go to the **Variables** page.

---

4 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**. Select Subdomain 1 and type `p_tot` in the **Name** edit field and `p` in the **Expression** edit field. This defines the integral of the pressure, p_{tot}, as the variable `p_tot`. Click **OK**.

PHYSICS SETTINGS—INCOMPRESSIBLE NAVIER-STOKES

Subdomain Settings

1 In the Model Tree (in Overview mode), right-click the **Mixture Model (chmm)** node and click **Subdomain Settings**. (Alternatively, choose **Mixture Model (chmm)** from the **Multiphysics** menu, then select **Subdomain Settings** from the **Physics** menu.)

2 Enter the following settings in the edit fields:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ_c	`rho_f`	Density of continuous phase
η_c	`eta_f`	Dynamic viscosity of continuous phase
ρ_d	`rho_s`	Density of dispersed phase

3 Go to the **Physics** page and type `g` in the right **Gravity** edit field. This edit field corresponds to the *y*-component of the gravity vector.

4 Click the **Artificial Diffusion** button and clear the **Streamline diffusion** check box. Click the **Dispersed Phase Transport** page and clear the **Isotropic diffusion** check box. Click **OK**.

5 On the **Mixture Model** page, select **User defined** from the **Slip model** list.

6 For the **Slip velocity**, type `J1/(phid*rho_s*(1-cd_chmm))` in the left edit field and `J2/(phid*rho_s*(1-cd_chmm))` in the right edit field.

7 In the $\phi_{\mathbf{max}}$ edit field, type `phi_max`.

8 Click the **Init** tab and type `phi0` in the **phid(t_0)** edit field.

9 Click **OK**.

You must add a condition on the integral of the pressure, because the pressure is not specified on any part of the boundary.

10 From the **Physics** menu, select **Equation System>Point Settings**. Select Point 1.

11 Click inside the **Constraint (constr = 0)** edit field. Five edit fields now appear. The third of these edit fields corresponds to the pressure equation; type `p_tot` in that field. Click in the **Constraint force** edit field. Type `test(p_tot)` in the third of the edit fields that appear. You have now added the constraint that the integral of the pressure should be equal to zero. Click **OK**.

Boundary Conditions

1 Open the **Boundary Settings** dialog box for the **Mixture Model (chmm)**.

2 Press Ctrl while clicking all the boundaries of the interior circle. Boundaries 3, 4, 6, and 7 should now be selected in the **Boundary selection** list.

3 From the **Boundary type** list, select **Inlet.** Verify that **Velocity** is selected in the **Boundary condition** list. Type `c_vel*y` in the **x-velocity** edit field and `-c_vel*x` in the **y-velocity** edit field.

4 The default boundary condition **No slip** is correct for the other boundaries.

5 For boundary conditions on the dispersed phase, the default condition **Insulation/ Symmetry** is correct for all boundaries.

6 Click **OK**.

PHYSICS SETTINGS—SHEAR RATE

Subdomain Settings

1 Right-click **PDE, General Form (g)** in the Model Tree and select **Subdomain Settings**.

2 Enter subdomain variables according to the following table; when done, click **OK**.

NAME	EXPRESSION
Γ	`0 0`
F	`gamma-sqrt(0.5*(4*ux^2+2*(uy+vx)^2+4*vy^2)+eps)`
e_a	`0`
d_a	`0`

Boundary Conditions

1 Right-click **PDE, General Form (g)** in the Model Tree and select **Boundary Settings**.

2 Select any of the boundaries, then press Ctrl+A to select all of them.

3 Select **Neumann boundary condition** and leave the value for **G** at zero.

4 Click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar. Type `[0 30 100 1000]` in the **Times** edit field. Click **OK**.

2 Click the **Solve** button on the Main toolbar.

The calculation takes about one minute.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 Select the **Arrow** tab and select the **Arrow plot** check box to create an arrow plot of the velocity field.

3 Click **OK** to generate the plot.

4 Click the **Animate** button on the Draw toolbar to create a movie corresponding to the plots shown in Figure 6-27.

Modeling Using the Graphical User Interface—Case 2

Next, modify the initial conditions to model the case with the particles initially gathered at the top. To build this model, you only have to make a few changes to the previous model.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Expressions>Scalar Expressions**. Add a variable with the **Name** `phi0_2` and the **Expression** `flc2hs(y[1/mm]-8,2)*0.59`.

2 Click **OK**.

PHYSICS SETTINGS—PARTICLE CONCENTRATION EQUATION

You must change the initial particle concentration distribution and add some isotropic artificial diffusion to stabilize the numerical calculations. In order to avoid dividing by zero in the region where the particle volume fraction is initially zero, modify the expression for the slip velocity.

Subdomain Settings

1 Open **Subdomain Settings** dialog box for **Mixture Model (chmm)**.

2 On the **Init** page, type `phi0_2` in the **phid(t_0)** edit field.

3 On the **Physics** page, click the **Artificial Diffusion** button.

4 On the **Dispersed Phase Transport** page, select the **Isotropic diffusion** check box. Type `1` in the $\delta_{\mathrm{scale},\,\rho}$ edit field. This is a suitable scale for high particle volume fractions. Click **OK**.

5 On the **Mixture Model** page, replace the expressions for the slip velocity by `J1/(phid*rho_s*(1-cd_chmm)+eps)` and `J2/(phid*rho_s*(1-cd_chmm)+eps)`.

6 Click **OK**.

MESH GENERATION

Click the **Refine Mesh** button on the Main toolbar to create a finer mesh compared to the one used for the previous model.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar. Type `0:10:100` in the **Times** edit field. Click **OK**.

2 Click the **Solver Manager** button on the Main toolbar. In the **Initial value** area, select **Initial value expression**. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

The computation takes about 6 minutes.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 Go to the **Surface** page and click the **Range** button.

3 Clear the **Auto** check box and type `-0.02` in the **Min** edit field and `0.64` in the **Max** edit field. Click **OK**.

4 Click **OK**.

5 Click the **Animate** button on the Draw toolbar to visualize the result shown in Figure 6-28 as a movie.

7

Microfluidics

This chapter contains examples of mass transport coupled to momentum transport, where typical systems of this type are found in microsystems and are often affected by electric fields. To transport fluid at very small scales, it is best to avoid small, moving parts. Instead, electric fields often transport a medium made up of an ionic solution.

COMSOL Multiphysics is well suited for these types of processes for two reasons:

- *Its ability to model multiphysics applications easily and quickly*—often you need to model momentum and mass transport to a description of the electric potential field. Other models might also require energy transport.
- *Its ability to handle equation-based modeling*—the coupling between the physics that describes such systems can be unusual and require user-defined functions. Furthermore, chemical kinetics can be involved along with sudden changes in time-based phenomena or phases. Further, such a system could depend on an arbitrary description of the double charge layer at a boundary or another description for the electric field, so the ability to quickly type in your own equations is therefore useful.

Electrokinetic Flow in a DNA Chip

This model was developed by Dr. Jordan MacInnes at the University of Sheffield, UK. The modeling work at his department has been combined with experimental studies.

Introduction

Miniature laboratories (Ref. 1) are required to efficiently analyze the information in human DNA, and they can facilitate tailor-made diagnosis and treatment of hereditary diseases for individuals. A problem that arises in these lab-on-chip devices concerns the transport of the liquid samples and other solutions in the chip, which are of very small dimensions. Moving parts of micrometer scale make the chips very expensive and fragile and are therefore to be avoided if at all possible. An alternative method for transporting fluid in the samples is through electrokinetic effects, where charged ions in the solutions are subjected to an electric field. These ions can drag the entire solution through the channels in the microchip from one analyzing point to the other.

Two mechanisms can drive the flow of a saline solution in an electric field. In the presence of solid surfaces, like the micromachined surfaces of the channels of a biochip, a charged solution is formed close to the wall surfaces. This layer is referred to as a *diffuse double layer*. Depending on the material used, it is formed by negatively or positively charged groups on the wall's surfaces. The electric field displaces the charged liquid in the charged double layer generating an *electroosmotic flow*. Figure 7-1 shows the velocity field shortly after the application of an electric field.

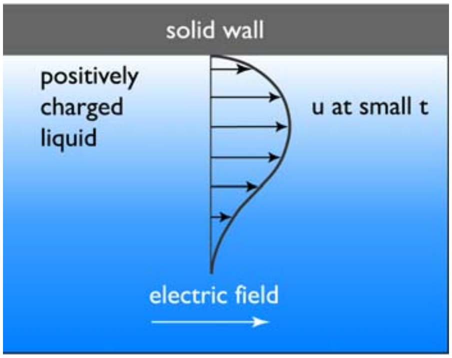


Figure 7-1: Velocity field near a solid wall. The fluid flows in the direction of the electric field.

A force is imposed on the positively charged solution close to the wall surface, and the fluid starts to flow in the direction of the electric field. The velocity gradients perpendicular to the wall give rise to viscous transport in this direction. In the absence of other forces, the velocity profile eventually becomes almost uniform in the cross section perpendicular to the wall. The time constant of the overall flow is roughly 1 ms, while the flow in the double layer responds to changes far more rapidly. The layer model of MacInnes (Ref. 1) replaces the double layer with the Helmholtz-Smoluchowski relationship between wall velocity and wall electric field (Ref. 2).

The second effect arises due to differences in mobility and charge of the ionic species. Negatively and positively charged ions migrate in different directions, and these ions drag water molecules, to different extents, through the channel system. Water is dragged by the sodium ions, which can coordinate more water molecules than the chloride ions in the solution. This type of flow is called electrophoretic flow; Figure 7-2 depicts its basic principle.

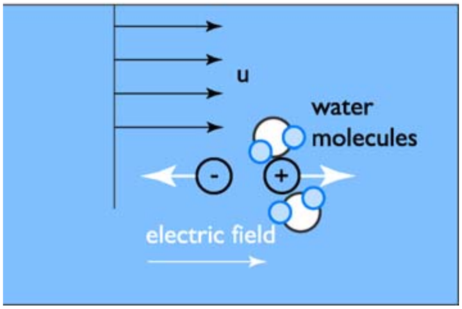


Figure 7-2: Electrophoretic flow.

This particular model does not include the mass transport of dissolved species in the sample (see Ref. 1), but you could easily add them through the Nernst-Plank application mode or the Convection and Diffusion application mode. As another possible model extension, you could use a time-dependent expression for the voltage at the inlet and outlet boundaries.

Model Definition

Flow in the chip occurs due to the electroosmotic effect just described. In order to simulate this type of flow, the model must couple the electric potential distribution in the ionic solution inside the chip and the Navier-Stokes equations for fluid flow.

Figure 7-3 shows the chip's geometry. The potential difference imposed between its different parts produces a flow in the vertical or horizontal direction, depending on the direction of the imposed field. Mode A generates a horizontal flow from right to left in the main channel; Mode B generates a flow that is vertical in the vertical channels and horizontal, from right to left, in the part of the main channel that unites the vertical branches.

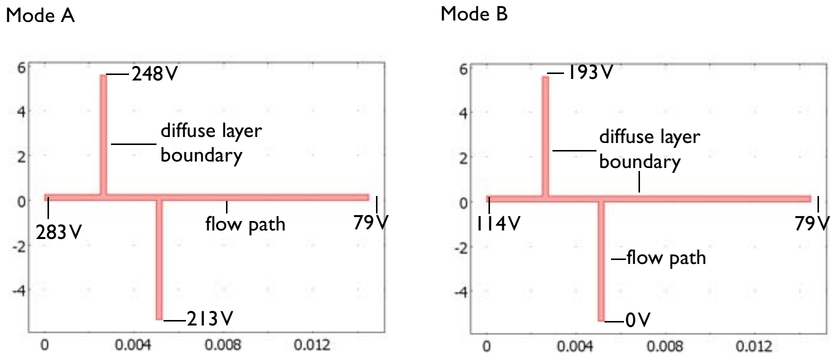


Figure 7-3: Geometry and electric field setup in the two modes: Mode A, where the flow is expected to flow in the horizontal branch, and Mode B, with flow in the vertical branch.

You set the potentials at the open boundaries, where the fluid is allowed to enter or leave the channel system. The wall boundaries are denoted diffuse layer boundaries. From the published work of Dr. MacInnes (Ref. 1) you can expect the flow to be laminar and of a low Reynolds number. This implies that it is adequate to use the Navier-Stokes equations to describe flow in the channels:

$$\rho\frac{\partial\mathbf{u}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 \qquad (7\text{-}1)$$
$$\nabla\cdot\mathbf{u} = 0$$

Here η denotes the dynamic viscosity (Pa·s), **u** is the velocity (m/s), ρ equals the fluid's density (kg/m^3), and p is the pressure (Pa).

The boundary conditions, according to this notation, are the following:

$$\begin{aligned} \mathbf{u} &= \frac{\varepsilon_\mathrm{w}\zeta_0}{\eta}\nabla V && \text{diffuse layer, wall} \\ \eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)\cdot\mathbf{n} &= 0 && \text{inlets and outlets} \end{aligned} \tag{7-2}$$

where ε_w (F/m) denotes the permittivity of water, ζ_0 (V) is the zeta potential at the channel wall, and V (V) refers to the applied potential. The boundary condition for the flow at the wall boundaries sets the velocity vector proportional to the gradient of the potential. For a more detailed review of the diffuse layer wall boundary condition, see Ref. 1 and Ref. 3.

Assuming that there are no concentration gradients for the ions carrying the current, it is possible to express the current balance in the channel through Ohm's law and the balance equation for current density:

$$\nabla\cdot(-\sigma\nabla V) = 0 \tag{7-3}$$

Here σ denotes the conductivity (S/m) and the expression within the brackets represents the current density (A/m^2).

The corresponding boundary conditions for the current balance are

$$\begin{aligned} -\sigma\nabla V\cdot\mathbf{n} &= 0 && \text{diffuse layer, wall} \\ V &= V_0 && \text{inlets and outlets} \end{aligned} \tag{7-4}$$

where V_0 corresponds to the voltage shown in the previous figure at the neutral boundaries. At these boundaries, the potential and current distributions in the chip determine if the fluid enters or exits the chip or stays at rest.

The input data used in this model is listed in the following table.

TABLE 7-1: INPUT DATA

PROPERTY	VALUE	DESCRIPTION
ρ	10^3 kg/m^3	Density
η	10^{-3} Pa·s	Dynamic viscosity
σ	0.11845 S/m	Electric conductivity
ε_w	$80.2\cdot 8.854\cdot 10^{-12}$ F/m	Electric permittivity
ζ_0	0.1 V	Zeta potential

Results

Figure 7-4 shows the potential distribution for Mode A in the chip. From this plot it is clear that the largest potential differences arise in the horizontal direction. This also implies that the main flow is in the same direction.

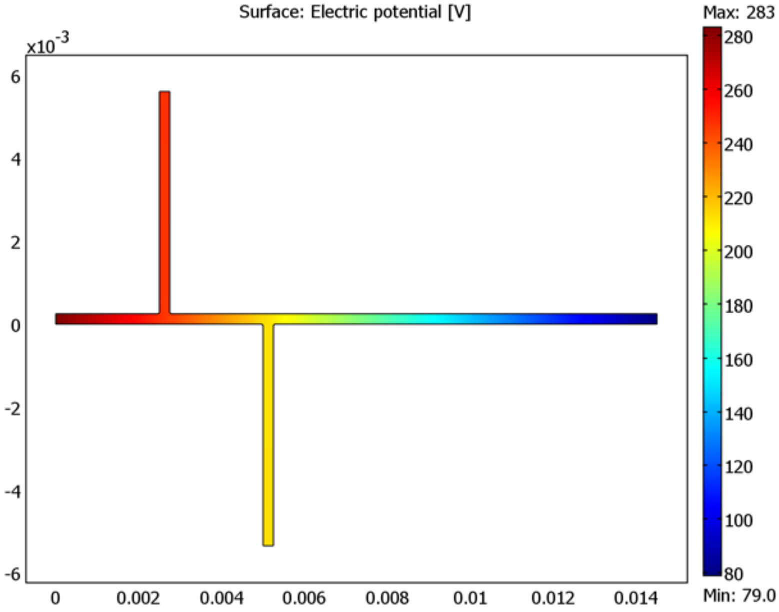


Figure 7-4: Potential distribution in the chip when the electric field from mode A is applied.

The plot in Figure 7-5 shows that the average velocity in the channel is approximately 1 mm/s. The largest velocity occurs at the corner walls where the electric field is large.

This clearly shows the effect of the driving force located at the walls. For regular pressure-driven flow, the velocity at the solid surfaces is zero.

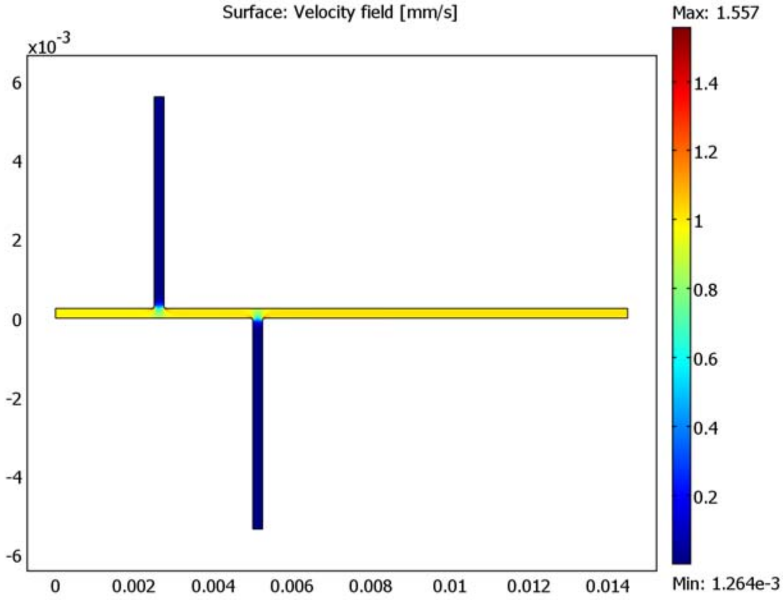


Figure 7-5: Velocity distribution in the chip with the electric field from Mode A applied.

Studying the velocity flow lines in the channel, Figure 7-6 shows that flow takes a small deviation at the T-junctions in the chip. This can also be detected in the color scale of the velocity, which decreases in the middle of the junction.

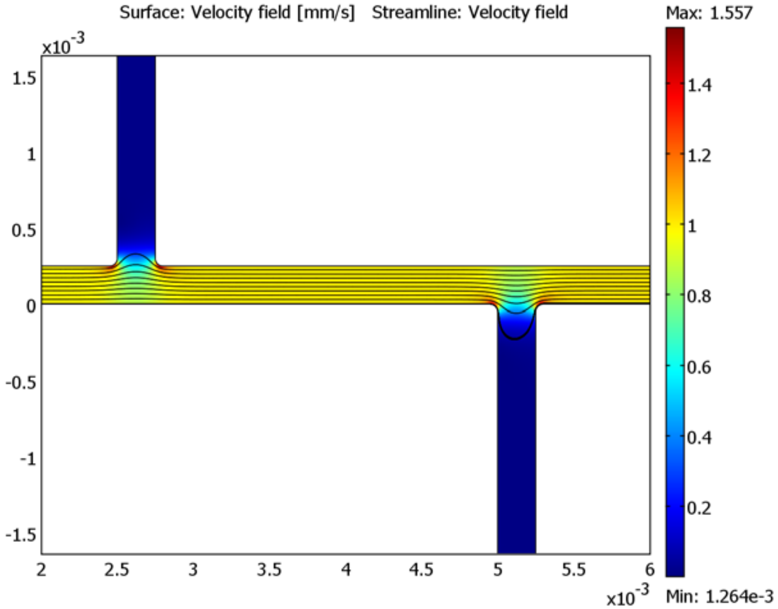


Figure 7-6: Close-up of the velocity field. The surface plot shows the modulus of the velocity vector and the lines the streamlines of the velocity field.

Regulating the potential can quickly and efficiently change the flow path in the channels. This makes it possible to mix solutions in different branches of the chip. Figure 7-7 shows a different flow direction with the same magnitude as the potential configuration given in Mode A. In this plot, you can also find the corner effects and the low velocity regions in the T-junctions as the channel width increases.

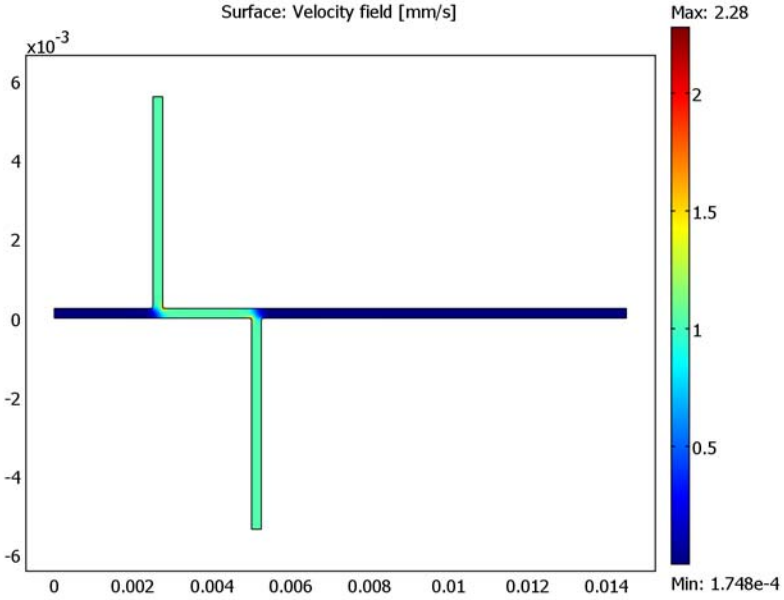


Figure 7-7: Flow distribution in the chip with the electric field from Mode B applied.

Figure 7-8 shows that the flow decreases in the outer parts of the turns while a maximum arises in the inner parts. The maximum velocity is actually larger in this case than in the previous one because the electric field is much stronger around the corners compared to the straight path in the first simulation.

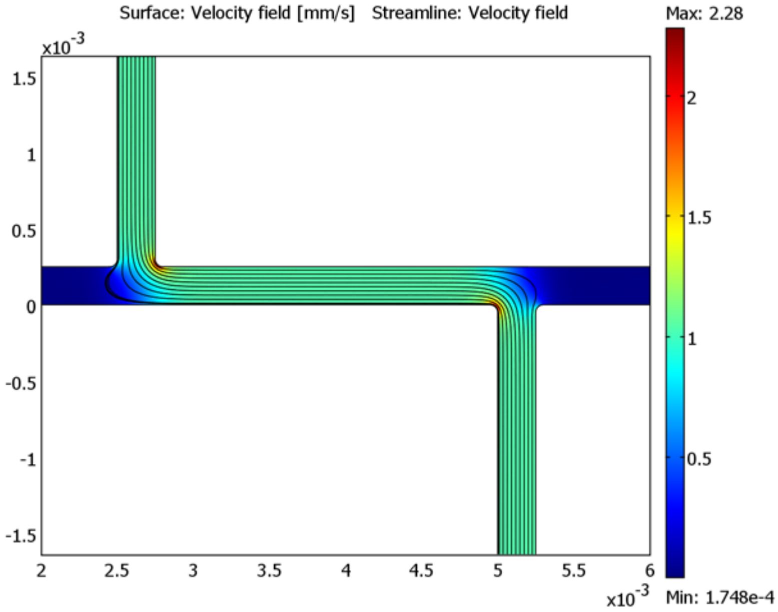


Figure 7-8: Close-up of the flow distribution near the T-junctions.

As the model demonstrates, it is easy to treat electrokinetic flow using the Chemical Engineering Module.

References

1. J.M. MacInnes, "Computation of Reacting Electrokinetic Flow in Microchannel Geometries," *J. Chem. Eng. Sci.*, vol. 57, no. 21, pp. 4539–4558, 2002.

2. R.F. Probstein, *Physicochemical Hydrodynamics*, Wiley-Interscience, 1994.

3. W. Menz, J. Mohr, and O. Paul, *Microsystems Technology*, WILEY-VCH Verlag GmbH, 2001.

Model Library path: `Chemical_Engineering_Module/Microfluidics/biochip`

Modeling Using the Graphical User Interface

1. In the **Model Navigator**, set the **Space dimension** to **2D**.
2. From the **Application Modes** list, select **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.
3. Click the **Multiphysics** button.
4. Click the **Add** button.
5. From the **Application Modes** list, select **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**, then click **Add**.
6. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Constants**.
2. Define the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1e3[kg/m^3]`	`Density`
`eta`	`1e-3[Pa*s]`	`Viscosity`
`sigma`	`0.11845[S/m]`	`Electric conductivity`
`eps_w`	`80.2*8.854[pF/m]`	`Electric permittivity`
`zeta0`	`0.1[V]`	`Zeta potential`

GEOMETRY MODELING

Create the geometry using the CAD tools in COMSOL Multiphysics.

1. Press the Shift key and click the **Rectangle/Square** button on the Draw toolbar.
2. In the **Size** area of the **Rectangle** dialog box, enter the **Width** `0.25e-3` and the **Height** `5.35e-3`. In the **Position** area, set **x** to `2.5e-3` and **y** to `2.5e-4`. Click **OK**.
3. Repeat this procedure to create two additional rectangles with the following properties:

SETTINGS	RECTANGLE 2	RECTANGLE 3
Width	`0.25e-3`	`1.45e-2`
Height	`5.35e-3`	`2.5e-4`
x	`5e-3`	`0`
y	`-5.35e-3`	`0`

4 Click the **Zoom Extents** button on the Main toolbar.

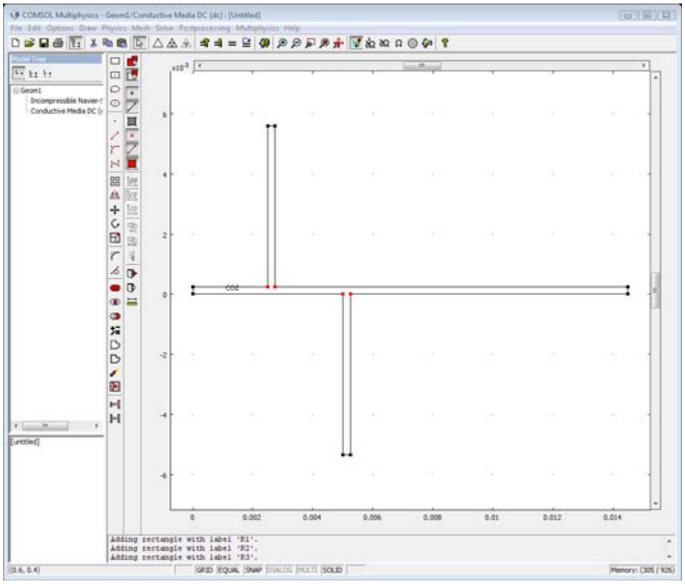
5 Press Ctrl+A to select all geometry objects.

6 Click the **Union** button on the Draw toolbar.

7 Click the **Delete Interior Boundaries** button.

8 From the **Draw** menu, select **Fillet/Chamfer**.

9 In the drawing area, Ctrl-click to select the four vertices connecting the vertical channels with the horizontal one (Vertices 3, 5, 8, and 10).



```
Adding rectangle with label 'R1'.
Adding rectangle with label 'R2'.
Adding rectangle with label 'R3'.
```

10 In the **Fillet/Chamfer** dialog box, specify the fillet **Radius** `0.5e-4`.

11 Click **OK** to close the dialog box.

This completes the geometry modeling stage.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Select Subdomain 1.

4 In the ρ edit field, type `rho`, and in the η edit field, type `eta`. Click **OK**.

5 In the **Multiphysics** menu, switch to the **2 Conductive Media DC (dc)** application mode.

6 From the **Physics** menu, open the **Subdomain Settings** dialog box.

7 In the σ edit field, type `sigma`. Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, open the **Boundary Settings** dialog box.

3 Specify boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2–4, 6–8, 10, 11, 13–16	BOUNDARIES 5, 9, 12
Boundary type	Outlet	Inlet	Open boundary
Boundary condition	Pressure, no viscous stress	Velocity	Normal stress
u_0		`(eps_w*zeta0/eta)*Vx`	
v_0		`(eps_w*zeta0/eta)*Vy`	
p_0	0		
f_0			0

4 From the **Multiphysics** menu, select **2 Conductive Media DC (dc)**.

5 From the **Physics** menu, open the **Boundary Settings** dialog box.

6 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 9	BOUNDARY 12	BOUNDARIES 2–4, 6–8, 10, 11, 13–16
Boundary condition	Electric potential	Electric potential	Electric potential	Electric potential	Electric insulation
V_0	283	248	213	79	

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** button, then set the **Mesh curvature factor** to `0.6`.

3 Click the **Boundary** tab. From the **Boundary selection** list, select **1**, **5**, **9**, and **12**.

4 In **Maximum element size** edit field, type `1e-4`.

5 Click the **Remesh** button to generate the mesh.

6 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Follow these instructions to generate the plot in Figure 7-4:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, make sure that only the **Surface** and **Geometry edges** plot types are selected.
3. On the **Surface** page, select **Conductive Media DC (emdc)>Electric potential** from the **Predefined quantities** list on the **Surface Data** page.
4. Click **Apply**.

Proceed to create the plots in Figure 7-5 and Figure 7-6 with these steps:

5. On the **Surface** page, select **Incompressible Navier-Stokes (chns)>Velocity field** from the **Predefined quantities** list on the **Surface Data** page. From the **Unit** list, select **mm/s**.
6. Click **Apply** to obtain the plot in Figure 7-5.
7. On the **Streamline** page, select the **Streamline plot** check box.
8. From the **Predefined quantities** list on the **Streamline Data** page, select **Incompressible Navier-Stokes (chns)>Velocity field**.
9. From the **Streamline plot type** list, select **Magnitude controlled**. Set the **Density** to `9`.
10. On the **Line Color** page, click first the **Uniform color** option button and then the **Color** button. In the **Streamline Color** dialog box, select the black swatch, then click **OK**.
11. Click the **Advanced** button. Set the **Maximum number of integration steps** to `4000`.
12. Click **OK** to close the **Advanced Streamline Parameters** dialog box.
13. Click **OK** in the **Plot Parameters** dialog box.
14. From the **Options** menu, select **Axes/Grid Settings**.
15. On the **Axis** page, specify these settings:

x min	`2e-3`
x max	`6e-3`
y min	`-1e-3`
y max	`1e-3`

16. Click **OK** to generate the plot in Figure 7-6.

PHYSICS SETTINGS—MODE B

Now switch the electric field to Mode B (see the right panel of Figure 7-3).

Boundary Conditions

1 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

2 From the **Physics** menu, open the **Boundary Settings** dialog box.

3 Modify the boundary conditions according to the table below; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 9
Boundary condition	Electric potential	Electric potential	Electric potential
V_0	114	193	0

COMPUTING THE SOLUTION—MODE B

Click the **Restart** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION—MODE B

The plot that appears in the drawing area when the solver has finished reproduces the one in Figure 7-8. To generate the plot in Figure 7-7, follow these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Streamline** page, clear the **Streamline plot** check box, then click **OK**.

3 Click the **Zoom Extents** button on the Main toolbar.

Filling of a Capillary Channel

Introduction

Surface tension and wall adhesive forces are often used to transport fluid through microchannels in MEMS devices or to measure, transport and position small amounts of fluid using micropipettes. Multiphase flow through a porous medium and droplets on solid walls are other examples where wall adhesion and surface tension strongly influence the dynamics of the flow.

To model the adhesive forces at the walls correctly, the treatment of the boundary conditions is important. If you fix the velocity to zero on the walls, the interface cannot move along the walls. Instead, you need to allow a non-zero slip velocity and to add a frictional force at the wall. With such a boundary condition, it is possible to explicitly set the contact angle, that is, the angle between the fluid interface and the wall. The correct value of the contact angle depends on properties of the fluids and the wall. You can determine the contact angle experimentally or calculate it from the surface energies related to the different phase interfaces using Young's law.

This example studies a narrow vertical cylinder placed on top of a reservoir filled with water. Because of wall adhesion and surface tension at the air/water interface, water rises through the channel. The model calculates the pressure field, the velocity field, and the water surface's shape and position. It uses a level set method to track the air/water interface and shows how to add friction and specify the contact angle at the channel walls.

Model Definition

The model consists of a capillary channel of radius 0.15 mm attached to a water reservoir. Water can flow freely into the reservoir. Because both the channel and the reservoir are cylindrical, you can use the axisymmetric model illustrated in Figure 7-9. Initially, the thin cylinder is filled with air. The wall adhesion causes water to creep up along the cylinder boundaries. The deformation of the water surface induces surface tension at the air/water interface, which in turn creates a pressure jump across the interface. The pressure variations cause water and air to move upward. The fluids continue to rise until the capillary forces are balanced by the gravity force that builds up as the water rises in the channel. In the present example, the capillary forces dominate over gravity throughout the simulation. Consequently, the interface moves upwards during the entire simulation.

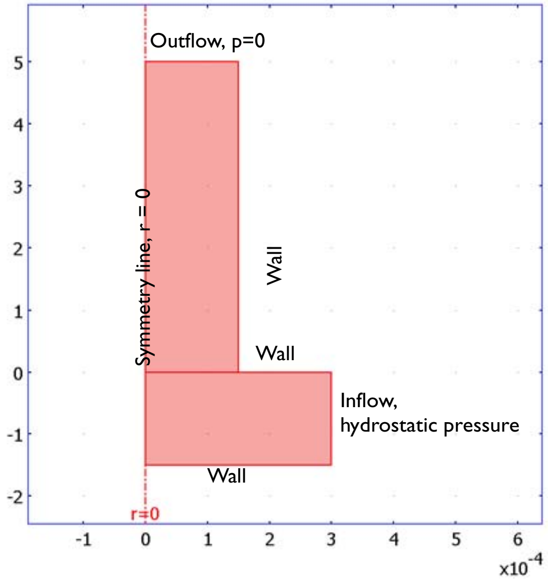


Figure 7-9: Axisymmetric geometry description.

MASS AND MOMENTUM TRANSPORT

The Navier-Stokes equations describe the transport of mass and momentum for fluids of constant density. In order to account for capillary effects, it is crucial to include surface tension in the model. The Navier-Stokes equations are then

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - \nabla \cdot (\eta(\nabla \mathbf{u} + \nabla \mathbf{u}^T)) + \nabla p = \mathbf{F}_{\mathrm{st}} + \rho \mathbf{g}$$

$$\nabla \cdot \mathbf{u} = 0$$

Here, ρ denotes the density (kg/m^3), η equals the dynamic viscosity (Ns/m^2), $\mathbf{u}$ represents the velocity (m/s), p denotes the pressure (Pa), and $\mathbf{g}$ is the gravity vector (m/s^2). $\mathbf{F}_{\mathrm{st}}$ is the surface tension force that acts at the air/water interface and is

$$\mathbf{F}_{\mathrm{st}} = \nabla \cdot \mathbf{T}$$

$$\mathbf{T} = \sigma(\mathbf{I} - (\mathbf{n}\mathbf{n}^T))\delta$$

Here, $\mathbf{I}$ is the identity matrix, $\mathbf{n}$ is the interface normal, σ equals the surface tension coefficient (N/m), and δ equals a Dirac delta function that is nonzero only at the fluid interface. When you use the finite element method to solve the Navier-Stokes equations, you multiply the equations by test functions and then integrate over the computational domain. If you use integration by parts, you can move derivatives of $\mathbf{T}$ to the test functions. This is used in the Level Set and Laminar Flow application mode and results in an integral over the computational domain plus a boundary integral of the form

$$\int_{\partial\Omega} \mathrm{test}(\mathbf{u}) \cdot [\sigma(\mathbf{n}_{\mathrm{wall}} - (\mathbf{n}\cos\theta))\delta]dS\,, \tag{7-5}$$

where θ is the contact angle (see Figure 7-10). If you apply a no-slip boundary condition, the boundary term vanishes because $\mathrm{test}(\mathbf{u}) = 0$ on that boundary, and you cannot specify the contact angle. Instead, the interface remains fixed on the wall. However, if you allow a small amount of slip, it is possible to specify the contact angle. The Wetted wall boundary condition adds the term given by Equation 7-5 and consequently allows you to set the contact angle.

REPRESENTATION AND CONVECTION OF THE FLUID INTERFACE

The Level Set Two-Phase Flow, Laminar application mode automatically sets up the equations for the convection of the interface, calculates normal and curvature of the interface, and adds surface tension and gravitation to the Navier-Stokes equations.

The application mode represents the interface as the 0.5 contour of the level set function ϕ. In air, $\phi = 0$ and in water $\phi = 1$. You can thus think of the level set function as the volume fraction of water. The transport of the interface is given by

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\phi\mathbf{u}) + \gamma\left[\left(\nabla \cdot \left(\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)\right) - \varepsilon\nabla \cdot \nabla\phi\right] = 0$$

The application mode uses the level set function to smooth the density and viscosity jump across the interface by letting

$$\rho = \rho_{\mathrm{air}} + (\rho_{\mathrm{water}} - \rho_{\mathrm{air}})\phi$$

$$\mu = \mu_{\mathrm{air}} + (\mu_{\mathrm{water}} - \mu_{\mathrm{air}})\phi$$

The delta function is approximated by

$$\delta = 6|\phi(1-\phi)||\nabla\phi|$$

and the interface normal is calculated from

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$$

INITIAL CONDITIONS

Initially, the reservoir is filled with water and the capillary channel is filled with air. The initial velocity is zero.

BOUNDARY CONDITIONS

Inlet

The hydrostatic pressure, $p = \rho g z$, gives the pressure at the inflow boundary. Only water enters through the inlet, so the level set function, that is, the volume fraction of water, is 1 here.

Outlet

At the outlet, the pressure is equal to zero, that is, equal to the pressure at the top of the inflow boundary. Because it is an outflow boundary, you do not have to set any condition on the level set function.

Walls

The boundary condition **Wetted wall** is suitable for solid walls in contact with a fluid interface. It sets the velocity component normal to the wall to zero, that is,

$$\mathbf{u} \cdot \mathbf{n}_{\mathrm{wall}} = 0$$

and adds a frictional boundary force

$$\mathbf{F}_{\mathrm{fr}} = -\frac{\eta}{\beta}\mathbf{u}$$

Here, β is the slip length. The boundary condition also allows you to specify the contact angle θ, that is, the angle between the wall and the fluid interface (see Figure 7-10 according to "Mass and Momentum Transport" on page 335). In this example, the contact angle is 67.5° and the slip length equals the mesh element size, h.

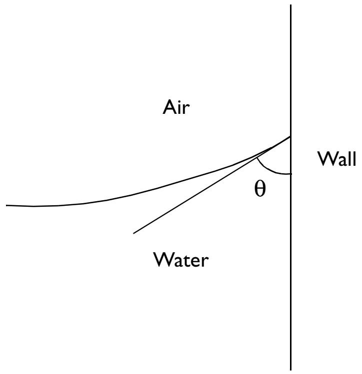
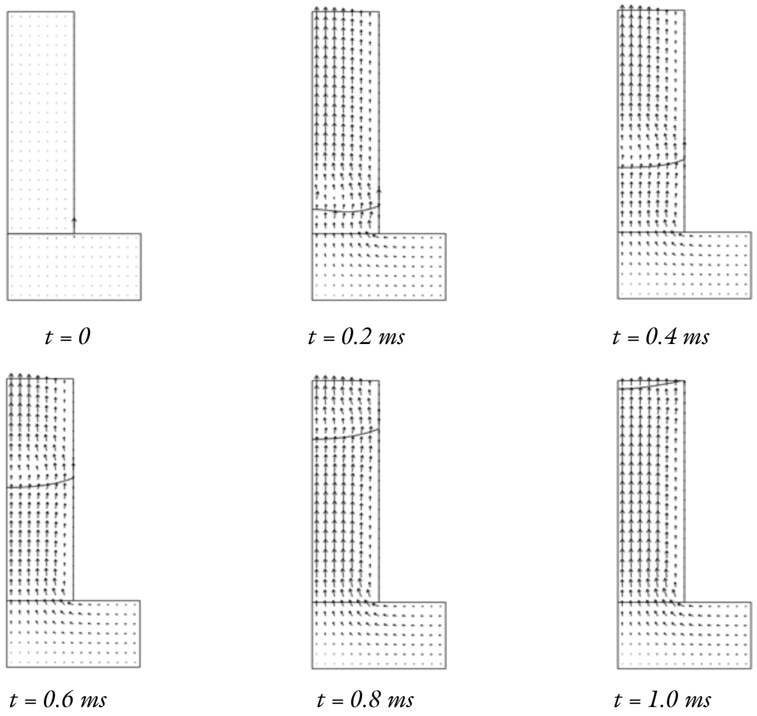


Figure 7-10: Definition of the contact angle θ.

Results and Discussion

Figure 7-11 shows the interface and the velocity field at different times. Initially, the shape of the interface changes dynamically (see Figure 7-12). After about 0.6 ms the shape of the water surface remains constant and forms a rising concave meniscus. Note that the slip velocity at the walls is almost zero, except close to the fluid interface/wall contact point.



$t = 0$

$t = 0.2$ ms

$t = 0.4$ ms

$t = 0.6$ ms

$t = 0.8$ ms

$t = 1.0$ ms

Figure 7-11: Interface and velocity field at different times.

Figure 7-12 shows how the interface dynamically deforms during the first 0.2 ms as a result of the surface tension at the water surface.

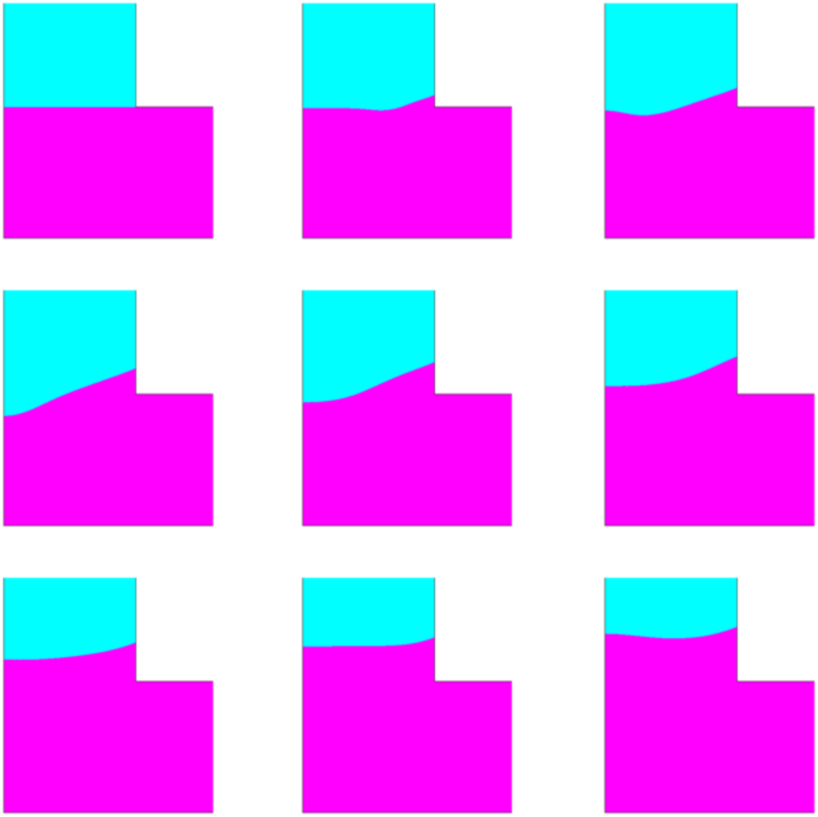


Figure 7-12: Snapshots of the position of the interface during the first 0.2 ms.

Figure 7-13 shows the pressure profile at $t = 0.6$ ms. At the fluid interface there is a pressure jump of roughly 300 Pa. The jump is caused by the surface tension, and forces water and air to rise through the channel.

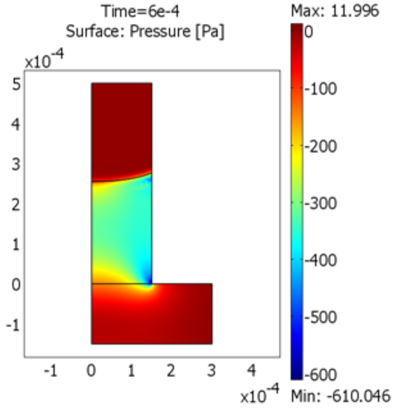


Figure 7-13: Pressure at t = 0.6 ms.

You can easily calculate the position of the interface/wall contact point by integrating the level set function along the thin cylinder wall. Figure 7-14 shows the position of the contact point as a function of time. After 0.6 ms, the contact point moves with an almost constant speed.

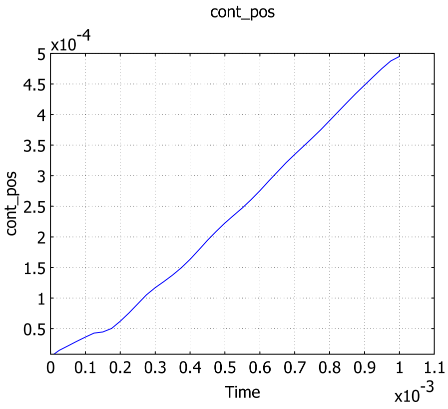


Figure 7-14: Position of the interface/wall contact point as a function of time. The velocity is approximately constant after t = 0.6 ms.

Finally, you can verify the obtained contact angle. It is defined by $\cos\theta = \mathbf{n}^T\mathbf{n}_{\text{wall}}$.

In this case, the normal to the wall is $\mathbf{n}_{\text{wall}} = (1, 0)$. The contact angle is thus $\theta = \text{acos}\, n_r$, where n_r is the radial component of the interface normal. At $t = 0.6$ ms, the contact angle is 1.16 rad $= 66°$, which can be compared with the imposed contact angle of $3\pi/8 = 1.18 = 67.5°$. The contact angle approaches the imposed value if you refine the mesh further.

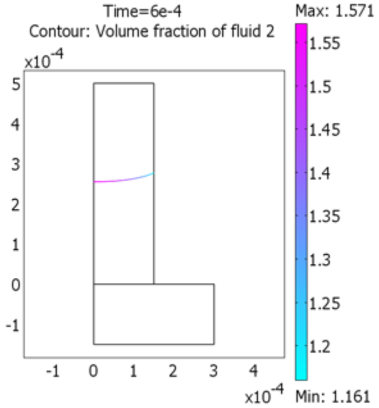


Figure 7-15: Plot of acos(n_r)*. At the wall, this gives the contact angle. In this case* $\theta = 1.16$ *rad* $= 66°$.

Modeling in COMSOL Multiphysics

It is straightforward to set up the model with the Level Set Two-Phase Flow, Laminar application mode. At the walls in contact with the fluid interface, use the Wetted wall boundary condition.

Model Library path:

`Chemical_Engineering_Module/Microfluidics/capillary_filling`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, go to the **Space dimension** list and select **Axial symmetry (2D)**.

2 From the list of application modes, select **Chemical Engineering Module>Momentum Transport>Multiphase Flow>Level Set Two-Phase Flow, Laminar**.

3 In the **Application mode name** edit field, type `twophase`, then click **OK**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar. Type `3e-4` in the **Width** edit field, `1.5e-4` in the **Height** edit field, `0` in the **r** edit field, and `-1.5e-4` in the **z** edit field. Click **OK**. Click the **Zoom Extents** button on the Main toolbar.

2 Create another rectangle with these settings:

WIDTH	HEIGHT	BASE	R	Z
`1.5e-4`	`5e-4`	Corner	0	0

3 Click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants:

NAME	EXPRESSION	DESCRIPTION
`theta`	`(3*pi/8)[rad]`	`Contact angle`
`p_ref`	`1e5[Pa]`	`Reference pressure`
`T_ref`	`293[K]`	`Temperature`
`sigma`	`0.073[N/m]`	`Surface tension coefficient`
`g`	`9.81[m/s^2]`	`Acceleration due to gravity`

3 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 In the **Model Tree**, right-click **Level Set Two-Phase Flow, Laminar (twophase)** and select **Subdomain Settings**.

Note: There are a number of different ways to open the **Subdomain Settings** and the **Boundary Settings** dialog boxes. This description assumes that you have the **Model Tree** visible in **Overview** mode. To open the **Model Tree** click the **Model Tree** button on the Main toolbar, then click the **Overview** button on the toolbar at the top of the **Model Tree**.

---

2 Press Ctrl and select both subdomains. In the **Fluid 1** area, click the **Load** button. Select **Liquids and Gases>Gases>Air, 1 atm** from the **Materials** list and click **OK**.

3 Click the **Load** button in the **Fluid 2** area. Select **Liquids and Gases>Liquids>Water, liquid** and click **OK**.

4 For both fluids, replace `p` and `T` in the expressions for the **Dynamic viscosity** and **Density** by `p_ref` and `T_ref`.

5 Go to the **Sources/Sinks** page. Type `sigma` in the **Surface tension coefficient** edit field and `-g` in the **Gravity, z component** edit field.

6 Click the **Init** tab. Select Subdomain 1 and select the option button **Fluid 2**.

7 Click **OK**.

Boundary Conditions

1 In the **Model Tree** right-click **Level Set Two-Phase Flow, Laminar (twophase)** and select **Boundary Settings**.

2 Assign boundary conditions for the exterior boundaries according to the following table.

SETTINGS	BOUNDARIES 1, 3	BOUNDARY 8	BOUNDARY 5	BOUNDARIES 6, 7
Boundary type	Symmetry boundary	Inlet	Outlet	Wall
Boundary condition	Axial symmetry	Pressure, no viscous stress	Pressure, no viscous stress	Wetted wall
p_0		`rho_twophase*z*gz_twophase`	0	
ϕ_0		1		
θ				`theta`
β				`h`

3 Select Boundary 4 and select the **Interior boundaries** check box. Select the boundary condition **Initial fluid interface**.

4 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu select **Mapped Mesh Parameters**.

2 Select both subdomains and select **Extremely fine** from the **Predefined mesh sizes** list.

3 Click the **Mesh Selected** button, then click **OK**.

COMPUTING THE SOLUTION

First reinitialize ϕ to obtain the correct shape of ϕ in the transition layer.

1 From the **Solve** menu select **Solver Parameters**.

2 Click the **General** tab and enter `1e-3` in the **Times** edit field. Click **OK**.

3 Click the **Solve** button on the Main toolbar. This creates a good initial solution to the level set function.

Use the obtained solution as an initial condition to the simulation of the droplet motion.

1 Click the **Solver Manager** button on the Main toolbar.

2 Click the **Store Solution** button. Select the time **0.001**. Click **OK**.

3 In the **Initial value** area click the **Stored solution** option button.

4 Select **0.001** from the **Solution at time** list, then click **OK**.

5 Click the **Solver Parameters** button on the Main toolbar.

6 Click the **General** tab, then enter `0:0.25e-4:1e-3` in the **Times** edit field. Click **OK**.

7 From the **Physics** menu, select **Properties**.

8 Change the **Analysis type** to **Transient**, then click **OK**.

9 Click the **Solve** button on the Main toolbar.

Note: The calculations take 2–3 hours.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, clear the **Surface** check box and select the **Contour** and **Arrow** check boxes.

3 On the **Contour** page, go to the **Contour levels** area and click the **Vector with isolevels** option button. Type `0.5` in the corresponding edit field.

4 Click the **Arrow** tab. From the **Predefined quantities** list on the **Subdomain Data** page, select **Velocity field**. In the **Number of points** edit field for **z points**, type `30`.

5 Click **Apply**.

6 On the **General** page, select a value from the **Solution at time** list and then click **Apply** to visualize the result at the corresponding value. Repeat to view the solution at other times.

7 Click **OK**.

8 To create a movie from the plots at the different times, click the **Animate** button on the Plot toolbar.

To create filled contour plots as in Figure 7-12, perform the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

3 On the **Contour** page, select the **Filled** check box.

4 Click **OK**.

Next, create the pressure plot in Figure 7-13.

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, clear the **Contour** check box and select the **Surface** check box in the **Plot type** area. In the **Solution to use** area, select `6e-4` from the **Solution at time** list.

3 Click the **Surface** tab. From the **Predefined quantities** list on the **Surface Data** page, select **Pressure**.

4 Click **OK**.

Follow the next steps to calculate and plot the position of the contact point as in Figure 7-14.

1 From the **Options** menu, select **Integration Coupling Variables>Boundary Variables**.

2 Select Boundary 6. Type `cont_pos` in the **Name** edit field on the first row of the table and `phi` in the corresponding **Expression** edit field. Click **OK**.

3 From the **Solve** menu, select **Update Model**.

4 From the **Postprocessing** menu, select **Global Variables Plot**.

5 Type `cont_pos` in the **Expression** edit field, then click the **Add Entered Expression** button next to the edit field. Click **OK** to generate the plot.

Finally, check the obtained contact angle.

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, clear the **Surface** check box and select the **Contour** check box in the **Plot type** area.

3 Click the **Contour** tab. On the **Color Data** page, click the **Color data** option button.

4 Clear the **Filled** check box.

5 In the **Expression** edit field, type `acos(normr_twophase)`, then click **OK**.

Transport in an Electrokinetic Valve

Introduction

This model presents an example of pressure-driven flow and electrophoresis in a microchannel system.

Researchers often use a device similar to the one in this model as an electrokinetic sample injector in biochips to obtain well-defined sample volumes of dissociated acids and salts and to transport these volumes. The model presents a study of a pinched injection cross valve during the focusing, injection, and separation stages. Inspiration for the model comes from a study by Ermakov and others (Ref. 1). Focusing is obtained through pressure-driven flow of the sample and buffer solution, which confines the sample in the focusing channel. When the system reaches steady state, the pressure-driven flow is turned off and an electric field is applied along the channels. This field drives the dissociated sample ions in the focusing zone at right angles to the focusing channel and through the injection channel. A clean separation of the sample ions is important, so the model examines the effect on ion separation of different configurations of the electric field.

This specific case does not account for electroosmosis because the channel surfaces are subjected to a treatment that minimizes the extension of the electric double layer. For a 3D version of this model, see “Transport in an Electrokinetic Valve, 3D Model” on page 365.

Model Definition

Figure 7-16 shows the model domain's geometry. The horizontal channel serves as the focusing channel and the vertical channel is the injection channel.

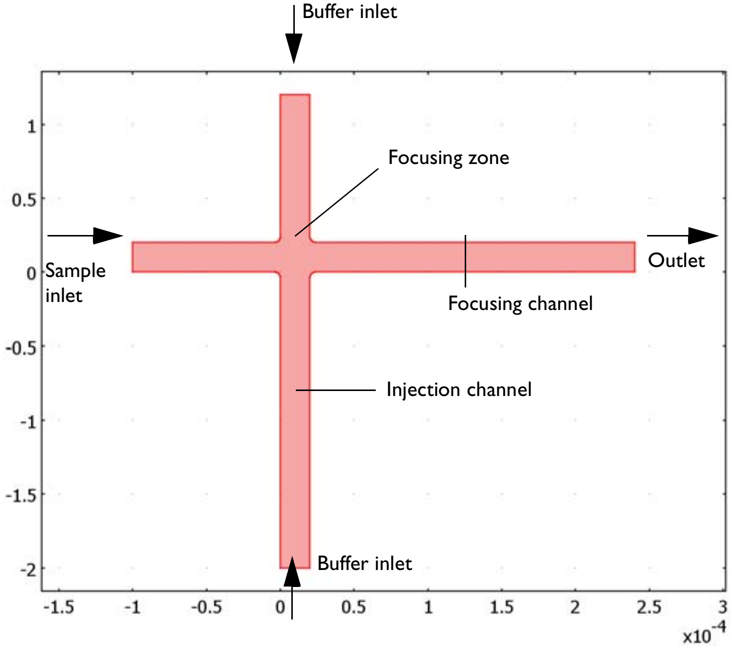


Figure 7-16: The focusing stage involves pressure-driven and electro-driven flow of the sample and the buffering solution from the left, top, and bottom to the right. An electric field is then applied over the focusing zone to induce transport down through the injection channel.

The device operation and hence the modeling procedure takes place in two stages: focusing and injection.

The focusing stage involves a buffering solution that is injected through pressure-driven convection and electro-driven migration into the vertical channel. The buffering solution neutralizes the acids contained in the sample except for a very thin region confined to the junction between the horizontal and vertical channels. This means that the dissociated ions are found only in the needle-shaped region in the focusing zone.

During the injection stage, convective flow is turned off and an electric field is applied in both the horizontal and vertical directions toward the upper end of the injection channel (see Figure 7-17).

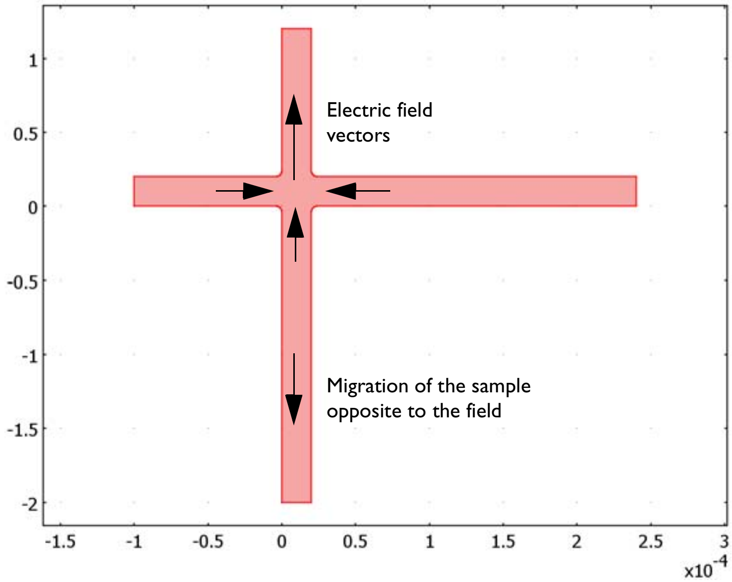


Figure 7-17: During the injection stage, the convective flow is turned off and an electric field is applied. The horizontal field prevents sample broadening while the vertical field injects the sample into the vertical channel in a direction opposite to the electric field.

The horizontal field focuses the sample during the initial part of the injection stage to produce a well-separated sample. The vertical field is applied to migrate the sample from the focusing channel to the injection point at the lower end of the vertical channel. The sample ions are negatively charged and thus migrate in the opposite direction to the electric field. To study the effect of sample distortion during the injection stage, the simulation also covers the case where the horizontal field has not been applied.

This study assumes that the concentration of charged samples is very low compared to that of other ions dissolved in the solution. This implies that the sample concentration does not influence the solution's conductivity and that you can neglect the concentration gradients of the charge-carrying species, which are present in a much higher concentration than the sample ions. Such an electrolyte is referred to as a supporting electrolyte.

Further assume that concentration variations of the sample species are small in the direction perpendicular to the *xy*-plane, which reduces a 3D model to a 2D approximation. This assumption is not entirely true for pressure-driven flow, and a detailed model would include the third dimension.

The model uses the Navier-Stokes equations, the equation for current balance, and a mass transport based on the Nernst-Planck equation. The steady-state solution for the focusing stage serves as the initial condition for the injection stages.

The boundary conditions are changed between the focusing and injection stages. Moreover, you do not solve the Navier-Stokes equations during the injection stage because the transport of the charged sample takes place through diffusion and migration (electrophoresis). The model equations are formulated below.

THE FOCUSING STAGE

The Navier-Stokes equations give the global momentum transport

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = 0, \tag{7-6}$$

which for incompressible flow is complemented by the mass-conservation equation

$$\nabla \cdot \mathbf{u} = 0. \tag{7-7}$$

Here η denotes the dynamic viscosity (Pa·s), $\mathbf{u}$ represents the velocity (m/s), ρ gives the fluid's density (kg/m^3), and p is the pressure (Pa).

The total balance of charges for a supporting electrolyte is given by the divergence of the current density, which in a supporting electrolyte satisfies Ohm's law,

$$\mathbf{i} = -\kappa\nabla V, \tag{7-8}$$

where κ is the electrolyte's conductivity (S/m) and V denotes the potential (V). Combined with the balance of current at steady state,

$$\nabla \cdot \mathbf{i} = 0, \tag{7-9}$$

this leads to a Laplace equation for the electric potential:

$$\nabla \cdot (-\kappa\nabla V) = 0. \tag{7-10}$$

The Nernst-Planck equation gives the flux vector for the sample ions with concentration, c (mol/m^3):

$$\mathbf{N} = -D\nabla c - zu_{\mathrm{m}}Fc\nabla V + c\mathbf{u}. \tag{7-11}$$

For the focusing stage, you solve the electrolyte mass-conservation equation at steady state, $\nabla \cdot \mathbf{N} = 0$, in a fixed background potential:

$$\nabla \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla V + c\mathbf{u}) = 0 . \qquad (7\text{-}12)$$

In Equations 7-11 and 7-12, D is the diffusivity (m^2/s), z is the charge number, u_{m} represents the mobility ($\mathrm{mol{\cdot}m^2/(J{\cdot}s)}$), and F equals Faraday's constant (C/mol).

Turning to the boundary conditions, assume laminar flow at the inlets with specified average inflow velocities. At the outlet, the shear-stress tensor components normal to the boundary are negligible,

$$\mathbf{n} \cdot \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) = 0 , \qquad (7\text{-}13)$$

and the pressure is constant,

$$p = 0 . \qquad (7\text{-}14)$$

The boundary conditions for the charge balance set the potential at the inlet and outlet boundaries:

$$V = V_{0,i} \qquad (7\text{-}15)$$

Here the index i runs over the inlet and outlet boundaries. Assume that all wall boundaries are insulating, so that

$$\nabla V \cdot \mathbf{n} = 0 . \qquad (7\text{-}16)$$

The boundary conditions for the mass transport of the sample during the focusing stage specify the concentration at the sample inlet and at the two buffer inlets located at the ends of the vertical channel:

$$\begin{aligned} c &= c_{\mathrm{in}} && \text{at the sample inlet} \\ c &= 0 && \text{at the buffer inlets} \end{aligned} \qquad (7\text{-}17)$$

The boundary condition at the outlet states that convection is the dominating transport mechanism there (that is, diffusion and migration are negligible):

$$\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla V) = 0 . \qquad (7\text{-}18)$$

THE INJECTION AND SEPARATION STAGES

During the injection and separation stages, you turn off the flow and modify the electric-field configuration. To account for the latter change, solve Equation 7-10 again using a new set of boundary conditions.

In the transient mass transport for the dilute species you assume the convective term to be zero, resulting in the equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c - z u_{\mathrm{m}} F c \nabla V) = 0 . \tag{7-19}$$

The boundary conditions for the current-balance equation implies that the potential is locked at all boundaries except for the walls:

$$V = V_{0,\,i} . \tag{7-20}$$

The walls, in contrast, you assume to be electrically insulated:

$$\nabla V \cdot \mathbf{n} = 0 . \tag{7-21}$$

The mass-transport boundary conditions are different from those during the focusing stage. During the injection and separation stages, you leave the inlet and outlet boundaries open and assume that migration is the dominating transport mechanism:

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_{\mathrm{m}i} F c_i \nabla V) \cdot \mathbf{n} . \tag{7-22}$$

The time-dependent solution requires an initial condition for the mass transport, namely

$$c(t = 0) = c_{\mathrm{focus}} \tag{7-23}$$

where the concentration comes from the steady-state solution reached at the end of the focusing stage.

Results and Discussion

This study covers two configurations for the potential. In the first, Mode A, the electric field in the injection stage is applied only over the injection channel. Figure 7-18 depicts the resulting concentration distribution in a time sequence.

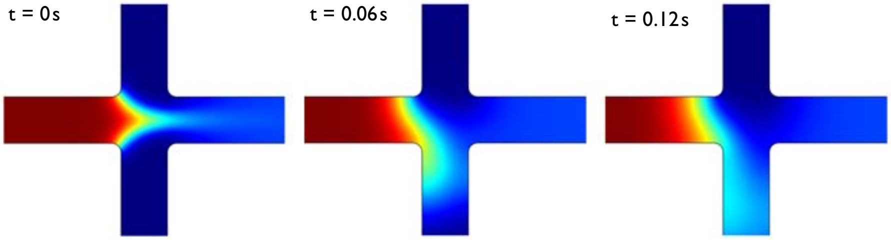


Figure 7-18: The concentration distribution during the focusing (left) and injection stages (middle and right) in the electrokinetic valve's junction. The separation stage is part of the injection stage. The right plot of the separation step shows that the detachment of the sample is incomplete.

The figure clearly shows that the detachment of the sample during the separation process is incomplete. In fact, if the separated sample is allowed to travel further down the injection channel, the poorly separated region remains attached to the focusing zone. This is clearly visible in Figure 7-19, which shows the cross-section of the concentration profiles at different time steps during the simulation 5 µm from the left wall of the injection channel. The concentration peak moves downwards along the injection channel, but a part of the sample remains attached to the focusing zone. This effect gives an unwanted distortion of the sample and a deviation from a required bell-curve shape for the concentration profile.

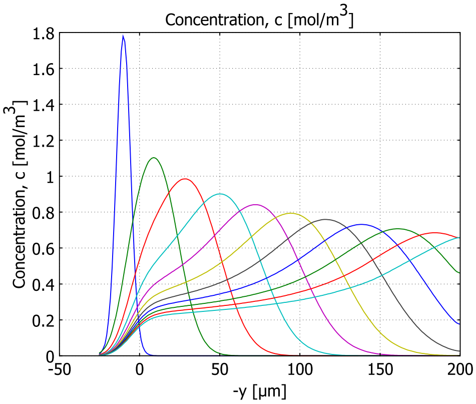


Figure 7-19: Mode-A concentration profiles along the injection channel at the times 0 s, 0.06 s, 0.12 s, 0.18 s, 0.24 s, 0.30 s, 0.36 s, 0.42 s, 0.48 s, 0.54 s, and 0.60 s after initiation of the injection stage. The incomplete detachment is clearly seen in the graph.

In Mode B, you apply an electric field in the horizontal direction, inward from both ends to the focusing zone, to avoid broadening of the sample top and to ensure complete detachment. The next two figures examine the results from that simulation.

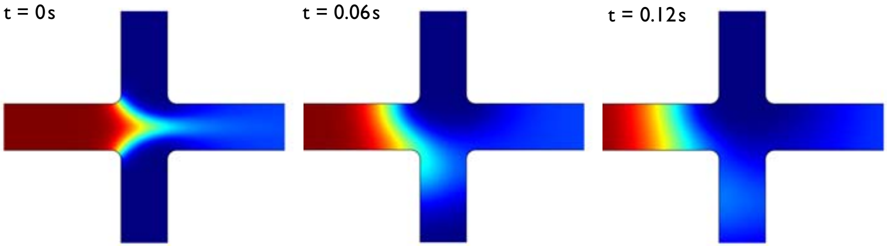


Figure 7-20: In this case the sample has almost completely detached during the separation stage compared to the results in Figure 7-18. It should be mentioned that the electric field strength has a different distribution, which gives a slightly lower migration rate.

Figure 7-20 shows the improved detachment effect that the horizontal field has on the separation of the sample. This is even clearer in Figure 7-21, in which the concentration profile forms a nice bell curve throughout the downward transport in the injection channel.

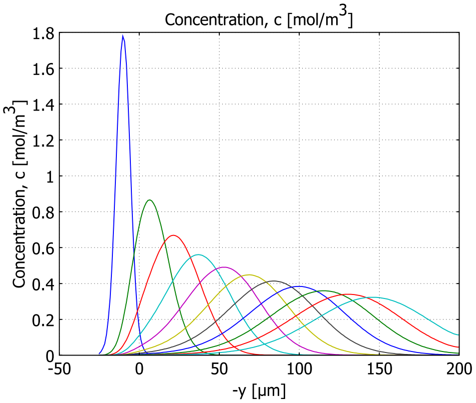


Figure 7-21: Mode-B concentration profiles along the injection channel at 0 s, 0.06 s, 0.12 s, 0.18 s, 0.24 s, 0.30 s, 0.36 s, 0.42 s, 0.48 s, 0.54 s, and 0.60 s after initiation of the injection stage. The separation of the sample is substantially improved compared to the Mode-A simulation in Figure 7-19.

This study clearly shows that modeling is extremely valuable in the investigation of electrophoretic transport. You can vary the configuration of the potential to obtain even better focusing and injection stages for the studied valve.

Reference

1. S.V. Ermakov, S.C. Jacobson, and J.M. Ramsey, "Computer Simulations of Electrokinetic Mass Transport in Microfabricated Fluidic Devices," *Tech. Proc. 1999 Intl. Conf. on Modeling and Simulation of Microsystems*, Computational Publications, 1999.

Modeling in COMSOL Multiphysics

The COMSOL Multiphysics implementation is reasonably straightforward but deserves a few comments. The main strategy is to first solve the equations for the focusing stage using the stationary solver and then solve the equations for the injection stage using both the stationary and time-dependent solvers. The following list provides a summary of the main steps:

1. Solve the steady-state problem for the focusing stage, which involves the Navier-Stokes, charge-balance, and mass-transport equations.
2. Store the solution.
3. Change the boundary conditions for the charge balance and re-solve the equation for this balance only. Keep the solution for the concentration field unchanged.
4. Store the solution.
5. Change the boundary conditions for the mass transport.
6. Change the settings to a time-dependent problem and set the velocity components u and v to zero in the Electrokinetic Flow application mode.
7. Re-solve the problem.

Model Library path:
`Chemical_Engineering_Module/Microfluidics/electrokinetic_valve_2d`

Modeling Using the Graphical User Interface

1. In the **Model Navigator** set the **Space dimension** to **2D**.
2. In the list of application modes select **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.

3 Click the **Multiphysics** button, then click **Add**.

4 Similarly add two more application modes: **Chemical Engineering Module>Mass Transport>Electrokinetic Flow>Transient analysis** and **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**.

Note that you must explicitly select the transient analysis type for the Electrokinetic Flow application mode; by not selecting an analysis type for Incompressible Navier-Stokes, you get the correct stationary analysis type for that application mode.

5 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the constants in the following table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`u_av`	`0.2[mm/s]`	`Average velocity, sample inlet`
`v_av`	`0.67[mm/s]`	`Average velocity, buffer inlets`
`rho`	`1e3[kg/m^3]`	`Fluid density`
`eta`	`1e-3[Pa*s]`	`Fluid viscosity`
`D`	`1e-9[m^2/s]`	`Sample ion diffusivity`
`Rg`	`8.314[J/(mol*K)]`	`Gas constant`
`T`	`298[K]`	`Temperature`
`nu`	`D/(Rg*T)`	`Sample ion mobility`
`sigma`	`1[S/m]`	`Electric conductivity, electrolyte`
`c_in`	`0.05*3.5[g/l]/(22+35)[g/mol]`	`Sample inlet concentration`

GEOMETRY MODELING

1 Hold the Shift key and click the **Rectangle/Square** button on the Draw toolbar.

2 In the **Rectangle** dialog box that appears, enter the following properties; when done, click **OK**.

PARAMETER	VALUE
Width	`2e-5`
Height	`3.2e-4`
x position	`0`
y position	`-2e-4`

3 Repeat this procedure for a second rectangle with the following dimensions.

PARAMETER	VALUE
Width	`3.4e-4`
Height	`2e-5`
x position	`-1e-4`
y position	`0`

4 Click the **Zoom Extents** button on the Main toolbar.

5 Press Ctrl+A to select both rectangles.

6 Click first the **Union** button and then the **Delete Interior Boundaries** button on the Draw toolbar.

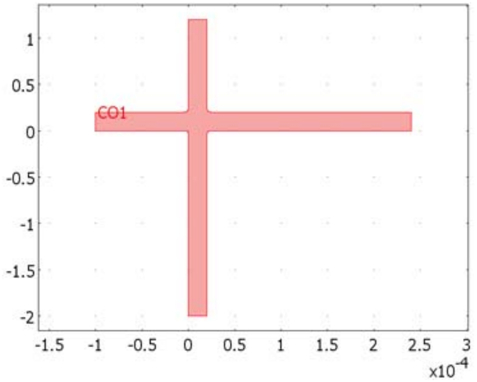
7 Click the **Fillet/Chamfer** button on the Draw toolbar.

8 In the drawing area, Ctrl-click to select the four vertices where the horizontal and vertical channels meet (Vertices 4, 5, 8, and 9).

9 In the **Fillet/Chamfer** dialog box, set the fillet **Radius** to `4e-6`.

10 Click **OK**.

The model geometry is now complete; it should look like that in the following figure.



PHYSICS SETTINGS—FOCUSING STAGE

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Select Subdomain 1, then enter these subdomain settings; when done, click **OK**.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

4 From the **Multiphysics** menu, select **2 Electrokinetic Flow (chekf)**.

5 From the **Physics** menu, open the **Subdomain Settings** dialog box.

6 With Subdomain 1 selected, enter these subdomain settings; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	`D`
R	`0`
u_m	`nu`
z	`-1`
u	`u`
v	`v`
V	`V`

7 From the **Multiphysics** menu, select **3 Conductive Media DC (dc)**.

8 From the **Physics** menu, open the **Subdomain Settings** dialog box.

9 Select Subdomain 1, then set σ to `sigma`. Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Specify boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 5, 7	BOUNDARY 12	BOUNDARIES 2–4, 6, 8–11, 13–16
Boundary type	Inlet	Inlet	Outlet	Wall
Boundary condition	Laminar inflow	Laminar inflow	Pressure, no viscous stress	No slip
U_0	`u_av`	`v_av`		
L_{entr}	`1e-4`	`1e-4`		
Constrain end points to zero	Yes	Yes		
p_0			`0`	

4 From the **Multiphysics** menu, select **2 Electrokinetic Flow (chekf)**.

5 Specify boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2–4, 6, 8–11, 13–16	BOUNDARIES 5, 7	BOUNDARY 12
Boundary condition	Concentration	Insulation/ Symmetry	Concentration	Convective flux
c_0	`c_in`		`0`	

6 From the **Multiphysics** menu, select **3 Conductive Media DC (dc)**.

7 Specify boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2–11, 13–16	BOUNDARY 12
Boundary condition	Electric potential	Electric insulation	Ground
V_0	`-1`		-

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** button.

3 Set the **Maximum element size** to `2e-6` and the **Mesh curvature factor** to `0.5`.

The latter setting increases the typical mesh-element size near the fillets compared to that obtained with the default parameter value 0.3, while maintaining a sufficient mesh resolution in these regions.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION—FOCUSING STAGE

First, compute the solution for the velocity field, and then use that solution when solving the mass-transport problem.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Incompressible Navier-Stokes (chns)** from the **Solve for variables** list.

3 Click the **Solve** button.

4 When the solver has finished, click the **Initial Value** tab.

5 Click the **Current solution** option button in the **Initial value** area, then return to the **Solve For** page.

6 From the **Solve for variables** list, select **Conductive Media DC (dc)**. Click **Solve**.

7 From the **Solve for variables** list, select **Electrokinetic Flow (chekf)**. Click **Solve**.

8 Click the **Initial Value** tab.

9 Click the **Store Solution** button, then click **OK** to close the dialog box.

The focusing stage is now complete. In the next step you solve the model for the transient problem that describes the injection and separation stages.

PHYSICS SETTINGS—INJECTION STAGE, MODE A

Subdomain Settings

1 From the **Multiphysics** menu, select **2 Electrokinetic Flow (chekf)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Change the values for **u** and **v** to `0`, then click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundaries 1, 5, 7, and 12 (the inlets and outlets).

3 From the **Boundary condition** list, select **Flux**.

4 In the $\mathbf{N_0}$ edit field, type `-nmflux_c_chekf`.

The predefined boundary variable `nmflux_c_chekf` gives the outward normal electrophoretic flux, $\mathbf{N}_i \cdot \mathbf{n}$ (see Equation 7-22 for its definition).

5 Click **OK**.

6 From the **Multiphysics** menu, select **3 Conductive Media DC (dc)**.

7 From the **Physics** menu, select **Boundary Settings**.

8 Modify the following boundary settings; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 12	BOUNDARY 5	BOUNDARY 7
Boundary condition	Electric insulation	Ground	Electric potential
V_0	-	-	`-3.2`

COMPUTING THE SOLUTION—INJECTION STAGE, MODE A

1 Click the **Solver Manager** button on the Main toolbar.

2 Click the **Script** tab. Select the **Automatically add commands when solving** check box.

This setting instructs the software to record the subsequent solver settings and commands, which you can then reuse when solving Mode B.

3. Click the **Initial Value** tab. Click the **Stored solution** option button in the **Initial value** area. This makes the steady-state solution from the focusing stage the initial solution.
4. Click the **Solve For** tab. In the **Solve for variables** list, select **Conductive Media DC (dc)**, then click **Solve**.
5. Click the **Initial Value** tab. In the **Initial value** area, click the **Current solution** option button.
6. Leaving the **Solver Manager** dialog box open, click the **Solver Parameters** button on the Main toolbar.
7. From the **Analysis** list, select **Transient**.
8. In the **Times** edit field, type `0:0.03:0.6`.
9. Click **OK** to close the **Solver Parameters** dialog box.
10. Return to the **Solver Manager** and click the **Solve For** tab.
11. In the **Solve for variables** list, select **Electrokinetic Flow (chekf)**.
12. Click **OK** to close the **Solver Manager**.
13. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION—MODE A

To generate the three plots in Figure 7-18 on page 354, follow these steps:

1. From the **Options** menu, open the **Axes/Grid Settings** dialog box.
2. On the **Grid** page, select the **Auto** check box.
3. On the **Axis** page, set **x min** and **y min** to `-4e-5`, and **x max** and **y max** to `6e-5`. Click **OK**.
4. From the **Postprocessing** menu, open the **Plot Parameters** dialog box.
5. Click the **Surface** tab. On the **Surface Data** page, choose **Electrokinetic Flow (chekf)>Concentration, c** from the **Predefined quantities** list.
6. On the **General** page, clear the **Auto** check box for **Element refinement** and type `5` in the associated edit field.
7. Select **0** from the **Solution at time** list.
8. Click **Apply** to generate the plot in the left panel.
9. On the **General** page, select **0.06** from the **Solution at time** list.
10. Click **Apply** to generate the plot in the center panel of Figure 7-18.
11. Select **0.12** from the **Solution at time** list.

12 Click **OK** to close the dialog box and generate the plot in the right panel.

Generate Figure 7-19 using the cross-section plot functionality:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 On the **General** page, select every other time step from the **Solutions to use** list starting with **0**.

3 Click the **Line/Extrusion** tab.

4 In the **y-axis data** area, choose **Electrokinetic Flow (chekf)>Concentration, c** from the **Predefined quantities** list.

5 In the **x-axis data** area, click the lower option button, then click the **Expression** button. In the **X-Axis Data** dialog box, type `-y` in the **Expression** edit field. From the **Unit** list, select **µm**, then click **OK**.

6 In the **Cross-section line data** area, specify the following settings:

PROPERTY	VALUE
x0	`0.1e-4`
x1	`0.1e-4`
y0	`0.25e-4`
y1	`-2e-4`

7 Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the plot.

PHYSICS SETTINGS—INJECTION STAGE, MODE B

The next step is to model the second configuration of the electric field—Mode B.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Modify the following boundary settings for the Conductive Media DC application mode; when done, click **OK**.

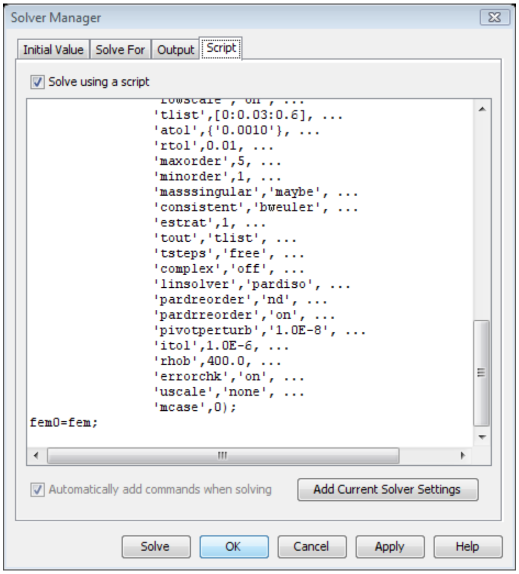
SETTINGS	BOUNDARY 1	BOUNDARY 12
Boundary condition	Electric potential	Ground
V_0	-1	-

COMPUTING THE SOLUTION—INJECTION STAGE, MODE B

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Script** page, select the **Solve using a script** check box.

3 Click **Solve** to execute the script you see in the edit window.



```
                 'tlist',[0:0.03:0.6], ...
                 'atol',{'0.0010'}, ...
                 'rtol',0.01, ...
                 'maxorder',5, ...
                 'minorder',1, ...
                 'masssingular','maybe', ...
                 'consistent','bweuler', ...
                 'estrat',1, ...
                 'tout','tlist', ...
                 'tsteps','free', ...
                 'complex','off', ...
                 'linsolver','pardiso', ...
                 'pardreorder','nd', ...
                 'pardrreorder','on', ...
                 'pivotperturb','1.0E-8', ...
                 'itol',1.0E-6, ...
                 'rhob',400.0, ...
                 'errorchk','on', ...
                 'uscale','none', ...
                 'mcase',0);
fem0=fem;
```

4 Click **OK** to close the **Solver Manager**.

POSTPROCESSING AND VISUALIZATION—MODE B

Generate the three plots in Figure 7-20 on page 355 as follows:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select **0** from the **Solution at time** list. Click **Apply**.

This generates the plot in the left panel.

3 Repeat Step 2 but select, in turn, **0.06** and **0.12** from the **Solution at time** list to generate the remaining two plots. When done, click **Cancel** to close the dialog box.

Finally, generate the plot in Figure 7-21 with the following steps:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 On the **General** page, select every other entry in the **Solutions to use** list starting with **0**, then click **OK**.

Transport in an Electrokinetic Valve, 3D Model

Introduction

This model presents an example of pressure-driven flow and electrophoresis in a microchannel system.

Researchers often use a device similar to the one in this model as an electrokinetic sample injector in biochips to obtain well-defined sample volumes of dissociated acids and salts and to transport these volumes. The model presents a study of a pinched injection cross valve during the focusing, injection, and separation stages. Inspiration for the model comes from a study by Ermakov and others (Ref. 1). Focusing is obtained through pressure-driven flow of the sample and buffer solution, which confines the sample in the focusing channel. When the system reaches steady state, the pressure-driven flow is turned off and an electric field is applied along the channels. This field drives the dissociated sample ions in the focusing zone at right angles to the focusing channel and through the injection channel. A clean separation of the sample ions is important, so the model examines the effect on ion separation of different configurations of the electric field.

This specific case does not account for electroosmosis because the channel surfaces are subjected to a treatment that minimizes the extension of the electric double layer.

Model Definition

Figure 7-16 shows a 2D cross section of the geometry in the xz-plane and points out the different channels and boundaries. The horizontal channel serves as the focusing channel, while the vertical channel is the injection channel. The actual model is in 3D with rectangular pipes whose corners are rounded. For geometry dimensions refer to Table 7-3 on page 374.

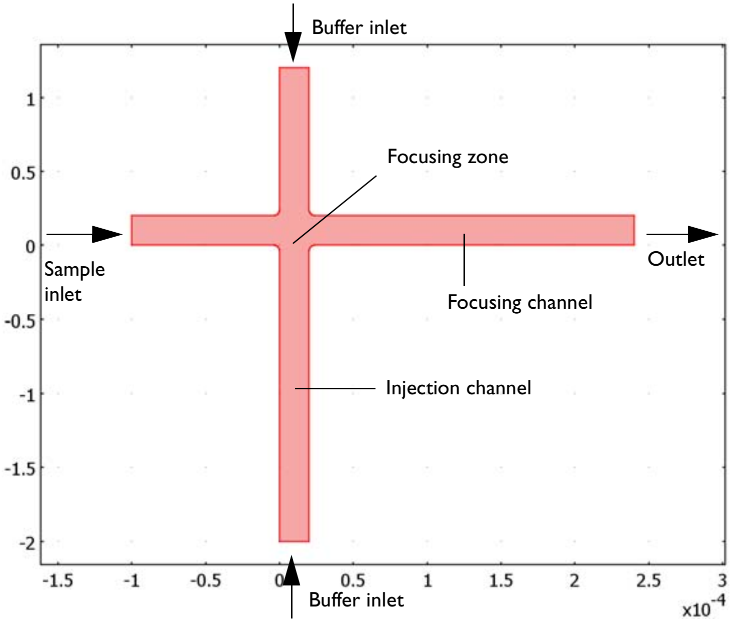


Figure 7-22: The focusing stage involves pressure-driven flow of both the sample and the buffering solution. The device applies an electric field over the focusing channel.

The device operation and hence the modeling procedure takes place in two stages: focusing and injection.

In the focusing stage, the device injects a buffering solution through pressure-driven convection into the vertical channels from the top and bottom. At the same time, it forces the sample solution through the horizontal focusing channel (see Figure 7-16). The buffering solution neutralizes the acids contained in the sample except for a very thin region confined to the crossing between the horizontal and vertical channels. This means that the dissociated ions are only in a needle-shaped region in the focusing zone.

Next, in the injection stage the device turns off the convective flow and then applies a vertical field to migrate the sample from the focusing channel to the injection point at the lower end of the vertical channel. The sample ions are negatively charged and migrate in opposite direction to the electric field. This model studies two different configurations (See Table 7-2) for the applied electric field. In the first configuration (Injection stage, Mode A) electric field is only applied in the vertical direction. In the second configuration (Injection stage, Mode B) the electric field is applied in both the horizontal and vertical directions (Figure 7-17).The horizontal field focuses the sample during the initial part of the injection stage in order to obtain a well-separated sample.

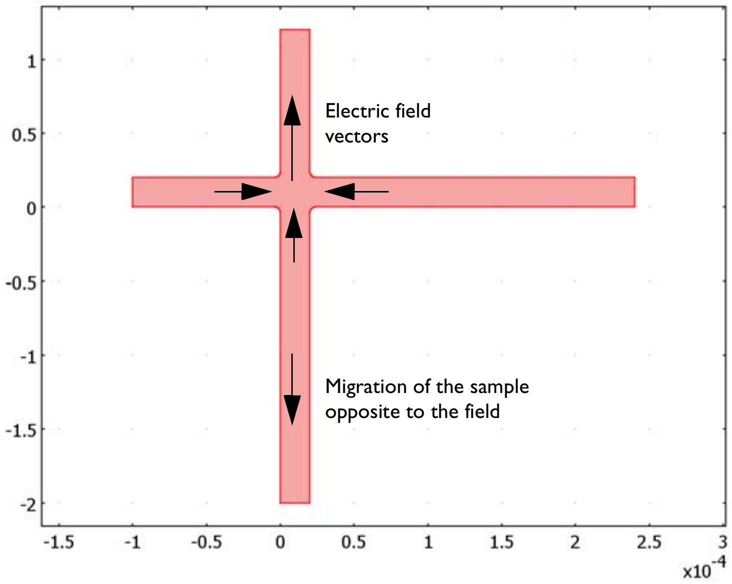


Figure 7-23: During the injection stage, the device turns off convective flow and applies an electric field. The horizontal field avoids the broadening of the sample, while the vertical field injects the sample into the vertical channel in the direction opposite to the electric field.

TABLE 7-2: APPLIED ELECTRIC FIELD CONFIGURATION

INLET	**MODE A**	**MODE B**
Sample inlet	Electric insulation	Electric potential, V = -1V
Outlet	Electric insulation	Electric potential, V = 0V
Upper buffer inlet	Electric potential, V = -3.2V	Electric potential, V = -3.2V
Lower buffer inlet	Electric potential, V = 0V	Electric potential, V = 0V

The model assumes that the charged sample concentration is very low compared to other ions dissolved in the solution. This implies that the sample concentration does not influence the solution’s conductivity and that you can neglect the concentration gradients of the charge-carrying species, which are present in a much higher concentration than the sample ions. Such an electrolyte is known as a supporting electrolyte.

Several equations describe the model: the Stokes flow equations, the equation for current balance, and a mass balance using the Nernst-Planck equation. This model uses the steady-state solution for the focusing stage as the initial condition for the injection stages.

Now consider the formulation of the model equations.

THE FOCUSING STAGE

The incompressible Navier-Stokes equations give the global mass a momentum balance in the focusing stage:

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

In these equations, η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ is the velocity (m/s), p is the pressure (Pa).

The total balance of charges for a supporting electrolyte comes from the divergence of the current-density vector, which in a supporting electrolyte is given by Ohm's law:

$$\mathbf{i} = -\kappa\nabla V$$

Here κ is the electrolyte's conductivity (S/m) and V is the potential (V). The balance of current at steady state then becomes

$$\nabla\cdot\mathbf{i} = 0$$

which gives

$$\nabla\cdot(-\kappa\nabla V) = 0$$

The flux vector for the sample ions comes from the Nernst-Planck equation

$$\mathbf{N}_i = -D_i\nabla c_i - z_i u_{\mathrm{m}i}Fc_i\nabla V + c_i\mathbf{u}$$

which leads to the following mass balance equation at steady state for species i:

$$\nabla\cdot(-D_i\nabla c_i - z_i u_{\mathrm{m}i}Fc_i\nabla V + c_i\mathbf{u}) = 0$$

Here c_i is the concentration (mol/m^3), D_i represents the diffusivity (m^2/s), z_i equals the charge number (which equals 1 for this model), $u_{\mathrm{m}i}$ is the mobility (s·mol/kg), and F is Faraday's constant (C/mol).

For the pressure-driven flow, assume that the flow has fully developed laminar form in all inlets, that all sides have no-slip conditions, and that the fluid flows freely out from the end of the focusing channel.

The boundary conditions for the charge balance determine the potential at the respective inlet and outlet boundary

$$V = V_{0,\,i}$$

where i denotes the index for each boundary. This model also assumes that all wall boundaries are insulating:

$$\nabla V \cdot \mathbf{n} = 0$$

The boundary conditions for the mass balance of the sample during the focusing stage appear below. The equation

$$c = c_{\mathrm{in}}$$

gives the concentration at the inlet of the sample, while the equation

$$c = c_{\mathrm{buffer}}$$

gives the concentration of the buffer at the inlet of the two vertical channels, and the buffer inlets are at both boundaries in the vertical channel. At the outlet boundary, convection and migration are the dominating transport mechanisms (that is, diffusion is negligible), so that

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_{\mathrm{m}i} F c_i \nabla V + c_i \mathbf{u}) \cdot \mathbf{n}$$

THE INJECTION STAGE

In the injection and separation stages, the device turns the flow off and changes the configuration of the electric field. You again solve the charge-balance equations but with new boundary conditions:

$$\nabla \cdot (-\kappa \nabla V) = 0$$

The mass balance for the dilute species comes from a time-dependent mass balance:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m}i} F c_i \nabla V) = 0$$

The model assumes that the convective contribution is zero.

The boundary conditions for the current-balance equation imply that the potential is locked at all boundaries except for the walls,

$$V = V_{0,i}$$

Further assume the walls are electrically insulated, which yields

$$\nabla V \cdot \mathbf{n} = 0$$

As opposed to the focusing state, the boundary conditions for the mass balance are changed. In the injection stage, set the concentration at the inlet boundary:

$$c = c_{\mathrm{in}}$$

For all other boundaries, assume that migration is the dominating transport mechanism, so that

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_{\mathrm{m}i} F c_i \nabla V) \cdot \mathbf{n} \tag{7-24}$$

The time-dependent solution requires an initial condition for the mass balance, which you obtain from the steady-state solution of the focusing stage:

$$c(t=0) = c_{\mathrm{focus}}$$

Results and Discussion

This example analyzes the focusing stage and two configurations for the injection stages. Recall that the first injection-stage configuration (Mode A) applies the electric field only over the injection channel while the inlet and outlet boundaries of the focusing channel are insulated; the second injection-stage configuration (Mode B) applies the electric field over both channels.

Figure 7-24 shows the steady-state concentration distribution during the focusing stage along with the distribution at the beginning of the injection stage. Note that the vertical flows from the upper and lower injection channels focus the concentration on a very narrow region near the crossing area of the channels. Further away from the crossing area, however, the concentration spreads again more equally over the channel.

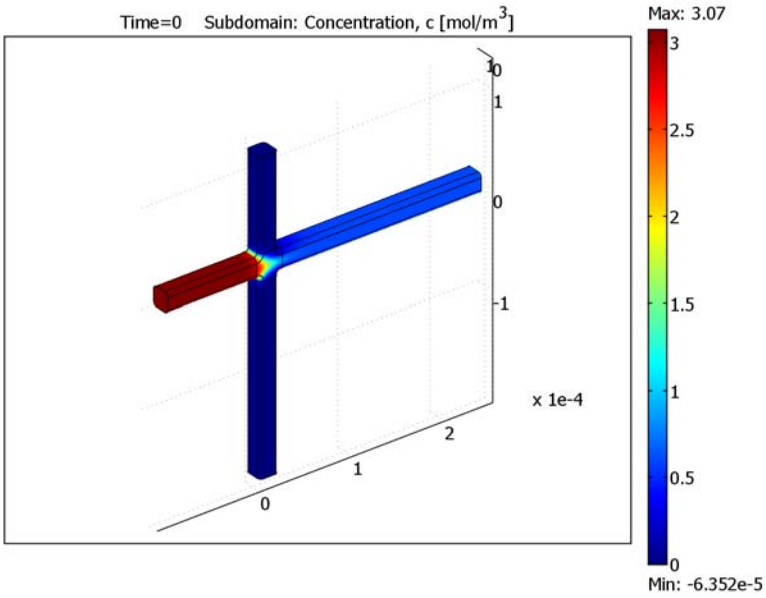


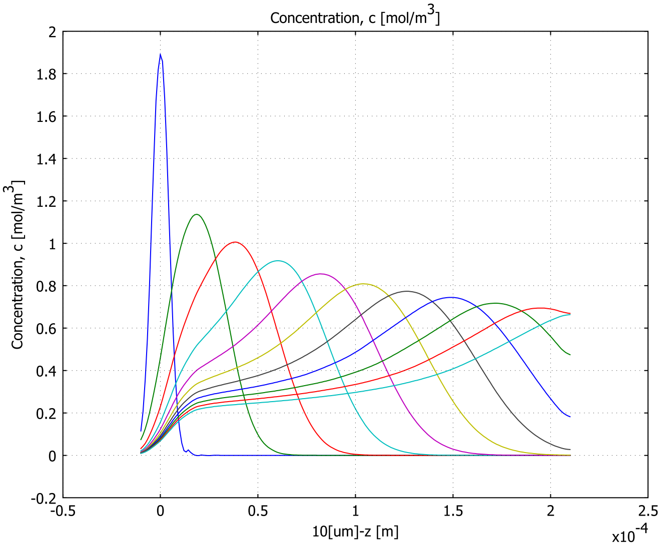
Figure 7-24: The steady-state concentration distribution during the focusing stage and prior to the injection stage.

Figure 7-25 and Figure 7-26 compare the concentration distribution for the two configurations at two times, specifically 0.06 s and 0.12 s after the beginning of the injection stage. The figures on the left show that for Mode A the concentration boundary is practically stationary in the horizontal direction. Consequently, the vertical electric field can continuously draw ions from the focusing channel, which results in poor separation and a poorly defined sample volume of the substance. For Mode B the situation is very different. The horizontal electric field draws the concentration boundary to the left, and the channels separate rapidly. Consequently, this scheme draws a well-defined sample volume of the substance into the injection channel.

Figure 7-25: The concentration distribution at a time 0.06 s after starting the injection stage for the Mode A configuration (left) and Mode B configuration (right).

Figure 7-26: The concentration distribution at a time 0.12 s after starting the injection stage for the Mode A configuration (left) and Mode B configuration (right).

It is also possible to observe the difference between the two configurations if you look at the concentration along a line through the middle of the injection channel, examining it at several times after the start of the injection stage (Figure 7-27). The maximum concentration moves down the injection channel with time. The peaks are higher in the upper axis corresponding to Mode A, but they are much wider than for Mode B. A considerable amount of concentration appears at the left of the peak, and the sample remains attached to the focusing area—resulting in an unwanted distortion of the sample package. The narrow peaks of Mode B, on the other hand, form nice bell curves throughout the downward transport in the injection channel, resulting in a well-defined sample package.



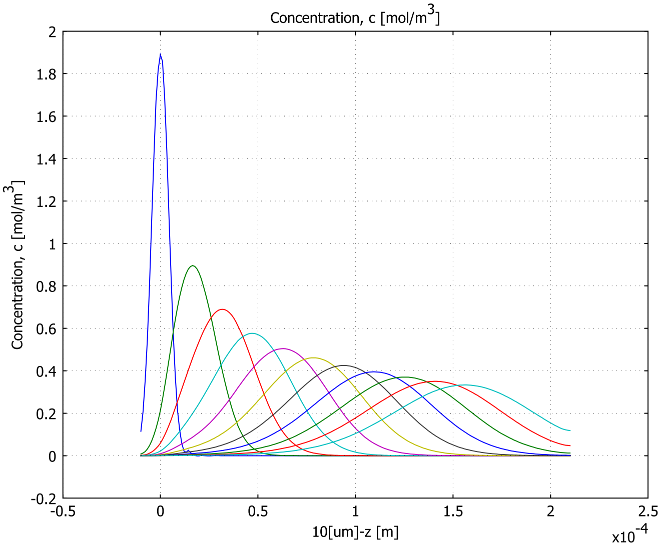


Figure 7-27: Concentration profile for Mode A (top) and Mode B (bottom) along the injection channel at various time steps: 0 s, 0.06 s, 0.12 s, 0.18 s, 0.24 s, 0.30 s, 0.36 s, 0.42 s, 0.48 s, 0.54 s, and 0.6 s after initialization of the injection stage. The origin of the x-axis marks the centerline of the focusing channel.

This study illustrates that modeling is extremely valuable in the investigation of electrophoretic transport. You can vary the configuration of the potential to obtain even better focusing and injection stages for the valve under study.

Modeling in COMSOL Multiphysics

APPLICATION MODES

In COMSOL Multiphysics you define the model with three application modes:

- The Incompressible Navier-Stokes application mode solves the fluid flow in the channels with Navier-Stokes equations.
- The Conductive Media DC application mode solves the equation for current balance.
- The Electrokinetic Flow application mode solves the Nernst-Planck equation.

GEOMETRY MODELING

Table 7-3 gives the dimensions of the model geometry. To draw it, proceed in four steps:

1. Initialize the geometry with simple blocks that represent the crossing of the channels.
2. Create a 2D work plane geometry in which you draw the cross section of the channel and a few assisting objects.
3. To finalize to channel crossing, apply the revolve operator to the 2D objects and subtract the resulting 3D objects from the original 3D blocks.
4. Finally apply the extrude operator to the 2D channel cross section to create the channels.

TABLE 7-3: MODEL DIMENSIONS

	HORIZONTAL CHANNEL	VERTICAL CHANNEL	CROSSING AREA
Dimensions (µm)			
- x	340	20	28
- y	20	20	20
- z	20	340	28
Position (µm)			
- x	-100	0	-4
- y	0	0	0

TABLE 7-3: MODEL DIMENSIONS

	HORIZONTAL CHANNEL	VERTICAL CHANNEL	CROSSING AREA
- z	0	-200	-4
Rounding (µm)			
- radius	4	4	4
- direction	in	in	out

COMPUTING THE SOLUTION

The operation of the actual device proceeds in two stages, the focusing stage and the injection stage. This model simulates two settings of the injection stage so in total it works in three phases.

The first phase defines the subdomain settings and boundary conditions for the focusing phase. Then the model solves the application modes sequentially with a nonlinear solver in the following sequence:

1. Incompressible Navier-Stokes Flow application mode
2. Conductive Media DC application mode
3. Electrokinetic Flow application mode

Each step uses the solution from the previous one. The model stores the last solution for use as the initial value for the consequent modeling.

In the second phase you change the subdomain settings and boundary conditions to handle the injection stage Mode A. In a real device you would turn off the convective flow; in the model you simulate this by setting the velocity parameters of the Electrokinetic Flow application mode to zero. Thus it uses no information from the Incompressible Navier-Stokes Flow application mode.

Solving the second phase starts from the stored solution of the first phase, and the model solves the Conductive Media DC application mode with a nonlinear solver. Then you select a time-dependent solver and solve the Electrokinetic Flow application mode. This solution is the result for the injection stage Mode A.

In the third phase you again change subdomain settings and boundary conditions but this time for the injection stage Mode B; you then solve for the final solution the same way as in the second phase.

Reference

1. S.V. Ermakov, S.C. Jacobson, and J.M. Ramsey, *Technical Proc 1999 Int'l Conf. on Modeling and Simulation of Microsystems*, Computational Publications, 1999.

Model Library path:
`Chemical_Engineering_Module/Microfluidics/electrokinetic_valve_3d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, select the **New** page, and from the **Space dimension** list select **3D**.

2 Click the **Multiphysics** button.

3 In the **Application Modes** tree, select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes**. Click **Add**.

4 In the **Application Modes** tree, select **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**. Click **Add**.

5 In the **Application Modes** tree, select **Chemical Engineering Module>Mass Transport>Electrokinetic Flow>Transient analysis**. Click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

Next define some constants for the model.

1 From the **Options** menu, choose **Constants**.

2 In the dialog box that opens, specify names, expressions, and (optionally) descriptions for the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`u_a`	`0.2[mm/s]`	`Average velocity, sample inlet`
`w_a`	`0.67[mm/s]`	`Average velocity, buffer inlets`
`rho`	`1e3[kg/m^3]`	`Fluid density`
`eta`	`1e-3[Pa*s]`	`Fluid viscosity`
`D`	`1e-9[m^2/s]`	`Sample ion diffusivity`

NAME	EXPRESSION	DESCRIPTION
`Rg`	`8.314[J/(mol*K)]`	`Gas constant`
`T`	`298[K]`	`Fluid temperature`
`nu`	`D/(Rg*T)`	`Sample ion mobility`
`sigma`	`1[S/m]`	`Electric conductivity, electrolyte`
`c_in`	`0.05*3.5[g/l]/(22+35)[g/mol]`	`Sample ion concentration, inlet`

GEOMETRY MODELING

3D Geometry—Step 1

Start the geometry by creating a simple set of rectangular blocks.

1 Click the **Block** tool on the 3D Draw toolbar and create two rectangular blocks using the settings from the following table; keep all other settings at their default values.

BLOCK	AXIS BASE POINT			LENGTH		
	X	Y	Z	X	Y	Z
BLK1	`-4e-6`	`0`	`-4e-6`	`28e-6`	`20e-6`	`28e-6`
BLK2	`-20e-6`	`0`	`-20e-6`	`60e-6`	`20e-6`	`60e-6`

2 Click the **Zoom Extents** button on the Main toolbar.

Work Plane Geometry

Next create a 2D geometry on a work plane. After you extrude and revolve the objects, they shape the 3D geometry.

1 From the **Draw** menu, choose **Work Plane Settings**.

2 On the **Quick** page, click the **y-z** option button. Type `-4e-6` in the associated **x** edit field. Click **OK**.

3 Click the **Geom2** tab to activate the 2D work plane geometry.

4 Shift-click the **Rectangle/Square** button on the Draw toolbar.

5 Create a rectangle as in the following table; when done, click **OK**.

SIZE		POSITION		
WIDTH	HEIGHT	BASE	X	Y
`20e-6`	`20e-6`	Corner	`0`	`0`

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

7 Click the **Fillet/Chamfer** button on the Draw toolbar.

8 In the dialog box go to the **Vertex selection** area, open the menu tree under **R1**, then select the four corners. Click the **Fillet** option button, and in the **Radius** edit field type `4e-6`. Click **OK**.

9 Shift-click the **Rectangle/Square** button on the Draw toolbar. Create a rectangle as in the following table; when done, click **OK**.

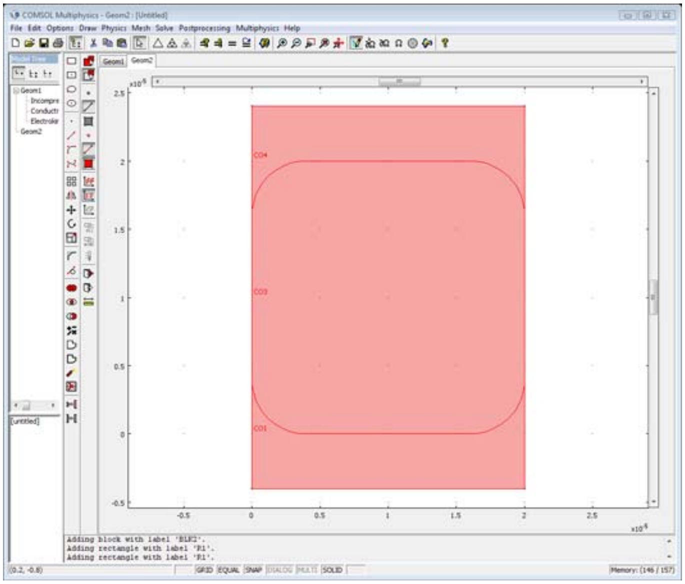
OBJECT	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	`20e-6`	`28e-6`	Corner	0	`-4e-6`

10 Click the **Create Composite Object** button on the Draw toolbar.

11 Verify that the **Keep interior boundaries** check box is selected.

12 In the **Set formula** edit field, type `CO1+R1`. Click **OK**.

13 Click the **Split Object** button on the Draw toolbar.



```
Adding block with label 'BLK2'.
Adding rectangle with label 'R1'.
Adding rectangle with label 'R1'.
```

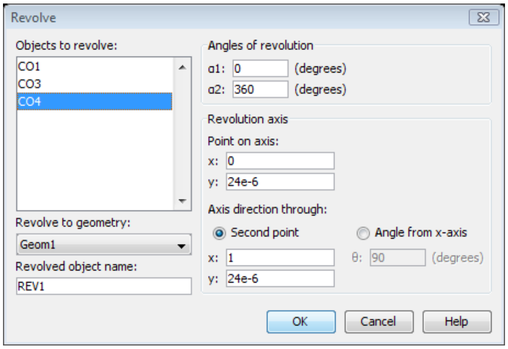
Zoom-in view of the completed 2D geometry.

3D Geometry—Step 2

After creating the work plane geometry, keep **Geom2** activated and use it to shape the 3D geometry.

1 From the **Draw** menu, choose **Revolve**.

2 In the resulting dialog box, enter settings as in the following figure.



Objects to revolve: CO1, CO3, CO4 (CO4 selected)
α1: 0 (degrees)
α2: 360 (degrees)
Point on axis:
x: 0
y: 24e-6
Axis direction through:
● Second point ○ Angle from x-axis
x: 1
y: 24e-6
θ: 90 (degrees)
Revolve to geometry: Geom1
Revolved object name: REV1

Settings for the Revolve operation.

3 Click **OK**. The revolved object automatically becomes activated in **Geom1**.

4 Click the **Array** button on the Draw toolbar.

5 In the dialog box that appears, specify the following settings, then click **OK**.

DISPLACEMENT			ARRAY SIZE		
X	Y	Z	X	Y	Z
28e-6	0	-28e-6	2	1	2

6 Click the **Create Composite Object** button on the Draw toolbar.

7 In the **Set formula** edit field, type `BLK2-REV1-REV2-REV3-REV4`. Click **Apply**.

8 In the **Set formula** edit field, type `BLK1*CO1`. Click **OK**.

9 Click the **Geom2** tab.

10 From the **Draw** menu, choose **Extrude**.

11 From the **Objects to extrude** list, select **CO3**. In the **Distance** edit field, type `-96e-6`. Click **OK**.

12 Click the **Geom2** tab.

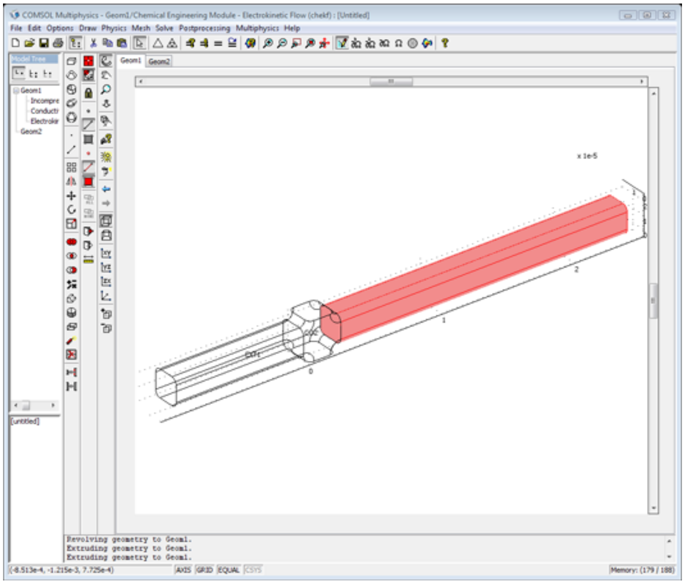
13 From the **Draw** menu, choose **Work Plane Settings**.

14 On the **Quick** page, click the **y-z** button, and in the corresponding **x** edit field type `24e-6`. Click **OK**.

15 From the **Draw** menu, choose **Extrude**.

16 In the dialog box that appears, set the **Distance** to `216e-6`. Click **OK**.

The following figure shows the 3D geometry when you have executed this step.



```
Revolving geometry to Geom1.
Extruding geometry to Geom1.
Extruding geometry to Geom1.
```

(-8.513e-4, -1.215e-3, 7.725e-4)

Memory: (179 / 188)

3D geometry after an extrusion operation on one of the arms.

17 Click the **Geom2** tab.

18 From the **Draw** menu, choose **Work Plane Settings**.

19 On the **Quick** page, click the **x-y** button. In the associated **z** edit field, type `-4e-6`. Click **OK**.

20 From the **Draw** menu choose **Extrude**. Set the **Distance** to `-196e-6`, then click **OK**.

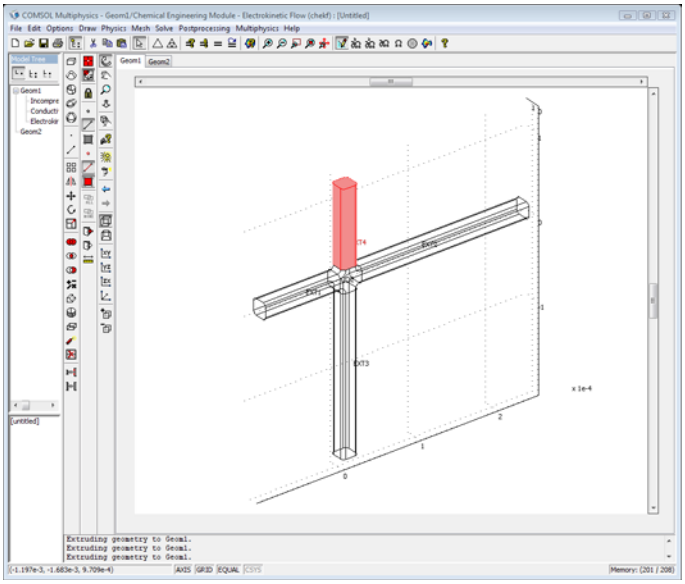
21 Click the **Geom2** tab.

22 From the **Draw** menu, choose **Work Plane Settings**.

23 On the **Quick** page, click the **x-y** button. In the associated **z** edit field type `24e-6`. Click **OK**.

24 From the **Draw** menu, choose **Extrude**. Set the **Distance** to `96e-6`, then click **OK**.

The completed geometry should look like that in the following figure.



```
Extruding geometry to Geom1.
Extruding geometry to Geom1.
Extruding geometry to Geom1.
```

The completed 3D geometry after extrusion of all four arms.

PHYSICS SETTINGS—THE FOCUSING STAGE

Subdomain Settings

1. From the **Multiphysics** menu, choose **1 Geom1: Incompressible Navier-Stokes (chns)**.
2. From the **Physics** menu, choose **Subdomain Settings**.
3. In the **Subdomain selection** list, select all the subdomains.
4. Enter the settings from the following table. When done, click **OK**.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

5. From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (dc)**.
6. From the **Physics** menu, choose **Subdomain Settings**.
7. For all subdomains, set σ to `sigma`. Click **OK**.
8. From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.
9. From the **Physics** menu, choose **Subdomain Settings**.

10 With all subdomains still selected, enter the settings in the following table; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	D
R	0
u_m	nu
z	-1
u	u
v	v
w	w
V	V

Boundary Conditions

1 From the **Multiphysics** menu, choose **1 Geom1: Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 Specify the following boundary conditions (for boundaries not listed in the table, the default No slip condition applies); when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 26	BOUNDARY 54
Boundary type	Inlet	Inlet	Outlet
Boundary condition	Laminar inflow	Laminar inflow	Pressure, no viscous stress
U_0	u_a	w_a	
L_{entr}	1e-4	1e-4	
Constrain outer edges to zero	Yes	Yes	
p_0			0

4 From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (dc)**.

5 From the **Physics** menu, choose **Boundary Settings**.

6 Click in the **Boundary selection** list and press Ctrl+A to select all boundaries. From the **Boundary condition** list, select **Electric insulation**.

7 Edit the boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 54
Boundary condition	Electric potential	Ground
V_0	`-1`	-

8 From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.

9 From the **Physics** menu, choose **Boundary Settings**.

10 Specify boundary settings as in the following table (for boundaries not listed, the default Insulation/Symmetry condition applies); when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 26	BOUNDARY 54
Boundary condition	Concentration	Concentration	Convective flux
c_0	`c_in`	`0`	-

MESH GENERATION

1 Click **Geom1** to activate the 3D geometry.

2 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION—THE FOCUSING STAGE

First, compute the solution for the velocity field, and then use that solution when solving the mass-transport problem.

1 Click the **Solver Manager** button on the Main toolbar.

2 Click the **Solve For** tab.

3 From the **Solve for variables** tree, select **Geom1 (3D)>Incompressible Navier-Stokes (chns)**.

4 Click the **Solve** button.

5 When the solver has finished, click the **Initial Value** tab.

6 Click the **Current solution** option button in the **Initial value** area, then return to the **Solve For** page.

7 From the **Solve for variables** tree, select **Geom1 (3D)>Conductive Media DC (dc)**.

8 Click **Solve**

9 From the **Solve for variables** tree, select **Geom1 (3D)>Electrokinetic Flow (chekf)**.

10 Click **Solve**.

11 On the **Initial Value** page, click the **Store Solution** button.

12 Click **OK** to close the **Solver Manager**.

PHYSICS SETTINGS—INJECTION STAGE, MODE A

Subdomain Settings

1 From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 In the **Subdomain selection** list, select all the subdomains, then change the settings for velocity parameters as in the following table; when done, click **OK**.

PROPERTY	VALUE
u	0
v	0
w	0

Boundary Conditions

1 From the **Physics** menu, choose **Boundary Settings**.

2 Select Boundaries 1, 21, 26, and 54 (the inlets and outlets).

3 From the **Boundary condition** list, select **Flux**.

4 In the $\mathbf{N_0}$ edit field, type `-nmflux_c_chekf`.

The predefined boundary variable `nmflux_c_chekf` gives the outward normal electrophoretic flux, $\mathbf{N}_i \cdot \mathbf{n}$.

5 Click **OK**.

6 From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (dc)**.

7 From the **Physics** menu, choose **Boundary Settings**.

8 Change the boundary settings as in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 54	BOUNDARY 21	BOUNDARY 26
Boundary condition	Electric insulation	Electric potential	Electric potential
V_0	-	0	`-3.2`

COMPUTING THE SOLUTION—INJECTION STAGE, MODE A

1 Click the **Solver Manager** button on the Main toolbar.

2 Click the **Script** tab. Select the **Automatically add commands when solving** check box.

This setting instructs the software to record the subsequent solver settings and commands, which you can then reuse when solving Mode B.

3 Click the **Initial Value** tab. In the **Initial value** area, click the **Stored solution** option button. This makes the steady-state solution from the focusing stage the initial solution.

4 Click the **Solve For** tab.

5 In the **Solve for variables** tree, select **Geom1 (3D)>Conductive Media DC (dc)**.

6 Click **Solve**.

7 Click the **Solver Parameters** button on the Main toolbar.

8 From the **Analysis** list, select **Transient**.

9 In the **Time stepping** area go to the **Times** edit field and enter `0:0.03:0.6`.

10 Click **OK**.

11 Activate the **Solver Manager** window.

12 Click the **Initial Value** tab.

13 In the **Initial value** area, click the **Current solution** option button.

14 Click the **Solve For** tab.

15 In the **Solve for variables** tree, select **Geom1 (3D)>Electrokinetic Flow (chekf)**.

16 Click **Solve**.

17 Click **OK**.

POSTPROCESSING AND VISUALIZATION—INJECTION STAGE, MODE A

Reproduce the plot in Figure 7-24 on page 371 with the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Subdomain** and **Geometry edges** check boxes in the **Plot type** area and clear all the others.

3 From the **Solution at time** list, select **0**.

4 Click the **Subdomain** tab. From the **Predefined quantities** list on the **Color Data** page, select **Electrokinetic Flow (chekf)>Concentration, c**. Click **Apply**.

5 Click the **Go to Default 3D View** button on the Camera toolbar, then click the **Zoom Extents** button on the Main toolbar.

To visualize the solution at two later times, as in the left panels of Figure 7-25 and Figure 7-26 on page 372, do as follows:

6 Return to the **Subdomain** page of the **Plot Parameters** dialog box.

7 Clear the **Color scale** check box in the **Element color** area.

8 Click the **General** tab. From the **Solution at time** list, select **0.06**. Click **Apply** to generate the plot in the left panel.

9 From the **Solution at time** list, select **0.12**. Click **OK** to generate the plot in the left panel.

To make an animation of the solution, click the **Animate** button on the Plot toolbar. On the **Animate** page of the **Plot Parameters** dialog box, you can customize the movie settings.

Generate the upper plot of Figure 7-27, by executing the following instructions:

1 From the **Postprocessing** menu, choose **Cross-Section Plot Parameters**.

2 On the **General** page, select **Interpolated times** from the **Select via** list.

3 In the **Times** edit field, type `0:0.06:0.6`.

4 Click the **Line/Extrusion** tab.

5 In the **Predefined quantities** list, select **Electrokinetic Flow (chekf)>Concentration, c**.

6 In the **x-axis data** area, click the option button next to the **Expression** button and then click **Expression**.

7 In the **Expression** edit field, type `10[um]-z`. Click **OK**.

8 In the **Cross-section line data** area, enter the settings listed in the following table; when done, click **OK**.

CROSS-SECTION LINE DATA			
x0	`1e-5`	x1	`1e-5`
y0	`1e-5`	y1	`1e-5`
z0	`2e-5`	z1	`-2e-4`
Line resolution			`200`

PHYSICS SETTINGS—INJECTION STAGE, MODE B

Boundary Conditions

1 From the **Physics** menu, choose **Boundary Settings**.

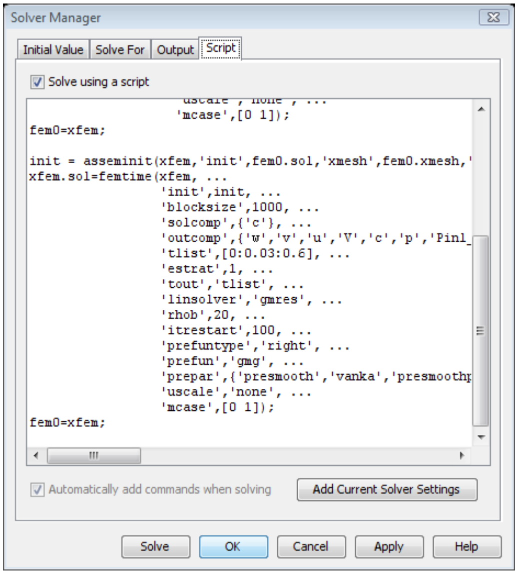
2 Change the boundary settings for the Conductive Media DC application mode to those in the following table:

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 54	BOUNDARY 26
Boundary condition	Electric potential	Electric potential	Electric potential
V_0	`-1`	`0`	`-3.2`

3 Click **OK**.

COMPUTING THE SOLUTION—INJECTION STAGE, MODE B

1. Click the **Solver Manager** button on the Main toolbar.
2. On the **Script** page, select the **Solve using a script** check box.
3. Click **Solve** to execute the script you see in the edit window.



☑ Solve using a script

```
                    'mcase',[0 1]);
fem0=xfem;

init = asseminit(xfem,'init',fem0.sol,'xmesh',fem0.xmesh,'
xfem.sol=femtime(xfem, ...
                  'init',init, ...
                  'blocksize',1000, ...
                  'solcomp',{'c'}, ...
                  'outcomp',{'w','v','u','V','c','p','Pinl_
                  'tlist',[0:0.03:0.6], ...
                  'estrat',1, ...
                  'tout','tlist', ...
                  'linsolver','gmres', ...
                  'rhob',20, ...
                  'itrestart',100, ...
                  'prefuntype','right', ...
                  'prefun','gmg', ...
                  'prepar',{'presmooth','vanka','presmoothp
                  'uscale','none', ...
                  'mcase',[0 1]);
fem0=xfem;
```

☑ Automatically add commands when solving

4. Click **OK** to close the **Solver Manager**.

POSTPROCESSING AND VISUALIZATION—INJECTION STAGE, MODE B

Generate the plots in the right panels of Figure 7-25 and Figure 7-26 on page 372 as follows:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, select **0.06** from the **Solution at time** list. Click **Apply**.

   This generates the right plot in Figure 7-25.
3. Repeat Step 2 but select **0.12** from the **Solution at time** list to generate the right plot in Figure 7-26.
4. From the **Solution** at time list, select **0**.
5. Click **OK** to close the dialog box and generate the plot you see when you open the model from the Model Library.

Finally, generate the lower plot in Figure 7-27 with the following steps:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 Accept the settings from Mode A by clicking **OK**.

Electroosmotic Flow in Porous Media

Introduction

This example treats the modeling of electroosmotic flow in porous media (Refs. 1, 2). The system consists of a compartment of sintered porous material and two electrodes that generate an electric field. The cell combines pressure-driven and electroosmotic flow.

The purpose of this model is to illustrate the modeling of electroosmosis and electrophoresis in porous media in COMSOL Multiphysics.

Model Definition

Figure 7-28 shows the system's geometry. It is made up of a domain of porous material containing the electrolyte and two electrodes that generate a potential difference. The conductivity is very small, and the model assumes that the effects of electrochemical reactions at the electrode surfaces are negligible.

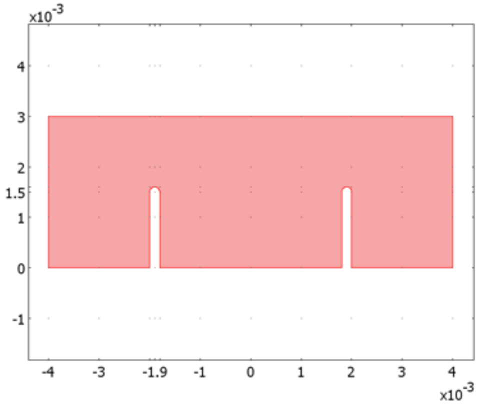


Figure 7-28: The modeled domain consists of an electrolyte contained in a porous structure and two electrodes that generate an electric field.

In the first part of the model, you solve the continuity equations for the flow velocity and the current density at steady state:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \nabla \cdot \mathbf{i} &= 0 \end{aligned} \qquad (7\text{-}25)$$

Here **u** denotes the velocity (m/s) and **i** represents the current-density vector (A/m^2). The velocity includes two driving forces—a pressure term and an electroosmotic term:

$$\mathbf{u} = -\frac{\varepsilon_p r^2}{8\eta\tau}\nabla p + \frac{\varepsilon_p \varepsilon_{\mathrm{w}} \zeta}{\eta\tau}\nabla V . \tag{7-26}$$

In this equation, ε_p denotes the porosity, r is the average radius of the pores (m), η gives the fluid's dynamic viscosity (Pa·s), τ represents the tortuosity of the porous structure, ε_{w} is the fluid's permittivity (F/m), p gives the pressure (Pa), ζ is the zeta potential (V), and V equals the potential (V). The current density is given by

$$\mathbf{i} = -\kappa \nabla V \tag{7-27}$$

where κ denotes the conductivity (S/m).

At the solid walls, the normal velocity component vanishes:

$$\mathbf{u} \cdot \mathbf{n} = 0 . \tag{7-28}$$

At the inlet and the outlet, the pressure is fixed:

$$p = p_1 \qquad \text{inlet} \tag{7-29}$$

and

$$p = p_0 \qquad \text{outlet} \tag{7-30}$$

The conditions for the current-density balance are insulating for all boundaries except the electrode surfaces. This is expressed as

$$\begin{array}{ll} \mathbf{i} \cdot \mathbf{n} = 0 & \text{all boundaries except the electrodes} \\ V = V_1 & \text{anode surface} \\ V = 0 & \text{cathode surface} \end{array} \tag{7-31}$$

In the second model stage, you use the steady-state velocity and potential fields in a transient simulation of the concentration of a charged tracer species injected into the system, assuming that the tracer species does not influence the conductivity or the set potential in the porous structure. The-mass transport equation for the tracer reads

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{N} = 0 \tag{7-32}$$

where **N** is the flux vector given by the Nernst-Planck equation

$$\mathbf{N} = -D\nabla c - zu_{\mathrm{m}}Fc\nabla V + c\mathbf{u}\,. \tag{7-33}$$

In this equation, D denotes the tracer's diffusivity (m^2/s), c gives its concentration ($\mathrm{mol/m}^3$), z represents the tracer's charge number, and F is Faraday's constant (C/mol). The mobility, u_{m} ($\mathrm{mol{\cdot}m^2/(J{\cdot}s)}$), is given by the Nernst-Einstein equation

$$u_{\mathrm{m}} = \frac{D}{R_{\mathrm{g}}T} \tag{7-34}$$

where $R_{\mathrm{g}} = 8.314$ J/(mol·K) is the gas constant and T (K) is the temperature.

The boundary conditions for the mass-transport equation Equation 7-32 are insulating, except for at the inlet and the outlet. There you use the *Flux* condition to set the diffusive and convective contributions to the flux through the boundaries to zero:

$$\begin{aligned} &\mathbf{n}\cdot(-D\nabla c + c\mathbf{u}) = 0 \qquad &&\text{(inlet and outlet)} \\ &\mathbf{n}\cdot\mathbf{N} = 0 &&\text{(all other boundaries)} \end{aligned} \tag{7-35}$$

The initial concentration is given by a distribution that is uniform in the y direction and bell-shaped in the x direction:

$$c(t{=}0) = c_{\mathrm{top}}\exp\left(-0.5\left(\frac{(x-x_{\mathrm{m}})}{\sigma}\right)^2\right) \tag{7-36}$$

Here c_{top} denotes the peak concentration, x_{m} is the position of the peak along the x-axis, and σ equals the base width of the peak.

Results

The upper plot in Figure 7-29 shows the flow distribution in the porous structure when only the pressure gradient acts as a driving force. In the lower plot, it is instead the electric field that drives the flow. In both cases, the velocity is large around the corners of the electrodes, where the field strength is large and the effect of the decrease in the geometry's cross section is most pronounced. Note by comparing the maximum values for the color scales that the pressure gradient is the dominating driving force.

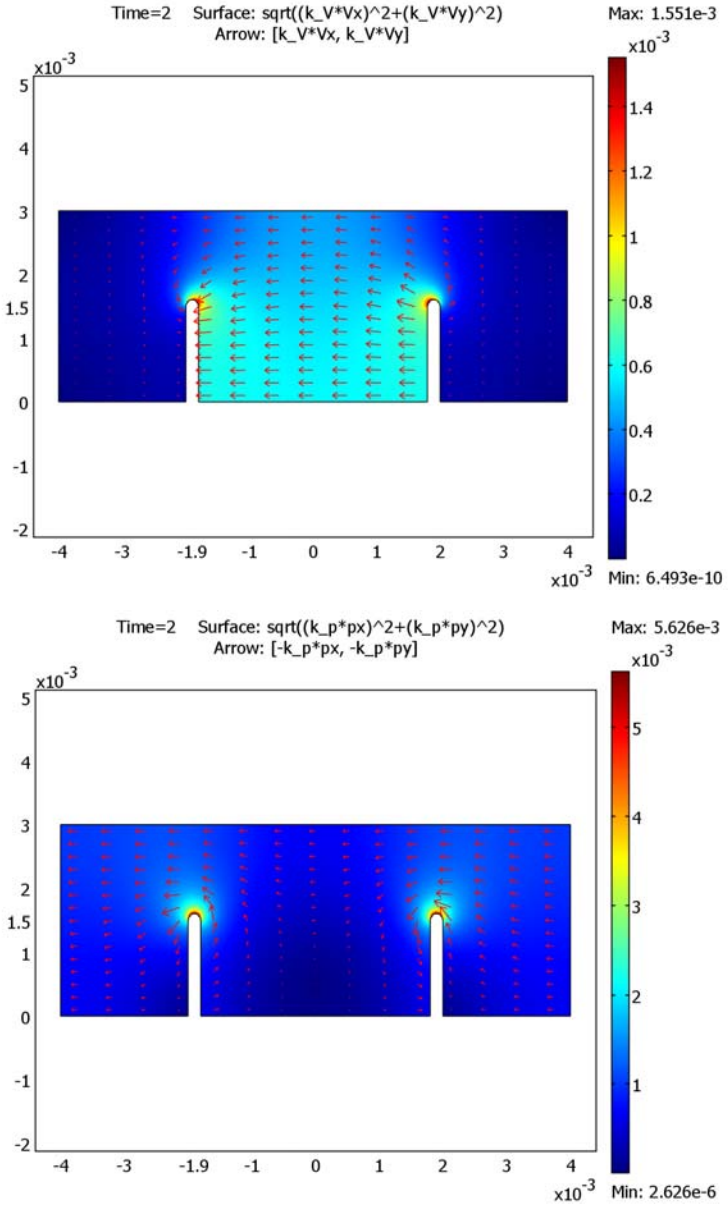


Figure 7-29: Velocity distributions in the cell with an applied pressure difference (top) and an applied electric field (bottom). The scale unit for the magnitude surface plot is m/s.

Figure 7-30 shows the concentration field in the case where both pressure and electroosmotic forces are included. The figure shows that the migration of the charged tracer also influences the transport rate. In this case, the tracer is transported both by the movement of the flow, due to pressure and electroosmotic terms, and the electrophoretic effect on the charged tracer itself. At $t = 0$, the tracer is introduced as a bell-shaped vertical distribution near the inlet. In the subsequent simulation, this distribution is sheared and transported by diffusion, migration, and convection.

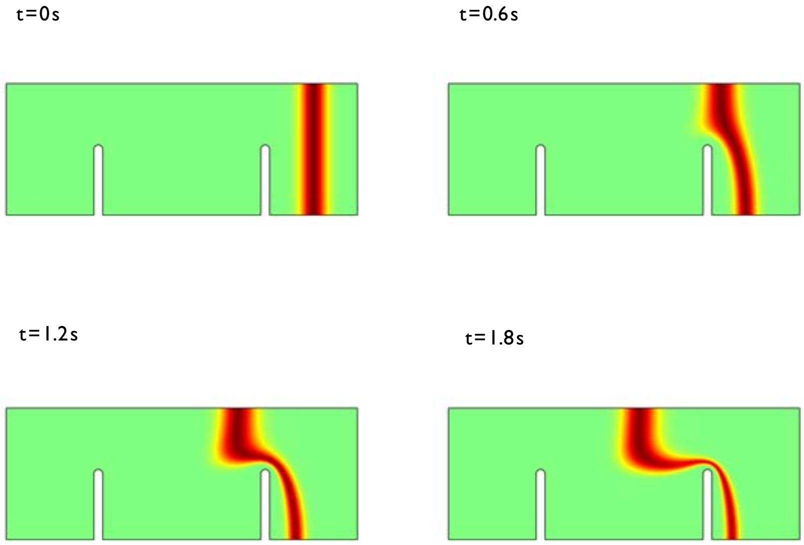


Figure 7-30: Concentration distribution in the domain at different times after injection. The effects of diffusion, convection, and migration deform the initial bell-shaped pulse.

Figure 7-31 shows the cross sections of the pulse along a line at $y = 2.5$ mm for the times $t = 0$, 0.5 s, 1.0 s, 1.5 s, and $t = 2.0$ s. Diffusion smears out the pulse, while migration and convection mainly translate and shear it depending on the pressure and the electric field.

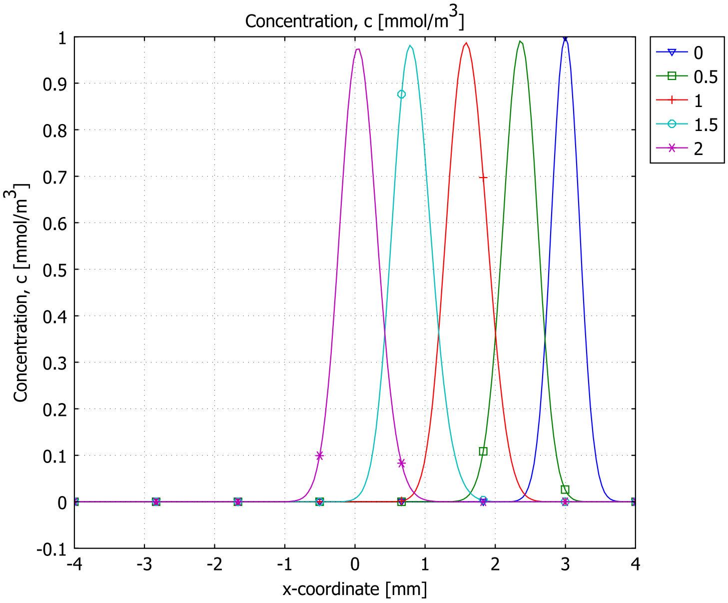


Figure 7-31: Cross-section plot of the concentration along a horizontal line at y = 2.5 mm for the times t = 0, 0.5 s, 1.0 s, 1.5 s, and 2.0 s.

Despite its geometrical simplicity, this model includes the components needed to model complex-shaped domains.

References

1. M-S. Chun, "Electrokinetic Flow Velocity in Charged Slit-like Microfluidic Channels with Linearized Poisson-Boltzmann Field," *Korean J. Chem. Eng.*, vol. 19, no. 5, pp. 729–734, 2002.

2. S. Yao, D. Huber, J. Mikkelsen, and J.G. Santiago, "A Large Flowrate Electroosmotic Pump with Micron Pores," *Proc. IMECE, 2001 ASME International Mechanical Engineering Congress and Exposition*, November 2001, New York.

Modeling in COMSOL Multiphysics

The COMSOL Multiphysics implementation is straightforward, and the only aspect to remember is to solve the steady-state problem first and then the time-dependent problem. Do this by following these steps:

1. Solve the nonlinear steady-state problem for the flow and current balances.
2. Store the solution.
3. Change the solver settings to transient.
4. Solve the problem only for the concentration, using the stored solution for the pressure and potential fields.

Model Library path:

`Chemical_Engineering_Module/Microfluidics/electroosmotic_flow`

Modeling Using the Graphical User Interface

1. Open the Model Navigator.
2. On the **New** page set the **Space dimension** to **2D**.
3. In the list of application modes select **Chemical Engineering Module>Mass Transport>Electrokinetic Flow>Transient analysis**.
4. Click the **Multiphysics** button, then click **Add**.
5. In the list of application modes select **COMSOL Multiphysics>PDE Modes>PDE, General Form**.
6. Click **Add**.
7. In the **Dependent variables** edit field, type `p V`.
8. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Axes/Grid Settings**.

2 Enter axis and grid settings as in the following table; on the **Grid** page clear the **Auto** check box.

AXIS		GRID	
x min	`-5e-3`	x spacing	`0.5e-3`
x max	`5e-3`	Extra x	`-1.9e-3, -1.8e-3`
y min	`-1e-3`	y spacing	`0.5e-3`
y max	`4e-1`	Extra y	`1.5e-3, 1.6e-3`

3 Click **OK**.

4 From the **Options** menu, select **Constants**.

5 Define the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`eps_p`	`0.6`	`Porosity`
`a`	`10[um]`	`Average pore radius`
`eta`	`1e-3[Pa*s]`	`Dynamic viscosity`
`eps_w`	`80.2*8.854[pF/m]`	`Electric permittivity`
`zeta`	`-0.1[V]`	`Zeta potential`
`p1`	`0.01*1.013e5[Pa]`	`Inlet pressure`
`k_p`	`eps_p*a^2/(8*eta)`	`Prefactor, flow-velocity pressure term`
`k_V`	`eps_p*eps_w*zeta/eta`	`Prefactor, flow-velocity electroosmotic term`
`kappa`	`3.5e-4[S/m]`	`Electric conductivity`
`V1`	`50[V]`	`Anode potential`
`sigma`	`0.2[mm]`	`Concentration-profile peak width`
`x_m`	`3[mm]`	`Concentration-profile peak position`
`D`	`1e-9[m^2/s]`	`Diffusion coefficient`
`Rg`	`8.314[J/(mol*K)]`	`Gas constant`
`T`	`298[K]`	`Temperature`
`nu`	`D/(Rg*T)`	`Tracer ion mobility`
`z`	`1`	`Tracer ion charge number`

You need also three expression variables for the model.

6 From the **Options** menu, select **Expressions/Scalar Expressions**.

7 Enter the expressions from this table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`u_flow`	`-k_p*px+k_V*Vx`	`Flow velocity, x-component`
`v_flow`	`-k_p*py+k_V*Vy`	`Flow velocity, y-component`
`c_init`	`1[mmol/m^3]*exp(-0.5*((x-x_m)/sigma)^2)`	`Initial concentration distribution`

GEOMETRY MODELING

1. Click the **Rectangle/Square** button on the Draw toolbar.
2. Draw a rectangle with its lower left corner at (-4e-3, 0) and its upper right corner at (4e-3, 3e-3).
3. Select the **Line** tool by clicking the **Line** button on the Draw toolbar.
4. Draw a line from (-2e-3, 0) to (-2e-3, 1.5e-3) by clicking at these positions.
5. Click the **2nd Degree Bézier** button on the Draw toolbar.
6. Click at the positions (-2e-3, 1.6e-3), (-1.9e-3, 1.6e-3), (-1.8e-3, 1.6e-3), and (-1.8e-3, 1.5e-3).
7. Click the **Line** button and click at (-1.8e-3, 0).
8. Close the geometry by clicking anywhere with the right mouse button.
9. Click the **Array** button on the Draw toolbar.
10. Set the **x displacement** to `3.8e-3` and the **Array size x** to `2`.
11. Click **OK**.
12. Click the **Create Composite Objects** button on the Draw toolbar.
13. In the **Set formula** edit field, type `R1-CO1-CO2`.
14. Finish the geometry by clicking **OK**.

PHYSICS SETTINGS

Subdomain Settings—Electrokinetic Flow

1. From the **Multiphysics** menu, select **1 Electrokinetic Flow (chekf)**.
2. From the **Physics** menu, open the **Subdomain Settings** dialog box.
3. Select Subdomain 1. On the **c** page, enter the following settings:

PROPERTY	VALUE
D (isotropic)	`D`
R	`0`

PROPERTY	VALUE
u_m	`nu`
z	`z`
u	`u_flow`
v	`v_flow`
V	`V`

4 Click the **Init** tab. In the **c(t$_0$)** edit field, type `c_init`.

5 Click **OK**.

Boundary Conditions—Electrokinetic Flow

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Select Boundaries 1 and 10. From the **Boundary condition** list, select **Flux**. In the **N$_0$** edit field, enter the inward-flux expression `-nmflux_c_chekf`. (The predefined variable `nmflux_c_chekf` gives the outward normal electrophoretic flux.)

For the remaining boundaries, the default Insulation/Symmetry condition applies.

3 Thus, click **OK** to confirm the settings and close the dialog box.

Subdomain Settings—PDE, General Form

1 From the **Multiphysics** menu, select **2 PDE, General Form (g)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 On the Γ page, enter the following components:

`u_flow`	`v_flow`
`-kappa*Vx`	`-kappa*Vy`

The first and second rows define the left-hand sides of the first and second of the Equations 7-25, respectively.

4 On the **F** page, set both source terms to `0`.

5 Click **OK**.

Boundary Conditions—PDE, General Form

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the boundary conditions according to the following table. The G coefficients defining the normal derivatives at the boundaries consistently take the default value zero, and you therefore do not need to set them.

SETTINGS	**BOUNDARIES 2, 3, 6, 9**	**BOUNDARIES 4, 5, 11, 12**	**BOUNDARIES 7, 8, 13, 14**	**BOUNDARY 1**	**BOUNDARY 10**
Type	Neumann	Dirichlet	Dirichlet	Dirichlet	Dirichlet
R	-	`0` `-V`	`0` `-V+V1`	`-p` `0`	`-p+p1` `0`

3 Click **OK**.

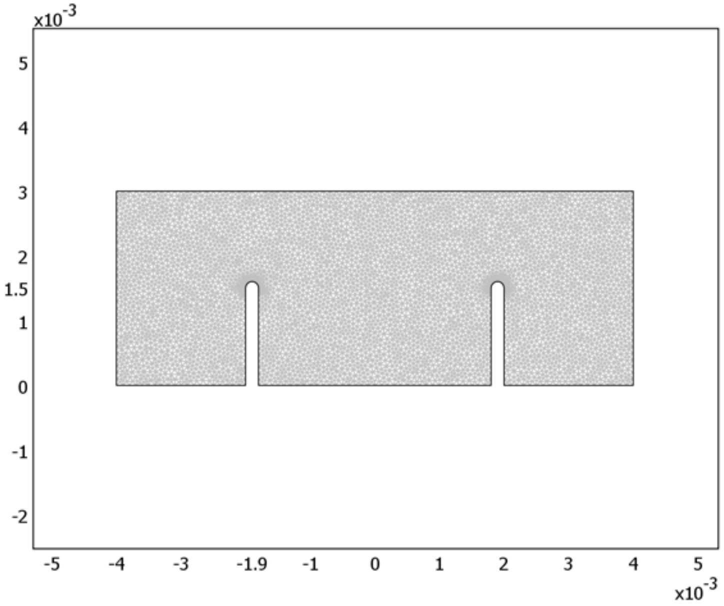
MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** button.

3 Set the **Maximum element size** to `1e-4`.

4 Click **Remesh** to generate the mesh. When the mesher has finished, click **OK**.



The meshed geometry.

COMPUTING THE SOLUTION

First solve for the two stationary fields: the pressure, p, and the potential, V.

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Analysis** list, select **Stationary**, then click **Apply**.

3 Click the **Solver Manager** button on the Main toolbar.

4 Click the **Solve For** tab.

5 From the **Solve for variables** list, select **PDE, General Form (g)**.

6 Click the **Solve** button to compute the solutions for p and V. The software uses the initial-value expression you specified earlier as the initial solution for c, which you do not solve for in this step.

When the solver has finished, turn to the transient problem for the concentration, c.

7 Still on the **Solve For** page in the **Solver Manager**, select **Electrokinetic Flow (chekf)** from the **Solve for variables** list.

8 Click the **Initial Value** tab.

9 Click the **Store Solution** button, then click the **Stored solution** option button in the **Values of variables not solved for and linearization point** area. With this setting, the p and V fields that you just computed serve as a stationary background when you solve for c.

10 Click **OK** to close the **Solver Manager**.

11 Return to the **Solver Parameters** dialog box.

12 From the **Analysis** list, select **Transient**.

13 In the **Times** edit field, type `0:0.1:2`. Set the **Absolute tolerance** to `1e-8`.

14 Click **OK**.

15 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create the upper part of Figure 7-29 follow these steps:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 Click the **Surface** tab and make sure the **Surface plot** check box is selected.

3 On the **Surface Data** page, type `sqrt((k_V*Vx)^2+(k_V*Vy)^2)` in the **Expression** edit field.

4 Click the **Arrow** tab and select the **Arrow plot** check box.

5 On the **Subdomain Data** page, enter the following settings:

x component	`k_V*Vx`
y component	`k_V*Vy`

6 Click **Apply** to generate the upper plot in Figure 7-29.

7 Change the arrow **x component** and **y component** to `-k_p*px` and `-k_p*py`, respectively.

8 Go to the **Surface** page and replace the **Expression** on the **Surface Data** page with `sqrt((k_p*px)^2+(k_p*py)^2)`.

9 Click **Apply** to generate the lower plot.

Generate the plots in Figure 7-30 by proceeding with the following instructions:

10 Still on the **Surface** page, select **Electrokinetic Flow (chekf)>Concentration, c** from the **Predefined quantities** list (or type `c` in the **Expression** edit field).

11 Edit the **Unit** expression to read `mmol/m^3` (that is, millimoles/cubic meter).

12 Click the **Range** button. In the **Color Range** dialog box, clear the **Auto** check box.

13 Set the **Min** and **Max** values to `-1` and `1`, respectively, then click **OK**.

Note that these max and min values refer to the current plot unit, for which the concentration lies between 0 and 1 (neglecting the numerical error in the solution). Using a symmetric interval around zero gives brighter-colored surface plots at the price of using only half the color scale.

14 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

15 Clear the **Auto** check box for **Element refinement**, then type `5` in the associated edit field.

16 Select **0** from the **Solution to use** list, then click **Apply** to generate the upper left plot.

17 Repeat the previous step using different selections from the **Solution at time** list to generate the other plots in Figure 7-30.

18 When finished, click **OK** or **Cancel** to close the **Plot Parameters** dialog box.

By clicking the **Animate** button on the Plot toolbar you can also generate a movie of the simulation.

Generate the plots in Figure 7-31 using the cross-section plot functionality:

1 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

2 From the **Solutions at time** list, select **0**, **0.5**, **1**, **1.5**, and **2.0**.

3 Click the **Line/Extrusion** tab.

4 In the **y-axis data** area, verify that **Concentration, c** is selected from the **Predefined quantities** list.

5 In the **x-axis** data area, click the lower option button and then the **Expression** button.

6 In the **X-Axis Data** dialog box, select **Geometry and Mesh>x-coordinate** from the **Predefined quantities** list (or type `x` in the **Expression** edit field).

7 From the **Unit** list, select **mm**, then click **OK** to close the **X-Axis Data** dialog box.

8 Set cross-section line data according to this table:

x0	`-4e-3`
x1	`4e-3`
y0	`2.5e-3`
y1	`2.5e-3`

9 Click the **Line Settings** button. From the **Line marker** list, select **Cycle**.

10 Select the **Legend** check box, then click **OK** to close the **Line Settings** dialog box.

11 Click **OK** to generate the plot in Figure 7-31.

Microchannel Cell

Introduction

This example was originally formulated by Albert Witarsa under Professor Bruce Finlayson's supervision at the University of Washington in Seattle. It was part of a graduate course in which the assignment consisted of using mathematical modeling to evaluate the potential of patents in the field of microfluidics.

This model treats a so-called H-microcell for separation through diffusion. The cell puts two different laminar streams in contact for a controlled period of time. The contact surface is well defined, and by controlling the flow rate it is possible to control the amount of species transported from one stream to the other through diffusion.

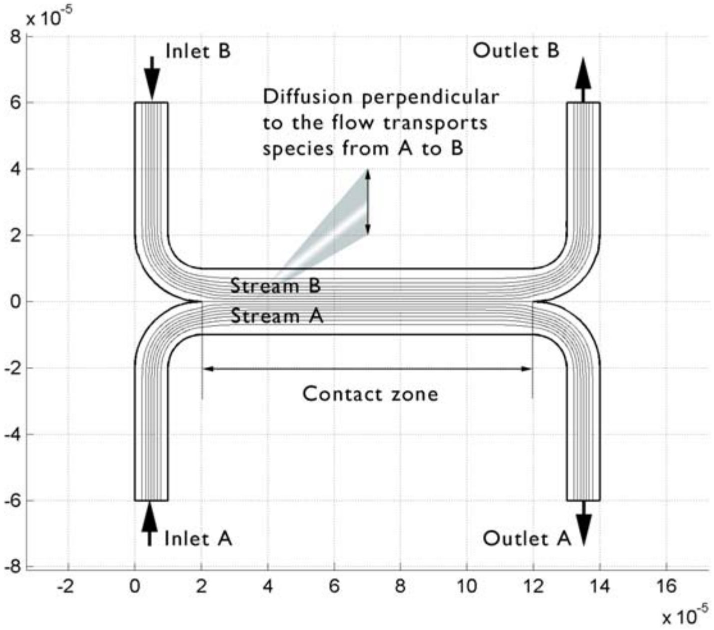


Figure 7-32: Diagram of the H-microcell.

Model Definition

The geometry of the microcell (Figure 7-33) is taken from Albert Witarsa's and Professor Finlayson's assignment. The cell geometry is divided in half because of symmetry. The design aims to avoid upsets in the flow field when the two streams, A and B, are united. This is to avoid the two streams mixing through convection, which would mix all species equally and lead to loss of control over the separation abilities. The transport of species between streams A and B should take place only by diffusion in order that species with low diffusion coefficients stay in their respective streams.

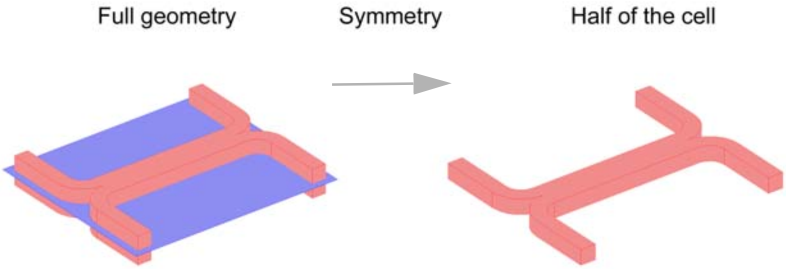


Figure 7-33: Model geometry. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

The simulations involve solving the fluid flow in the H-cell. According to the specifications, the flow rate at the inlet is roughly 0.1 mm/s. This implies a low Reynolds number, well inside the region of laminar flow:

$$\mathrm{Re} = \frac{d\rho u}{\eta} = \frac{1\cdot 10^{-5}\cdot 1\cdot 10^{3}\cdot 1\cdot 10^{-4}}{1\cdot 10^{-3}} \tag{7-37}$$

Equation 7-37 gives a Reynolds number of 0.001 for a water solution and the channel dimensions given in Figure 7-33, a value typical for microchannels. Thus it is easy to get a numerical solution of the full momentum balance and continuity equations for incompressible flow with a reasonable number of elements. The equations that you need to solve are the Navier-Stokes equations at steady state:

$$\begin{gathered} -\nabla\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p = 0 \\ \nabla\cdot\mathbf{u} = 0 \end{gathered} \tag{7-38}$$

Here ρ denotes density (kg/m^3), $\mathbf{u}$ is the velocity (m/s), η denotes viscosity (Pa·s), and p equals pressure (Pa).

Separation in the H-cell involves species in relatively low concentrations compared to the solvent, in this case water. This means that the solute molecules interact only with water molecules, and it is safe to use Fick's law to describe the diffusive transport in the cell. This mass-balance equation for a solute appears in the Convection and Diffusion application mode and reads

$$-\nabla \cdot (-D\nabla c + c\mathbf{u}) = 0\,. \tag{7-39}$$

In this equation, D denotes the diffusion coefficient (m^2/s) and c represents the concentration ($\mathrm{mol/m}^3$). In this model, you use the parametric solver to solve Equation 7-39 for three different values of D—$1\cdot 10^{-11}\ \mathrm{m}^2/\mathrm{s}$, $5\cdot 10^{-11}\ \mathrm{m}^2/\mathrm{s}$, and $1\cdot 10^{-10}\ \mathrm{m}^2/\mathrm{s}$—to simulate the mixing of different species.

You solve two versions of the model:

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

  $$\eta = \eta_0(1 + \alpha c^2)\,. \tag{7-40}$$

  Here α is a constant of dimension $(\text{concentration})^{-2}$. An influence of concentration on viscosity of this kind is usually observed in solutions of larger molecules.

Next, consider the boundary conditions, starting with the Navier-Stokes equations. For the relevant boundary groupings, refer to Figure 7-34.

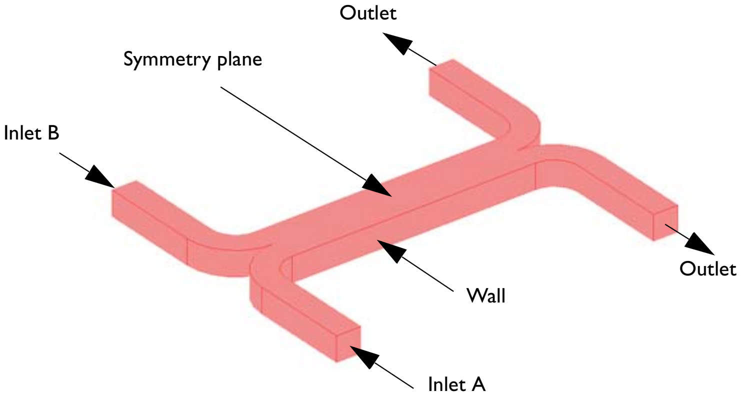


Figure 7-34: Model domain boundaries.

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

$$\begin{aligned} p &= p_0 \\ \mathbf{n}\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T) &= 0 \end{aligned} \tag{7-41}$$

Setting the pressure at the outlets to zero, the pressure at the inlets represents the pressure drop over the cell. These inlet and outlet conditions comply with the H-cell being a part of a channel system of constant width, which justifies the assumption of developed flow.

At the symmetry plane, choosing the boundary type *Symmetry boundary* sets the velocity component in the normal direction of the surface to zero:

$$\begin{aligned} \mathbf{n}\cdot\mathbf{u} &= 0 \\ \mathbf{t}\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)\mathbf{n} &= 0 \end{aligned} \tag{7-42}$$

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

$$(u, v, w) = (0, 0, 0) \qquad \text{at the walls} \tag{7-43}$$

For the mass balances, the assumption that solute molecules interact only with water molecules implies that it is sufficient to consider a single species A of concentration c. At the inlets, use the *Concentration* boundary condition with the following values:

$$\begin{aligned} c &= c_0 \qquad \text{at inlet A} \\ c &= 0 \qquad \text{at inlet B} \end{aligned} \tag{7-44}$$

Model the symmetry plane and cell walls with the *Insulation/Symmetry* condition:

$$(-D\nabla c + c\mathbf{u})\cdot\mathbf{n} = 0 \qquad \text{at the symmetry plane and walls} \tag{7-45}$$

This equation states that the flux of species perpendicular to the boundary equals zero. At the outlets, the *Convective flux* condition applies, stating that the diffusive transport perpendicular to the boundary normal is negligible:

$$(-D\nabla c)\cdot\mathbf{n} = 0 \qquad \text{at the outlets} \tag{7-46}$$

This condition eliminates concentration gradients in the flow direction.

Results

Figure 7-35 shows the velocity field. The flow is symmetric and is not influenced by the concentration field.

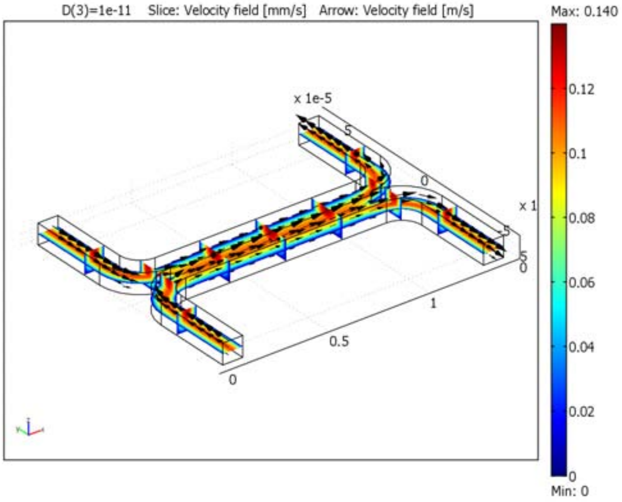


Figure 7-35: Flow velocity field.

Figure 7-36 shows the concentration distribution for the lightest species in this study.

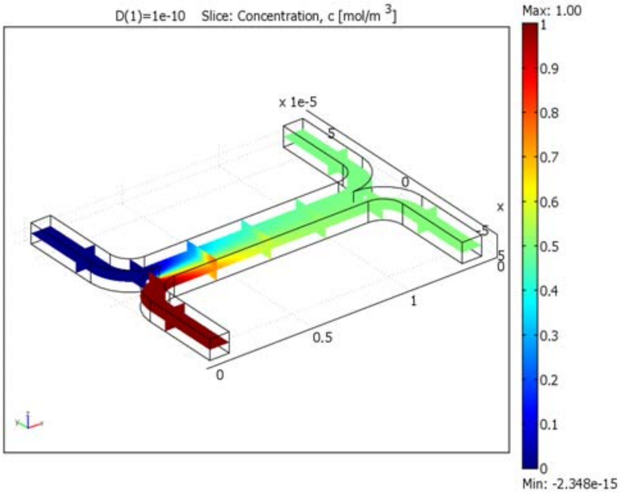


Figure 7-36: Concentration distribution for a species with diffusivity $1\cdot10^{-10} m^2/s$.

Because of the relatively large diffusion coefficient, the degree of mixing is almost perfect for the lightest species. The species with a diffusion coefficient ten times smaller than that of the lightest species shows a different result.

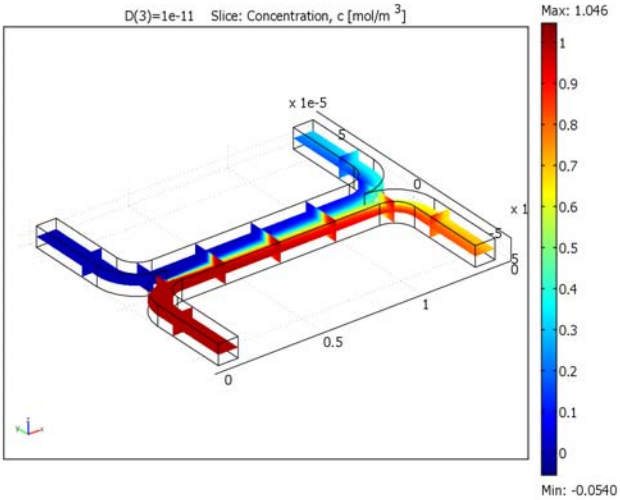


Figure 7-37: Concentration distribution for a species with diffusivity $1\cdot10^{-11} m^2/s$.

The concentration distribution in Figure 7-37 indicates that the diffusion coefficient for the species is low enough to avoid any significant mixing between streams A and B. The simulation clearly shows that the H-cell can separate lighter molecules from heavier ones. A cascade of H-cells can achieve a very high degree of separation.

In some cases, especially those involving solutions of macromolecules, the macromolecule concentration has a large influence on the liquid's viscosity. In such situations, the Navier-Stokes and the convection-diffusion become coupled, and they therefore must be solved simultaneously. Figure 7-38 shows the results of such a simulation, which you repeat in the second version of this model. You can see that changes in the concentration influence the flow field. It is clear from this plot that the velocity becomes asymmetric due to changes in viscosity. As a consequence of the modified flow field, the transport of molecules to the outlet B is also different from the result using a constant flow field. You can see the difference by comparing Figure 7-39 with Figure 7-37 on page 408.

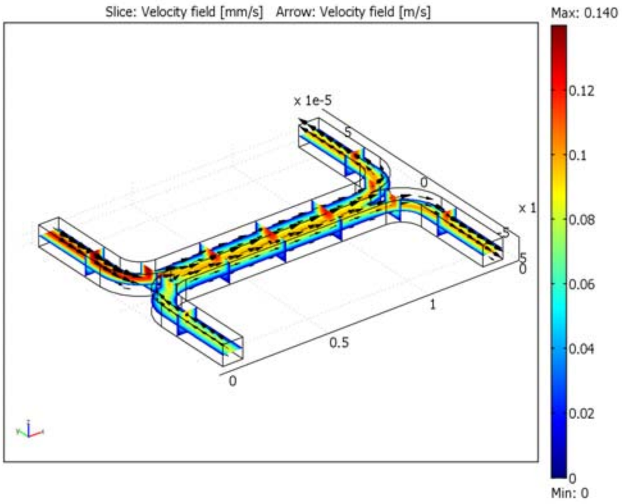


Figure 7-38: Velocity field. The viscosity varies with the concentration according to $\eta = \eta_0(1+\alpha c^2)$ *with* $\alpha = 0.5$ *(m*^{3}*/mol)*^{2}*. The figure shows that the velocity field is affected by variations in concentration. Compare it to the velocity field in Figure 7-35.*

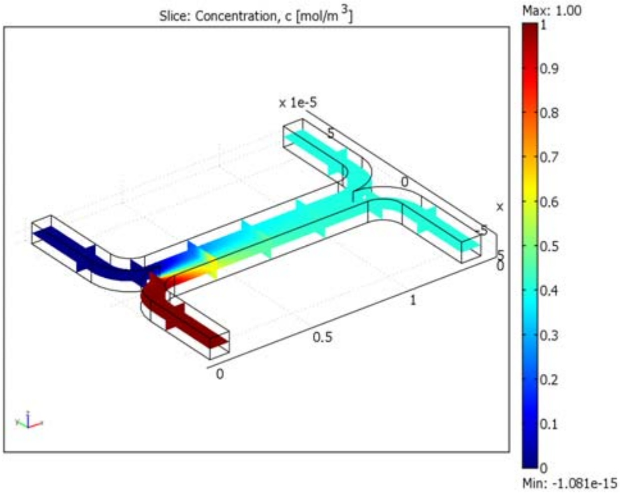


Figure 7-39: Concentration distribution for the species with diffusivity $1\cdot10^{-11}$ *m*^{2}*/s for the case where the fluid viscosity varies with concentration. Comparison with the plot in Figure 7-37 shows that fewer molecules of the species are transported to outlet B.*

Model Library path: `Chemical_Engineering_Module/Microfluidics/h_cell`

Modeling Using the Graphical User Interface

1. Start COMSOL Multiphysics.
2. On the **New** page, set the **Space dimension** to **3D**.
3. From the list of application modes, select **Chemical Engineering Module>Momentum Transport>Laminar Flow> Incompressible Navier-Stokes**.
4. Click the **Multiphysics** button, then click **Add**.
5. From the list of application modes, select **Chemical Engineering Module>Mass Transport>Convection and Diffusion**.
6. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Constants**.
2. Enter the following variable names, expressions, and (optionally) descriptions in the **Constants** dialog box; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1e3[kg/m^3]	Density
eta	1e-3[Pa*s]	Viscosity
D	1e-10[m^2/s]	Diffusion constant
p0	2[Pa]	Pressure drop
c0	1[mol/m^3]	Inlet concentration
alpha	0.5[(m^3/mol)^2]	Viscosity c^2-term prefactor

GEOMETRY MODELING

1. From the **Draw** menu, select **Work-Plane Settings**.
2. Use the default **Quick** work plane (the xy-plane at $z = 0$) by clicking **OK**.
3. From the **Options** menu, open the **Axes/Grid settings**.

4 On the **Axis** page, enter the following settings:

PROPERTY	VALUE
x min	-1
x max	15
y min	-7
y max	7

5 On the **Grid** page, clear the **Auto** check box and set both the **x spacing** and the **y spacing** to 1. Click **OK**.

6 Click the **Line** button on the Draw toolbar, then click the points with the *x*- and *y*-coordinates at (0, 6) and (0, 2).

7 Select the **2nd Degree Bezier Curve** tool on the Draw toolbar and click at the coordinate pairs (0, 0) and (2, 0).

8 Select the **Line** tool and click at the coordinates (12, 0).

9 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (14, 0) and (14, 2).

10 Select the **Line** tool and click at the coordinates (14, 6). Continue by clicking at the coordinates (13, 6) and (13, 2).

11 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (13, 1) and (12, 1).

12 Select the **Line** tool and click at the coordinates (2, 1).

13 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (1, 1) and (1, 2).

14 Select the **Line** tool and click at the coordinates (1, 6).

15 Click the right mouse button to close the set of lines and create a solid object, CO1.

You have now created half of the 2D cross section and can use copy, paste, and rotate operations to create the other half.

1 Click first the **Copy** button and then the **Paste** button, both on the Main toolbar. Let the **Displacements** remain at 0 and click **OK** to create the composite object CO2.

2 Click the **Scale** button on the Draw toolbar. Change the **y** component of the **Scale factor** to -1 (leave the other parameters at their default values).

3 Click **OK** to flip CO2 over the *x*-axis.

4 From the **Edit** menu, choose **Select All**. (Alternatively, press Ctrl+A.)

5 Click the **Create Composite Object** button on the Draw toolbar.

6 Clear the **Keep interior boundaries** check box. Click **OK**.

The cross section is now finished and you can extrude it to the full 3D geometry.

7 Select **Extrude** from the **Draw** menu. Let the **Distance** remain equal to `1`. Click **OK**.

The final geometry-modeling step is to scale the geometry to the correct scale.

8 Click the **Scale** button on the Draw toolbar.

9 Type `1e-5` in all three **Scale factor** edit fields. Click **OK**.

10 Click the **Zoom Extents** button on the Main toolbar.

You do not need the 2D workplane any more, so you can remove it from the model:

1 From the **Multiphysics** menu, choose **Model Navigator**.

2 In the **Multiphysics** area to the right, select **Geom2 (2D)** and then click **Remove**.

3 Click **OK** to close the **Model Navigator**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then specify the settings in this table; when done, click **OK**.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

5 From the **Physics** menu, select **Subdomain Settings**.

6 Select Subdomain 1.

7 Specify the following settings:

PROPERTY	VALUE
D (isotropic)	`D`
u	`u`
v	`v`
w	`w`

8 Click **OK** to confirm the settings and close the dialog box.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Specify boundary conditions as in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 2, 8	BOUNDARIES 20, 22	BOUNDARY 4	ALL OTHERS
Boundary type	Inlet	Outlet	Symmetry boundary	Wall
Boundary condition	Pressure, no viscous stress	Pressure, no viscous stress		No slip
p_0	p0	0	-	-

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

5 From the **Physics** menu, select **Boundary Settings**.

6 Specify the boundary conditions in the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARY 8	BOUNDARIES 20, 22	ALL OTHERS
Type	Concentration	Concentration	Convective flux	Insulation/ Symmetry
c_0	c0	0	-	-

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Extra fine**.

3 Click the **Remesh** button.

4 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Start by first computing the solution for the velocity field and then use that solution for solving the mass transport problem.

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, select **Direct (PARDISO)** from the **Linear system solver** list.

3 Click **OK**.

4 Click the **Solver Manager** button on the Main toolbar.

5 On the **Solve For** page, select **Incompressible Navier-Stokes (chns)**.

6 On the **Initial Value** page, click the **Initial value expression** option button in the **Initial value** area.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar.

You have now computed the velocity field and can use that solution to make a parametric analysis for the mass transport problem with varying diffusivity.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Convection and Diffusion (chcd)**.

3 Click the **Initial Value** tab, then click the **Current solution** option button in the **Initial value** area.

4 Click **OK**.

5 Click the **Solver Parameters** button on the Main toolbar.

6 From the **Solver** list, select **Parametric**.

7 In the **Parameter name** edit field, type `D`.

8 In the **Parameter values** edit field, type `1e-10 5e-11 1e-11`.

9 Click **OK**.

10 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 7-35 follow these steps:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 On the **General** page, select the **Slice** and **Arrow** check boxes in the **Plot type** area.

3 Clear the **Element refinement Auto** check box and type `5` in the associated edit field.

4 Click the **Slice** tab.

5 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (chns)>Velocity field**.

6 From the **Unit** list, select **mm/s**.

7 In the **Slice positioning** area, set **x levels** to `5`, **y levels** to `2`, and **z levels** to `1`.

8 Click the **Arrow** tab.

9 On the **Subdomain Data** page, verify that **Velocity field** is selected in the **Predefined quantities** list.

10 In the **Arrow positioning** area, set the numbers of **x points**, **y points**, and **z points** to `14`, `21`, and `3`, respectively.

11 In the **Arrow parameters** area, click the **Color** button. Select the black swatch from the palette in the **Arrow Color** dialog box, then click **OK**.

12 Select **3D arrow** from the **Arrow type** list.

13 Click **Apply** to generate the plot.

To generate Figure 7-36, continue with the following steps:

1 Clear the **Arrow plot** check box, then click the **Slice** tab.

2 From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

3 On the **General** page, select **1e-10** from the **Parameter value** list. Click **OK**.

Generate Figure 7-37 the same way as Figure 7-36, except use the parameter value **1e-11**.

PHYSICS SETTINGS—STUDY 2

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Change the viscosity expression to `eta*(1+alpha*c^2)`. Click **OK**.

COMPUTING THE SOLUTION—STUDY 2

When the viscosity is concentration dependent you must solve all equations simultaneously.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Geom1 (3D)** from the **Solve for variables** list. Click **OK**.

3 Click the **Solver Parameters** button on the Main toolbar.

4 From the **Solver** list, select **Stationary**. Click **OK**.

5 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION—STUDY 2

Finally, generate Figure 7-38 and Figure 7-39 with the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Arrow** check box in the **Plot type** area.

3 Click the **Slice** tab.

4 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (chns)>Velocity field**.

5 In the **Unit** list, select **mm/s**, then click **Apply** to generate Figure 7-38.

6 In the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

7 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

8 Click **OK** to close the dialog box and generate Figure 7-39.

8

Transport, Reactions, and Reaction Engineering

This chapter contains examples of mass transport coupled to transport of momentum and energy, where the systems are affected by chemical reaction kinetics. The Chemical Engineering Module is well suited for these types of processes for two reasons:

- *Its ability to model multiphysics applications easily and quickly* —often you need to model mass transport to a description of a fluid flow, both in free and porous media. Other models may also require energy transport. The reaction kinetics are often functions of concentration (mass transport), temperature (energy transport), and sometimes pressure (momentum transport). The multiphysics feature allows for all physical descriptions to be coupled and solved simultaneously.
- *Its ability to handle equation-based modeling*—chemical-kinetics equations can be convoluted and laborious to include. In COMSOL Multiphysics, however, you can quickly enter such equations. Furthermore, other material properties, such as diffusion coefficients and viscosity, can be functions of the dependent variables. It is also easy to account for such dependencies by directly entering the functions in the user interface.

Fixed-Bed Reactor for Catalytic Hydrocarbon Oxidation

Introduction

This example treats the partial oxidation of o-xylene in air to phthalic anhydride (PA) in a multitube fixed-bed reactor—the dominating process for producing this important industrial chemical.

In this process, temperature is usually kept between 400–475 °C and the residence time varies between 0.5–5 seconds. The catalyst of choice is usually a mix of vanadium oxide and potassium sulfate on a silica support. The most important factor to consider for this process is the temperature inside the reactor. The reactions taking place in the reactor are highly exothermic, and the reactor needs to be cooled to avoid runaway conditions. The temperature distribution also affects phthalic anhydride yield. It is possible to control the temperature distribution by varying tube diameter, residence time, wall temperature (cooling rate), and the inlet temperature of the feed. This example covers some of these factors by creating a detailed model of the system using the 2D pseudo-homogeneous model as described in the literature (Ref. 3, and Ref. 4).

Tubular reactors are usually modeled with the assumption that concentration and temperature gradients only occur in the axial direction. The only transport mechanism operating in this direction is the overall flow itself, which is considered to be of plug-flow type, that is, all the fluid elements are assumed to move with a uniform velocity along parallel streamlines. This example takes a more general approach by accounting for variations of the concentrations and the temperature in the axial direction. Through the use of effective diffusivities and conductivities, the model also includes the mixing in the axial direction that occurs in a reactor as a result of turbulence and the presence of packing.

Model Definition

Assume rotational symmetry to set up a 2D axisymmetric model.

The reaction kinetics of the rather complex process under study can, to a satisfactory degree, be described by the scheme in Figure 8-1 (References 1–4).

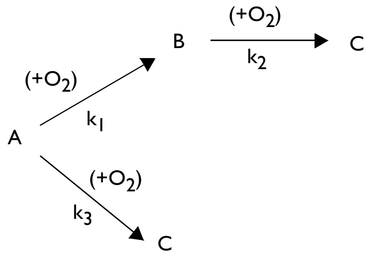


Figure 8-1: Reaction paths. A represents o-xylene, B refers to phthalic anhydride, and C is the total amount of carbon monoxide and carbon dioxide.

Owing to a very high excess of oxygen, the reactions are pseudo-first-order. It follows that the reaction rates can be described by the equations

$$\begin{aligned} r_1 &= \rho_b y_0 y_{A0} k_1 (1 - x_A) \\ r_2 &= \rho_b y_0 y_{A0} k_2 x_B \\ r_3 &= \rho_b y_0 y_{A0} k_3 (1 - x_A) \end{aligned} \qquad (8\text{-}1)$$

where ρ_b is the catalyst bulk density (kg/m^3), y_0 is the mole fraction of oxygen, y_{A0} is the inlet mole fraction of o-xylene, x_A is the total conversion of o-xylene, and x_B is the conversion of o-xylene into phthalic anhydride (similarly, x_C represents the total conversion into carbon monoxide and carbon dioxide). In the above equations, the conversions are dimensionless and the reaction rates have the SI unit mol/(m^3·s).

The rate coefficients (mol/(kg catalyst·s) depend on temperature as described by the Arrhenius law

$$k_i = A_i \exp\left(\frac{-B_i}{T}\right) \qquad (8\text{-}2)$$

where T is the reactor temperature, and A_i and B_i are characteristic parameters for each reaction ($i = 1, 2, 3$).

A schematic description of the reactor is given in Figure 8-2. The convective flow of gas takes place from the bottom to the top. Axisymmetry is assumed, which reduces the 3D geometry to two dimensions.

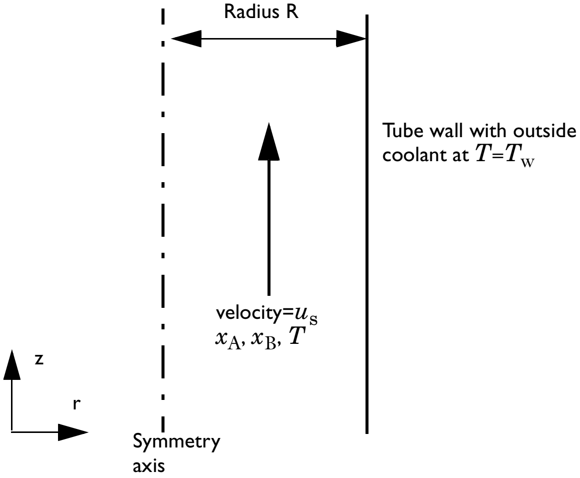


Figure 8-2: Schematic representation of the reactor.

The design equations for this system—a mass transport equation and an energy transport equation—read (Ref. 3 and Ref. 4)

$$\begin{aligned}\nabla\cdot(-D_\mathrm{eff}\nabla x_i+u_\mathrm{s}x_i) &= \frac{1}{c_\mathrm{tot}y_\mathrm{A0}}r_i\\ u_\mathrm{s}\rho_\mathrm{g}C_p\nabla\cdot T-\nabla\cdot(\lambda_\mathrm{eff}\nabla T) &= \sum\nolimits_{i=1}^{3}(-\Delta H_i)r_i\end{aligned}\tag{8-3}$$

Here u_s is the superficial velocity (m/s), c_tot is the total concentration (mol/m^3), ρ_g denotes the gas density (kg/m^3), y_A0 is the inlet mole fraction of o-xylene, λ_eff represents the bed's effective thermal conductivity (W/(m·K)), and ΔH_i is the enthalpy of adsorption for reaction i. Because $x_\mathrm{A} = x_\mathrm{B} + x_\mathrm{C}$, it is only necessary to solve two mass transport equations, which results in the following design equations:

$$\begin{aligned}\nabla\cdot(-D_\mathrm{eff}\nabla x_\mathrm{B}+u_\mathrm{s}x_\mathrm{B}) &= \frac{1}{c_\mathrm{tot}y_\mathrm{A0}}r_\mathrm{B}\\ \nabla\cdot(-D_\mathrm{eff}\nabla x_\mathrm{C}+u_\mathrm{s}x_\mathrm{C}) &= \frac{1}{c_\mathrm{tot}y_\mathrm{A0}}r_\mathrm{C}\\ \nabla\cdot(-\lambda_\mathrm{eff}\nabla T'+u_\mathrm{s}\rho_\mathrm{g}C_pT') &= \rho_\mathrm{b}[(-\Delta H_1)r_\mathrm{B}+(-\Delta H_3)r_\mathrm{C}]\end{aligned}\tag{8-4}$$

The rate equations can be rewritten accordingly:

$$
\begin{aligned}
r_{\mathrm{B}} &= y_{\mathrm{A}0} y_0 c_{\mathrm{tot}} [k_1 (1 - x_{\mathrm{B}} - x_{\mathrm{C}}) - k_2 x_{\mathrm{B}}] \\
r_{\mathrm{C}} &= y_{\mathrm{A}0} y_0 c_{\mathrm{tot}} [k_2 x_{\mathrm{B}} + k_3 (1 - x_{\mathrm{B}} - x_{\mathrm{C}})]
\end{aligned}
\tag{8-5}
$$

The boundary conditions for this system are as follows (see Figure 8-2 for the appropriate references):

$$
\begin{array}{ll}
\dfrac{\partial x_{\mathrm{B}}}{\partial r}(0, z) = \dfrac{\partial x_{\mathrm{C}}}{\partial r}(0, z) = 0 & \dfrac{\partial T}{\partial r}(0, z) = 0 \\
\dfrac{\partial x_{\mathrm{B}}}{\partial r}(R, z) = \dfrac{\partial x_{\mathrm{C}}}{\partial r}(R, z) = 0 & \lambda_{\mathrm{eff}} \dfrac{\partial T}{\partial r}(R, z) = -\alpha (T - T_0)
\end{array}
\tag{8-6}
$$

At the reactor inlet, the concentrations are zero and the temperature equals T_0. At the outlet, assume that the convective parts of the mass transport and the heat transport dominate.

Results and Discussion

A temperature plot (Figure 8-3) shows a maximum not far from the reactor inlet.

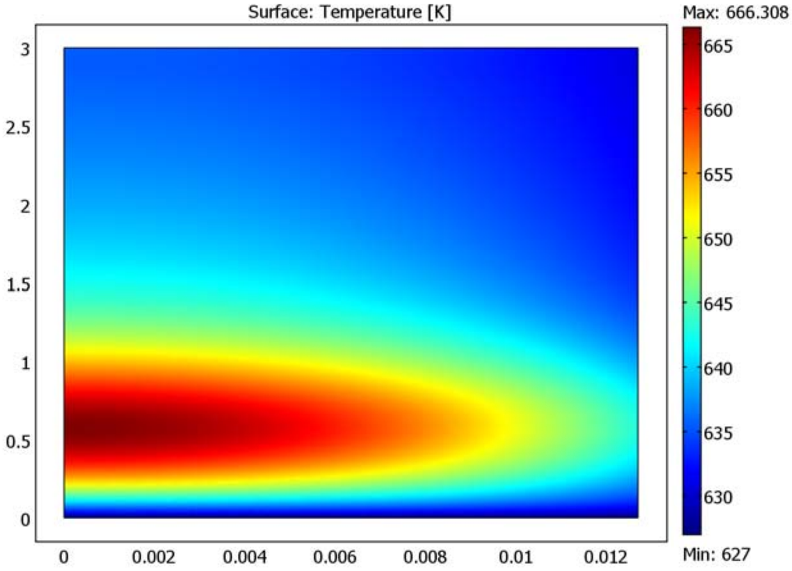


Figure 8-3: Temperature distribution across the tubular half plane.

This so-called hotspot is a common phenomenon for systems with exothermic reactions to which cooling is applied. Also, note that the radial temperature gradients are quite large around this hotspot.

Figure 8-4 shows the composition in the reactor along the axial direction. The graphs give the bulk mean conversions for an inlet temperature of 627 K (354 °C). You can see from the middle line that the phthalic anhydride production rate falls off somewhat along the tube, which is a typical behavior for consecutive reactions.

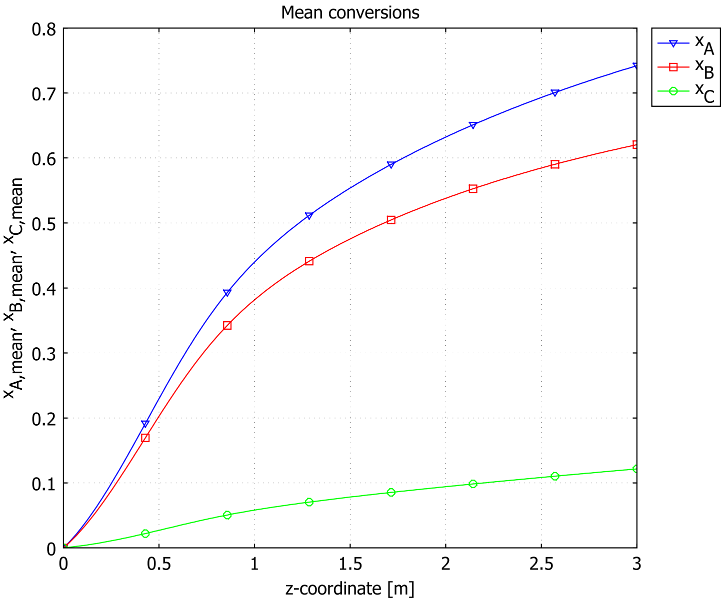


Figure 8-4: Composition versus axial coordinate in the reactor.

In Figure 8-5, note that the radial temperature gradients are quite severe, as the temperature along the symmetry axis is well above the mean temperature. On the basis of this information you can draw the conclusion that a 1D model with axial mixing would not be good enough to describe this system.

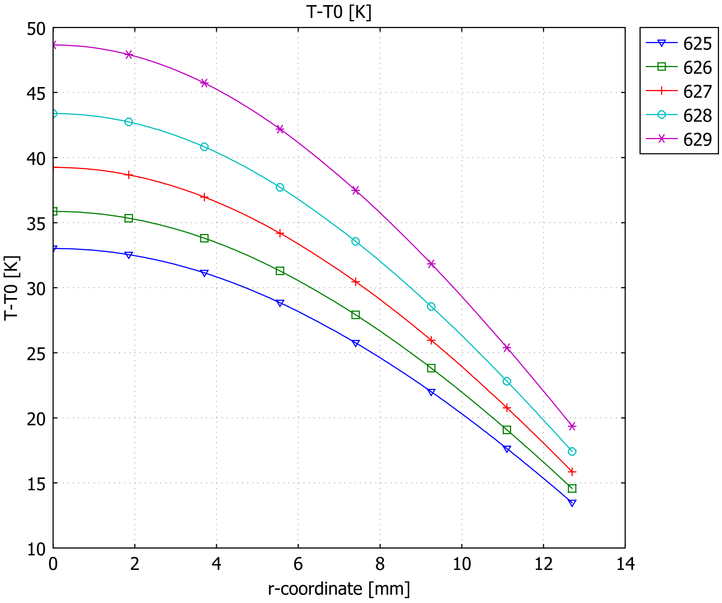


Figure 8-5: Temperature versus radial coordinate in the reactor (z=0.6 m) for a number of inlet of different inlet temperatures.

A parameter study of the inlet temperature gives the results displayed in Figure 8-6 for the average temperature along the reactor centerline. As this figure shows, the reactor's inlet temperature affects the centerline temperature quite dramatically. A high temperature increases the production rate of phthalic anhydride, but it can also increase the production of carbon monoxide and carbon dioxide. Furthermore, too high a temperature might be detrimental to the catalyst, which means that good control of the reactor's feed temperature is essential.

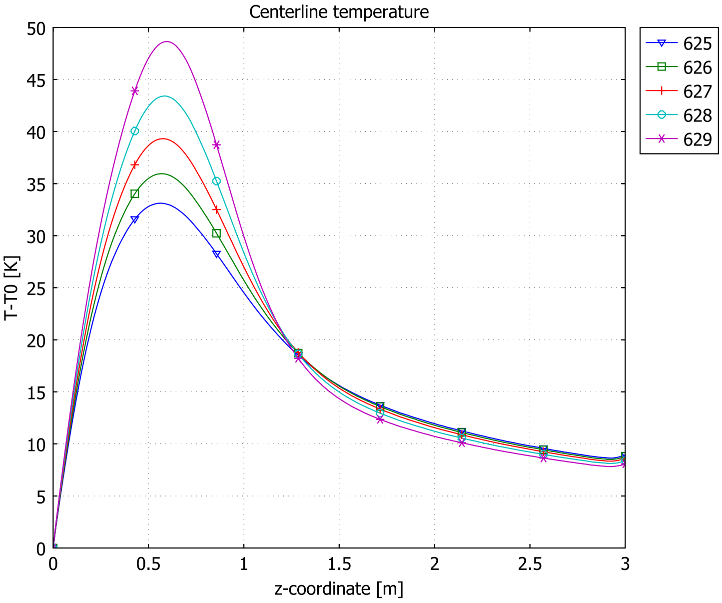


Figure 8-6: Average temperature along the reactor centerline vs. axial coordinate for different inlet temperatures.

Although the results presented here describe the process running at steady-state, the model can be easily generalized to a time-dependent version for use in automatic control and start-up simulations.

Modeling in COMSOL Multiphysics

To make use of the unit-handling capabilities that COMSOL Multiphysics offers, use $c_B \equiv x_B c_{tot}$ and $c_C \equiv x_C c_{tot}$ as the basic dependent variables in place of the dimensionless conversions x_B and x_C. For the latter, as well as for $x_A = x_B + x_C$, define scalar expressions to use for postprocessing. Furthermore, make the mean conversions over a circular cross section of the tube of area $A = \pi R^2$,

$$x_{\alpha,\,\mathrm{mean}}(z) = \frac{1}{A}\int_{\Omega} x_\alpha(r,z)\,d\Omega = \frac{2}{R^2}\int_0^R x_\alpha(r,z)\,r\,dr, \quad \alpha = \mathrm{A, B, C}, \tag{8-7}$$

available for postprocessing by defining corresponding projection coupling variables.

References

1. G.F. Froment, “Fixed Bed Catalytic Reactors,” *Ind. Eng. Chem.*, vol. 59, no. 2, pp. 18–27, 1967.

2. J.J. Lerou and G.F. Froment, “Velocity, Temperature and Conversion Profiles in Fixed Bed Catalytic Reactors,” *Chem. Eng. Science*, vol. 32, pp. 853–861, 1977.

3. G.F. Froment and K.B. Bischoff, *Chemical Reactor Analysis and Design*, 2nd ed., John Wiley & Sons, 1990.

4. C.N. Satterfield, *Heterogeneous Catalysis in Industrial Practice*, 2nd ed., Krieger, 1996.

Model Library path: `Chemical_Engineering_Module/Transport_and_Reactions/fixed_bed_reactor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click the **Multiphysics** button, and set the **Space dimension** list to **Axial symmetry (2D)**.

3 Select **Chemical Engineering Module>Mass Transport>Convection and Diffusion** from the **Application Modes** list. In the **Dependent variables** edit field type `cB cC` (space separated) and in the **Application mode name** edit field type `massbal`.

4 Click the **Add** button.

5 Select **Chemical Engineering Module>Energy Transport>Convection and Conduction** from the **Application Modes** list. Name the application mode `energybal` and leave the dependent variables to the default, `T`. Click **Add**.

6 Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1. Click the **Rectangle/Square** button on the Draw toolbar and draw a rectangle of arbitrary dimension. Double-click on the rectangle and type the values listed below in the corresponding edit fields; when done, click **OK**.

PROPERTY	VALUE
Width	`0.0127`
Height	3
Base	Corner
r	0
z	0

2. Double-click the **EQUAL** button on the status bar at the bottom of the user interface to allow for different scales on the r- and z-axes.
3. Click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

Constants

1. In the **Options>Constants** dialog box, define the constants listed in the following table. You can either type them in or import them from a file included in the Chemical Engineering Module. To do the latter, click the **Import Variables From File** button, browse to the folder listed in the Model Library path on page 425, select the file `fixed_bed_reactor_const.txt`, and then click **Open**.

NAME	EXPRESSION	DESCRIPTION
`R`	`1.27[cm]`	`Tube radius`
`D_eff`	`3.19e-7[m^2/s]`	`Effective diffusion constant`
`u_s`	`1.064[m/s]`	`Superficial velocity`
`rho_b`	`1300[kg/m^3]`	`Catalyst bulk density`
`k_eff`	`0.779[W/(m*K)]`	`Effective thermal conductivity`
`C_p`	`1046[J/(kg*K)]`	`Fluid heat capacity`
`rho_g`	`1.293[kg/m^3]`	`Gas density`
`c_tot`	`44.85[mol/m^3]`	`Total concentration`
`alpha`	`156[W/(m^2*K)]`	`Heat transfer coefficient`
`T0`	`627[K]`	`Inlet temperature`
`DeltaH1`	`-1.285[MJ/mol]`	`Enthalpy of adsorption, reaction 1`
`DeltaH2`	`-3.276[MJ/mol]`	`Enthalpy of adsorption, reaction 2`

NAME	EXPRESSION	DESCRIPTION
DeltaH3	DeltaH1+DeltaH2	Enthalpy of adsorption, reaction 3
yA0	0.00924	Inlet mole fraction of o-xylene
y0	0.208	Mole fraction of oxygen
A1	1[kmol/kg]*exp(19.837)/1[h]	Pre-exponential factor, reaction 1
A2	1[kmol/kg]*exp(20.86)/1[h]	Pre-exponential factor, reaction 2
A3	1[kmol/kg]*exp(18.97)/1[h]	Pre-exponential factor, reaction 3
B1	13588[K]	Activation temperature, reaction 1
B2	15803[K]	Activation temperature, reaction 2
B3	14394[K]	Activation temperature, reaction 3

2 Click **OK**.

Scalar Expressions

1 Define the following expressions in the **Options>Expressions>Scalar Expressions** dialog box, either by typing them in or by importing them from the file `fixed_bed_reactor_expr.txt`, which you find in the same directory as the constants text file.

NAME	EXPRESSION	DESCRIPTION
k1	A1*exp(-B1/T)	Forward rate constant, reaction 1
k2	A2*exp(-B2/T)	Forward rate constant, reaction 2
k3	A3*exp(-B3/T)	Forward rate constant, reaction 3
r1	rho_b*yA0*y0*k1*(1-xB-xC)	Reaction rate, reaction 1 (A->B)
r2	rho_b*yA0*y0*k2*xB	Reaction rate, reaction 2 (B->C)
r3	rho_b*yA0*y0*k3*(1-xB-xC)	Reaction rate, reaction 3 (A->C)
rB	r1-r2	Net production rate of phthalic anhydride
rC	r2+r3	Production rate of carbon oxides
xA	(cB+cC)/c_tot	Conversion, species A
xB	cB/c_tot	Conversion, species B
xC	cC/c_tot	Conversion, species C

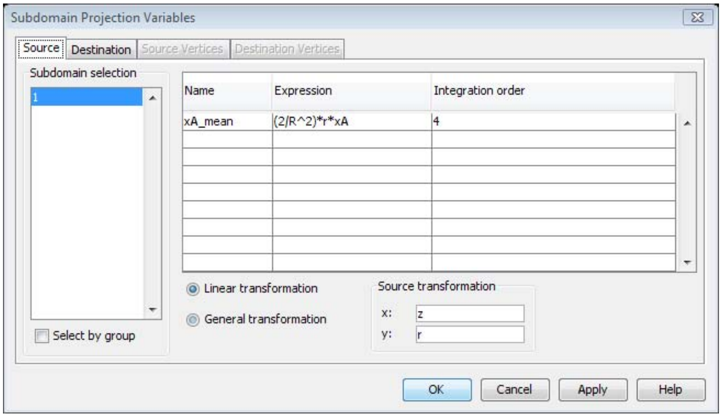
2 Click **OK**.

Projection Coupling Variables

Next, define the mean conversions (see Equation 8-7) as projection coupling variables and make them available on the reactor centerline, which corresponds to Boundary 1. (For information on coupling variables in COMSOL Multiphysics, see the section

"Using Coupling Variables" on page 255 of the *COMSOL Multiphysics User's Guide*.)

1 From the **Options** menu, select **Projection Coupling Variables>Subdomain Variables**.
2 On the **Source** page, select Subdomain 1 from the **Subdomain selection** list.
3 On the first empty row in the table, type `xA_mean` in the **Name** column and `(2/R^2)*r*xA` in the **Expression** column. (Use the default integration order.)
4 Click the **General transformation** option button. In the **Source transformation** area, set **x** to `z` and **y** to `r`.



Name	Expression	Integration order
xA_mean	(2/R^2)*r*xA	4

● Linear transformation
○ General transformation

Source transformation
x: z
y: r

5 On the **Destination** page, select **Boundary** from the **Level** list.
6 Select Boundary 1 as well as the **Use selected boundaries as destination** check box.
7 In the **Destination transformation** area, set **x** to `r`.
8 Click the **Source** tab.
9 Repeat Steps 3–8 twice to define `xB_mean` and `xC_mean` as the radial mean values of the conversions `xB` and `xC`, respectively.
10 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Mass Transport

1 From the **Multiphysics** menu, select **1 Convection and Diffusion (massbal)**.
2 From the **Physics** menu, select **Subdomain Settings**. Select Subdomain 1.

3 Specify the following subdomain settings:

SPECIES	CB	CC
D (isotropic)	`D_eff`	`D_eff`
R	`rB/yA0`	`rC/yA0`
u	`0`	`0`
v	`u_s`	`u_s`

4 On the **cB** and **cC** pages, in turn, click the **Artificial Diffusion** button. Select the **Streamline diffusion** check box. Click **OK** to confirm the default parameters.

5 Click **OK** in the **Subdomain Settings** dialog box.

Boundary Conditions—Mass Transport

1 Choose **Physics>Boundary Settings**.

2 On both the **cB** and the **cC** page, specify the following boundary conditions:

SETTINGS	BOUNDARY 2	BOUNDARY 3
Type	Concentration	Convective flux
cB_0, cC_0	0	

On Boundaries 1 and 4, the default **Insulation/Symmetry** condition applies.

3 Click **OK**.

Subdomain Settings—Energy Transport

1 From the **Multiphysics** menu, select **2 Convection and Conduction (energybal)**.

2 Choose **Physics>Subdomain Settings**.

3 For Subdomain 1, enter the settings listed in the following table:

PROPERTY	VALUE
k (isotropic)	`k_eff`
ρ	`rho_g`
C_p	`C_p`
Q	`(-DeltaH1)*rB+(-DeltaH3)*rC`
$\mathbf{u}$	`0 u_s`

4 Click the **Artificial Diffusion** button, then select the **Streamline diffusion** check box. Click **OK** to confirm the default parameters and close the dialog box.

5 On the **Init** page, set **T(t_0)** to `T0`.

6 Click **OK**.

Boundary Conditions—Energy Transport

1 Choose **Physics>Boundary Settings**.

2 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY 4
Type	Axial symmetry	Temperature	Convective flux	Heat flux
q_0				`-alpha*(T-T0)`
T_0		`T0`		

3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Finer**.

Because of the large aspect ratio of the model geometry—the reactor is 3 meters long and 0.0127 meters in radius—it is necessary to rescale the mesh in the radial direction; use a scale factor of 200.

3 Click the **Advanced** tab. In the **r-direction scale factor** edit field, type `200`.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

1 Click the **Plot Parameters** button on the Main toolbar.

2 Click the **Surface** tab. Type `T` in the **Expression** edit field on the **Surface Data** page.

3 Click **OK**.

4 From the **Postprocessing** menu, select **Domain Plot Parameters**.

5 Click the **Line/Extrusion** tab and select Boundary 1.

6 In the **Expression** edit field, type `xA_mean`.

7 In the **x-axis data** area, select the option button next to the **Expression** button, then click the **Expression** button. Type `z` in the **Expression** edit field, then click **OK**.

8 Click the **Line Settings** button.

9 Select **Triangle** from the **Line marker** list. Click **OK**.

10 Go to the **General** page and click the **Title/Axis** button. Click the option button next to the **Title** edit field and type `Mean conversions` in the edit field.

11 Click the option button next to the **Second axis label** edit field and type
`x<sub>A,mean</sub>, x<sub>B,mean</sub>, x<sub>C,mean</sub>`
in the edit field. Click **OK**.

12 Click **Apply**.

13 Return to the **Domain Plot Parameters** dialog box and select the **Keep current plot** check box.

14 Click the **Line/Extrusion** tab and type `xB_mean` in the **Expression** edit field.

15 Click the **Line Settings** button and select **Square** from the **Line marker** list.

16 Click **OK** then click **Apply**.

17 Type `xC_mean` in the **Expression** edit field.

18 Click the **Line Settings** button and select **Circle** from the **Line marker** list. Click **OK**.

19 Click **OK** to close the **Domain Plot Parameters** dialog box and generate the third graph.

20 In the figure window, click the **Edit Plot** toolbar button. In the **Edit Plot** dialog box, for each line, in turn, select the **Show legend** check box and edit the entry in the **Legends** edit field. When done, click **OK**.

PARAMETRIC STUDY

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Solver** list, select **Parametric**.

3 Type `T0` in the **Parameter name** edit field and `625 626 627 628 629` in the **Parameter values** edit field.

4 Click **OK**.

5 Click the **Solve** button on the Main toolbar.

6 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.

7 Click the **Line/Extrusion** tab and type `T-T0` in the **Expression** edit field.

8 In the **x-axis data** area, select the option button next to the **Expression** button, then click the **Expression** button. Type `r` in the **Expression** edit field, select **mm** from the **Unit** list and click **OK**.

9 In the **Cross-section line data** area, type in the following values:

R0	**R1**	**Z0**	**Z1**
`0`	`0.0127`	`0.6`	`0.6`

10 Click the **Line Settings** button.

11 Select **Cycle** from the **Line marker** list and select the **Legend** check box. Click **OK**.

12 Click **OK** to create the plot in Figure 8-5.

Finally, perform the following steps to produce Figure 8-6.

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.
2. On the **Line/Extrusion** tab, type `T-T0` in the **Expression** edit field.
3. Click the **Line Settings** button and select **Cycle** from both the **Line color** and the **Line marker** list. Select the **Legend** check box, then click **OK**.
4. Go to the **General** page and click the **Title/Axis** button.
5. Type `Centerline temperature` in the **Title** edit field and select the **Auto** option button for the **Second axis label**. Click **OK**.
6. From the **Plot in** list, select **New figure**.
7. Click **OK**.

Absorption in a Falling Film

Introduction

The absorption process of gases in liquids is thoroughly treated in the chemical engineering literature (References 1–3). When modeling reactors and equipment for unit operations, you are dependent on experimental data for the relation between gas and liquid composition. In the process of measuring absorption, you have to design your experiments in such a way that relevant data is obtained.

In this example[1], you model an experimental setup for studies of gas absorption, more specifically the absorption of chlorine, diluted in hydrogen, in a caustic solution containing low amounts of carbonate. In many electrolysis processes, hydrogen is generated at the cathode and is often contaminated by chlorine, which is produced at the anode in chloride solutions. The chlorine-contaminated hydrogen is cleaned in caustic soda scrubbers.

There are a number of different experimental methods for determining the absorption of a gas in a liquid. Most methods share the same basic principle: create a well-defined velocity profile in the liquid phase to obtain an analytic estimation of the diffusion boundary layer (References 1–3). Such a well-defined velocity profile can be obtained by using laminar jets, rotating drums with thin liquid films, falling films, etc. (see Ref. 4). The mass transport properties in the gas phase are estimated from the relative velocity between the liquid flow and the gas flow. In most cases, the gas flow velocity is negligible in comparison with the liquid velocity. Consequently, the magnitude of the forced convection in the gas is negligible and the transport properties can be

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[1] This model was developed in cooperation with Fredrik Herlitz, Eka Chemicals R&D.

obtained from the free convection that is induced in the gas phase by the flow of the liquid.

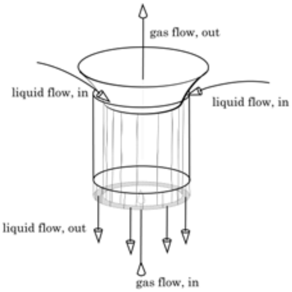


Figure 8-7: Schematic view of a falling film stripper.

The model describes measuring equipment for gas absorption based on the principle of a falling laminar film. The setup of this apparatus appears in Figure 8-7. A liquid film is formed by a guiding funnel that creates an annular flow with a free liquid surface facing a hollow tubular region. The gas is introduced in the tube from below and is absorbed on the free surface of the liquid. The liquid and gas compositions are measured before and after entering the apparatus. This setup implies that the liquid-gas contact area and the convection of the phase boundary are well defined.

The model shows that it is simple to treat fairly large systems of nonlinear partial differential equations in COMSOL Multiphysics.

Model Definition

The model describes a falling film apparatus for the absorption of low amounts of chlorine in hydrogen. The gas is further contaminated with low amounts of carbon dioxide, which in some cases can limit the absorption rate of chlorine. To obtain a more transparent model, use the following assumptions about the system:

- Assume that chlorine in hydrogen is diluted to such an extent that the volume of the gas is not influenced by the absorption process.
- Do not account for condensation and evaporation of water in the system.
- Neglect any homogeneous gas phase reactions.
- Assume laminar flow in the liquid phase.
- Assume that the radius of the tube is large enough in comparison to the thickness of the falling film that tube curvature effects are negligible.
- Assume the tube to be short enough that you can neglect gravitational acceleration.

- Assume that the contribution of diffusion to the flux of species is negligible in the direction of the convective flow, that is, in the vertical direction.
- Assume that the system is isothermal.

You find the thermodynamic and kinetic data for the system, as well as a detailed description of the chemistry, in Ref. 5. The chemical species in this example are given in Table 8-1.

TABLE 8-1: PARTICIPATING SPECIES

INDEX	1	2	3	4	5	6	7	8	9	10
SPECIES	Cl_2	OH^-	$HClO$	Cl^-	H^+	ClO^-	HCO_3^-	CO_2	CO_3^{2-}	H_2CO_3

The chemical reactions that appear in the mass balances for the species in the previous table are:

$$\begin{array}{ll}
Cl_2 + OH^- = HClO + Cl^- & (1) \\
H_2O = H^+ + OH^- & (2) \\
HClO + OH^- = ClO^- + H_2O & (3) \\
Cl_2 + H_2O = HClO + HCl & (4) \\
Cl_2 + HCO_3^- = CO_2 + HClO + Cl^- & (5) \\
Cl_2 + CO_3^{2-} = CO_2 + ClO^- + Cl^- & (6) \\
CO_2 + H_2O = H_2CO_3 & (7) \\
CO_2 + OH^- = HCO_3^- & (8) \\
HCO_3^- + OH^- = CO_3^{2-} + H_2O & (9) \\
HCO_3^- + H^+ = H_2CO_3 & (10)
\end{array} \qquad (8\text{-}8)$$

The model accounts for the kinetics in every reaction. Denote the kinetic parameters in the equations above `ki` and `k_i`, for the forward and backward reaction, respectively, where `i` is the number of the reaction. Denote the equilibrium constants for the reactions `Ki`.

The assumptions listed above allow you to define the mass balance equations for the system from the chemical reaction formulas. In addition, you can neglect the component of the flow velocity vector in the horizontal direction, which makes it possible to obtain an analytic expression for this vector (Ref. 2). The result of this is that you can reduce the 3D problem to a 1D time-dependent model, using time to represent the space coordinate in the vertical direction. The following sketch shows the domain that the model includes. The domain is confined by the gas phase on the left side and by the wall of the tube on the right side. It is also bounded by the inlet at the top and the outlet at the bottom.

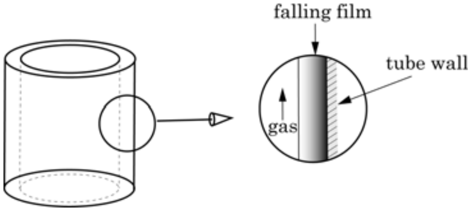


Figure 8-8: Schematic of the falling film at the tube wall in the experimental device.

The following general expression describes the flux vector of every species:

$$\mathbf{N}_i = \left(-D_i \frac{\partial c_i}{\partial x}, c_i v_y\right) \quad \text{in } \Omega \qquad i = 1, \ldots, 10 \tag{8-9}$$

Here $\mathbf{N}_i$ (mol/(m^2·s)) represents the flux, D_i (m^2/s) the diffusion coefficient in the liquid phase, and c_i (mol/m^3) the concentration of species i. Further, x (m) is the space coordinate in the horizontal direction and v_y (m/s) refers to the liquid-flow velocity component in the vertical direction. Ref. 1 gives the velocity profile, v_y, as

$$v_y = 1.5 v_{\mathrm{av}} \cdot \left(1 - \left(\frac{x}{\delta}\right)^2\right) \tag{8-10}$$

where v_{av} represents the average relative velocity and δ the thickness of the film. The space coordinate x is 0 at the gas phase boundary and δ at the wall of the tube. The coordinate y is 0 at the inlet and equal to the length of the tube, L, at the outlet.

You can now define the mass balance at steady state for the species:

$$(\nabla \cdot \mathbf{N}_i - \Sigma R_j = 0) \quad \text{in } \Omega, \qquad i = 1, \ldots, 10 \tag{8-11}$$

In this equation R_j (mol/(m^3·s)) represents the reaction rate for each of the reactions j that the species i takes part in. You can obtain the kinetic expressions for these reactions from Ref. 4, and they are also listed in the modeling instructions below. The equations above can be expressed in the following form:

$$\left(-D_i \frac{\partial^2 c_i}{\partial x^2} + v_y \frac{\partial c_i}{\partial y} - \sum R_j = 0\right) \quad \text{in } \Omega, \qquad i = 1, \ldots, 10 \tag{8-12}$$

You can rewrite these equations by using the transformation $y = v_{\mathrm{av}}t$ to get the following final system of equations in the domain:

$$1.5\left(1-\left(\frac{x}{\delta}\right)^2\right)\frac{\partial c_i}{\partial t} - D_i\frac{\partial^2 c_i}{\partial x^2} - \sum R_j = 0 \quad \text{in } \Omega, \qquad i = 1, \ldots, 10 \qquad (8\text{-}13)$$

The concentration at the inlet of each involved species is 0 except for those of the hydrogen and hydroxide ions. The transformation from vertical coordinate to time implies that the boundary conditions at $y = 0$ become initial conditions at $t = 0$, which thus read

$$\begin{aligned} &c_i(x, 0) = 0 \qquad i = 1, 3, 4, 6, \ldots, 10 \\ &c_2(x, 0) = C_{\mathrm{OH}} \\ &c_5(x, 0) = C_{\mathrm{H}} \end{aligned} \qquad (8\text{-}14)$$

The outlet corresponds to the time $t_{\mathrm{f}} = L/v_{\mathrm{av}}$. In this model, the parameters L and v_{av} are adjusted to give $t_{\mathrm{f}} = 1$ s.

The boundary conditions for the system at the gas phase boundary are

$$\begin{aligned} &-D_i\frac{\partial c_i}{\partial x}(0, t) = 0 \qquad\qquad i = 2, \ldots, 7, 9, 10 \\ &-D_1\frac{\partial c_1}{\partial x}(0, t) = k_{\mathrm{ga,\,Cl_2}}(p_{\mathrm{Cl_2}} - c_1 H_{\mathrm{Cl_2}}) \\ &-D_8\frac{\partial c_8}{\partial x}(0, t) = k_{\mathrm{ga,\,CO_2}}(p_{\mathrm{CO_2}} - c_8 H_{\mathrm{CO_2}}) \end{aligned} \qquad (8\text{-}15)$$

where k_{ga} (mol/(m^2·s·Pa)) denotes the mass transport coefficient in the gas phase, p (Pa) is the partial pressure, and H (Pa·m^3/mol) refers to the Henry constant.

The boundary conditions at the tube wall are

$$-D_i\frac{\partial c_i}{\partial x}(\delta, t) = 0 \qquad i = 1, \ldots, 10 \qquad (8\text{-}16)$$

which implies that there is no flux of species out of the domain at this boundary.

Results

Table 8-9 shows the concentration of chlorine inside the film as a function of distance from the gas-liquid interface at t = 1 s, which corresponds to the outlet of the tube.

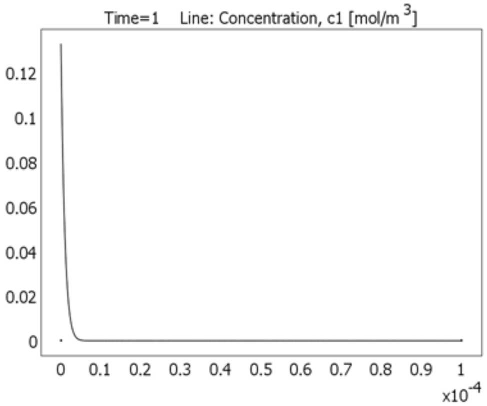


Figure 8-9: Concentration profile for chlorine.

The graph shows that chlorine does not penetrate the film to a larger extent. This is explained by chlorine's reaction with the hydroxide ion leading to hypochlorous acid and the hypochlorite ion. This reaction is very fast and limits the spreading of chlorine in the falling film. The low pH at the surface of the film, and thus the low content of hydroxide ions, allows for a high chlorine concentration. The acidic surface of the film reduces the scrubbing capacity in the falling film. For this reason, a scrubber is equipped with filling material that enhances the mixing through convection in the film.

The reaction products from chlorine's reaction with the hydroxide ion and water penetrate the falling film during the absorption process. You can see the concentration profile of the hypochlorite ion, from the inlet to the outlet of the tube in Figure 8-10.

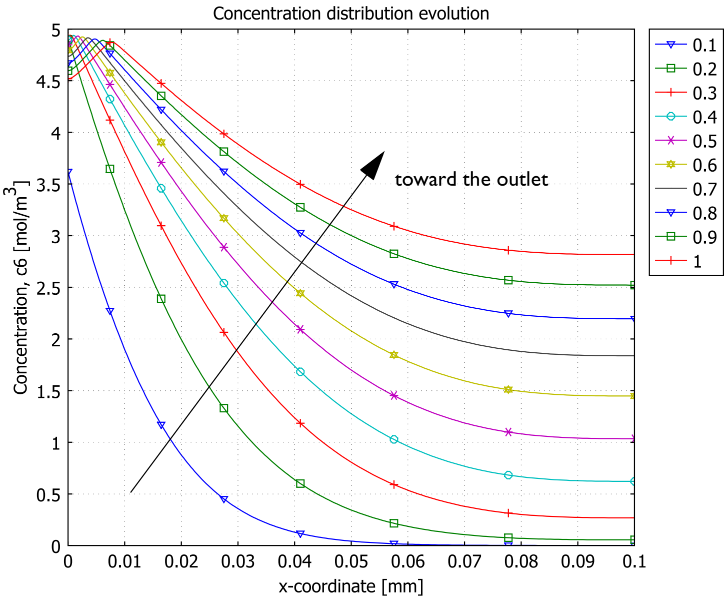


Figure 8-10: Radial concentration distribution at the distances 0.1L, 0.2L, …, L from the tube inlet (L = tube length).

You can see from this figure that the hypochlorite ion increases in concentration throughout the absorption process. At a certain stage, a maximum appears in the profile. This maximum is caused by the consumption of hypochlorite, through the formation of hypochlorous acid, at the low pH at the surface of the film ($x = 0$). The low pH is caused by the reaction of chlorine with hydroxide and water.

Modeling in COMSOL Multiphysics

When modeling a stationary convection-diffusion process that has negligible convective transport in one direction (in this case the radial direction) and negligible diffusive transport in the other direction (in this case the axial direction), it is possible to reformulate the convection-diffusion equation by switching the axial derivative to a time derivative. To be able to do so, you also need to have a nonchanging velocity field along the axial direction. This enables us to reduce one space dimension of the problem, making it a much smaller 1D problem, albeit time dependent. In COMSOL Multiphysics this is a "pseudo-2D equation,"

$$u_{\mathrm{dl}}\frac{\partial c}{\partial t}+\frac{\partial}{\partial x}\left(-D\frac{\partial c}{\partial x}\right) = R\,, \tag{8-17}$$

where u_{dl} is the dimensionless velocity.

References

1. R. Perry and D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

2. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

3. G.F. Froment and K.B. Bischoff, *Chemical Reactor Analysis and Design*, 2nd ed., John Wiley & Sons, 1990.

4. C.W. Spalding, "Reaction Kinetics in the Absorption of Chlorine into Aqueous Media," *AIChE J.*, vol. 8, no. 5, p. 685–689, 1962.

5. S.S. Ashour, E.B. Rinker, and O.C. Sandall, "Absorption of Chlorine into Aqueous Bicarbonate Solutions and Aqueous Hydroxide Solutions," *AIChE J.*, vol. 42, no. 3, pp. 671–682, 1996.

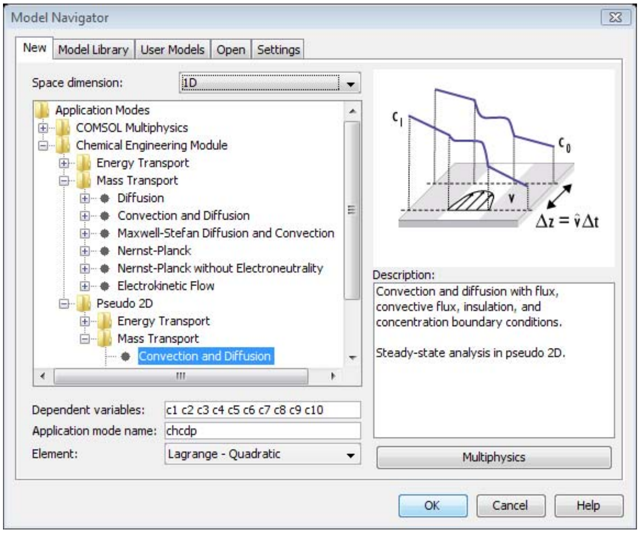
Model Library path:
`Chemical_Engineering_Module/Transport_and_Reactions/falling_film`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator,** select **1D** from the **Space dimension** list.
3. From the **Application Modes** list, select **Chemical Engineering Module>Pseudo 2D>Mass Transport>Convection and Diffusion**.

4 In the **Dependent variables** edit field, type the names of the concentration variables as space-separated entries: `c1 c2 c3 c4 c5 c6 c7 c8 c9 c10`.



Space dimension: 1D

Description:
Convection and diffusion with flux, convective flux, insulation, and concentration boundary conditions.

Steady-state analysis in pseudo 2D.

Dependent variables: c1 c2 c3 c4 c5 c6 c7 c8 c9 c10

Application mode name: chcdp

Element: Lagrange - Quadratic

5 Select **Lagrange - Cubic** from the **Element** list. Using higher order elements gives more accurate results compared to lower order elements.

6 Click **OK**.

OPTIONS AND SETTINGS

1 In the **Options>Axes/Grid settings** dialog box, set the axis limits to **x min:** `-1e-5` and **x max:** `11e-5`.

2 Click **OK**.

3 Define the following constants in the **Options>Constants** dialog box (the descriptions are optional); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
D1	1.47e-9[m^2/s]	Diffusivity, species 1
D2	3.43e-9[m^2/s]	Diffusivity, species 2
D3	1.54e-9[m^2/s]	Diffusivity, species 3
D4	1.565e-9[m^2/s]	Diffusivity, species 4
D5	3.43e-9[m^2/s]	Diffusivity, species 5
D6	3.43e-9[m^2/s]	Diffusivity, species 6
D7	1.5e-9[m^2/s]	Diffusivity, species 7

NAME	EXPRESSION	DESCRIPTION
D8	1.92e-9[m^2/s]	Diffusivity, species 8
D9	1.5e-9[m^2/s]	Diffusivity, species 9
D10	1.5e-9[m^2/s]	Diffusivity, species 10
T	298[K]	Temperature
k1	1.565e6[m^3/(mol*s)]	Forward rate constant 1
K1	4.491e10	Equilibrium constant 1
k_1	k1/K1	Reverse rate constant 1
k2	1e9[mol/(m^3*s)]	Forward rate constant 2
K2	1.002e-8[(mol/m^3)^2]	Equilibrium constant 2
k_2	k2/K2	Reverse rate constant 2
k3	2.79e12[m^3/(mol*s)]	Forward rate constant 3
K3	2.79e3[m^3/mol]	Equilibrium constant 3
k_3	k3/K3	Reverse rate constant 3
k4	1.4527e10[1/s]*exp(-6138.6[K]/T)	Forward rate constant 4
K4	4.5e10[(mol/m^3)^2]	Equilibrium constant 4
k_4	k4/K4	Reverse rate constant 4
k5	5.63e7[m^3/(mol*s)]* exp(-4925[K]/T)	Forward rate constant 5
K5	1.092e6[mol/m^3]	Equilibrium constant 5
k_5	k5/K5	Reverse rate constant 5
k6	k5	Forward rate constant 6
K6	6.569e9[mol/m^3]	Equilibrium constant 6
k_6	k6/K6	Reverse rate constant 6
k7	10^(329.85-110.541*log(T[1/K])/ log(10)-17265.4[K]/T)[1/s]	Forward rate constant 7
K7	2.06e-3	Equilibrium constant 7
k_7	k7/K7	Reverse rate constant 7
k8	10^(13.635-2895[K]/T) [m^3/(mol*s)]/1000	Forward rate constant 8
K8	4.112e4[m^3/mol]	Equilibrium constant 8
k_8	k8/K8	Reverse rate constant 8
k9	1e10[m^3/(mol*s)]	Forward rate constant 9
K9	4.640[m^3/mol]	Equilibrium constant 9
k_9	k9/K9	Reverse rate constant 9
k10	2.155e9[m^3/(mol*s)]	Forward rate constant 10

NAME	EXPRESSION	DESCRIPTION
K10	5[m^3/mol]	Equilibrium constant 10
k_10	k10/K10	Reverse rate constant 10
delta	0.1[mm]	Film thickness
Coh	10[mol/m^3]	Initial concentration, OH-
Ch	K2/Coh	Initial concentration, H+
kgaCl2	0.244[mol/(m^2*s*atm)]	Mass transport coefficient
pCl2	3[matm]	Partial pressure
HCl2	0.01636[atm*m^3/mol]	Henry constant
kgaCO2	0.244[mol/(m^2*s*atm)]	Mass transport coefficient
pCO2	1[matm]	Partial pressure
HCO2	0.0266[atm*m^3/mol]	Henry constant

4 Define the following expressions in the **Options>Expressions>Scalar Expressions** dialog box; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
udl	1.5*(1-(x/delta)^2)	Dimensionless velocity

GEOMETRY MODELING

Click the **Line** button on the Draw toolbar and draw a line from 0 to 1e-4.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, choose **Subdomain Settings**. Select Subdomain 1.

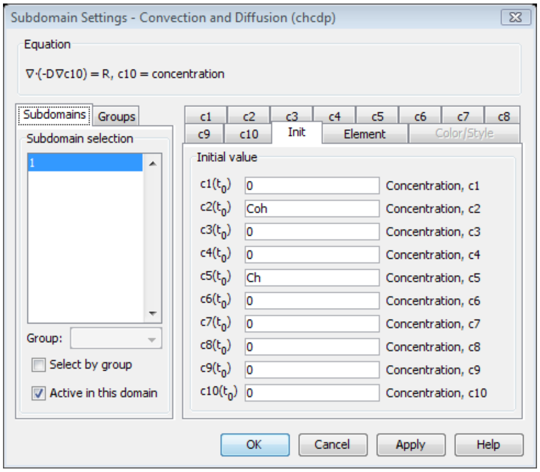
2 On each species page, **c1**, …, **c10**, enter the applicable settings for diffusion constant, reaction rate, and dimensionless velocity from this table:

SPECIES	D	R	u_{dl}
1	D1	(-k1*c1*c2+k_1*c3*c4 -k4*c1+k_4*c3*c4*c5)-(k5*c1*c7-k_5*c3*c4*c8) -(k6*c1*c9-k_6*c4*c6*c8)	udl
2	D2	(-k1*c1*c2+k_1*c3*c4+k2- k_2*c2*c5-k3*c2*c3+k_3*c6) -(k8*c2*c8-k_8*c7)-(k9*c2*c7-k_9*c9)	udl
3	D3	(k1*c1*c2-k_1*c3*c4-k3*c2*c3+ k_3*c6+k4*c1-k_4*c3*c4*c5) +(k5*c1*c7-k_5*c3*c4*c8)	udl

SPECIES	D	R	u_{dl}
4	`D4`	`(k1*c1*c2-k_1*c3*c4+k4*c1-k_4*c3*c4*c5)+(k5*c1*c7-k_5*c3*c4*c8)+(k6*c1*c9-k_6*c4*c6*c8)`	`udl`
5	`D5`	`(k2-k_2*c2*c5+k4*c1-k_4*c3*c4*c5)-(k10*c5*c7-k_10*c10)`	`udl`
6	`D6`	`(k3*c2*c3-k_3*c6)+(k6*c1*c9-k_6*c4*c6*c8)`	`udl`
7	`D7`	`-(k5*c1*c7-k_5*c3*c4*c8)+(k8*c2*c8-k_8*c7)-(k9*c2*c7-k_9*c9)-(k10*c5*c7-k_10*c10)`	`udl`
8	`D8`	`(k5*c1*c7-k_5*c3*c4*c8)+(k6*c1*c9-k_6*c4*c6*c8)-(k7*c8-k_7*c10)-(k8*c2*c8-k_8*c7)`	`udl`
9	`D9`	`-(k6*c1*c9-k_6*c4*c6*c8)+(k9*c2*c7-k_9*c9)`	`udl`
10	`D10`	`(k7*c8-k_7*c10)+(k10*c5*c7-k_10*c10)`	`udl`

3 On the **Init** page, set **c2(t_0)** to `Coh` and **c5(t_0)** to `Ch`.

The other concentrations are zero at the beginning of the process.



Subdomain Settings - Convection and Diffusion (chcdp)

Equation

$\nabla\cdot(-D\nabla c10) = R$, c10 = concentration

Initial value

c1(t_0)	0	Concentration, c1
c2(t_0)	Coh	Concentration, c2
c3(t_0)	0	Concentration, c3
c4(t_0)	0	Concentration, c4
c5(t_0)	Ch	Concentration, c5
c6(t_0)	0	Concentration, c6
c7(t_0)	0	Concentration, c7
c8(t_0)	0	Concentration, c8
c9(t_0)	0	Concentration, c9
c10(t_0)	0	Concentration, c10

☐ Select by group

☑ Active in this domain

4 Click **OK** to close the dialog box.

Boundary Conditions

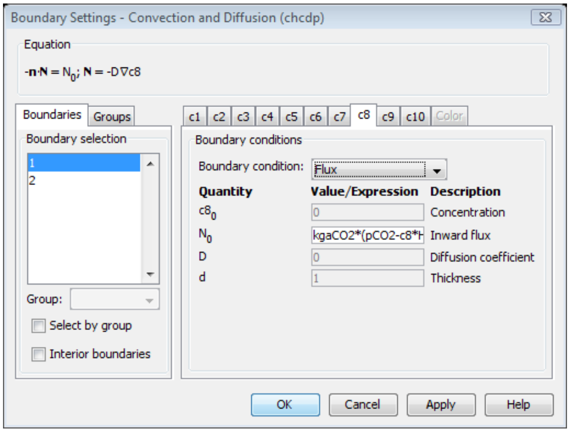
1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Select Boundary 1.

3 On the pages **c1** and **c8**, enter the corresponding settings from this table:

PROPERTY	**c1**	**c8**
Type	Flux	Flux
N_0	`kgaCl2*(pCl2-c1*HCl2)`	`kgaCO2*(pCO2-c8*HCO2)`

For the remaining species, leave the default condition (Insulation/Symmetry).



Equation

$-\mathbf{n}\cdot\mathbf{N} = N_0;\ \mathbf{N} = -D\nabla c8$

Boundary conditions

Boundary condition: Flux

Quantity	**Value/Expression**	**Description**
$c8_0$	0	Concentration
N_0	kgaCO2*(pCO2-c8*H	Inward flux
D	0	Diffusion coefficient
d	1	Thickness

4 Click **OK** to close the dialog box.

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 On the **Global** page, set the **Element growth rate** to `1.03`.

3 On the **Boundary** page, select Boundary 1 and enter a **Maximum element size** of `1e-6`.

4 Click the **Remesh** button.

5 When the mesher has finished, click **OK** to close the dialog box.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Timestepping** area, type `0:0.02:1` in the **Times** edit field. Set the **Relative tolerance** to `2e-6` and the **Absolute tolerance** to `1e-7` to improve accuracy in the time stepping.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar. Because you are using cubic elements and low error tolerances for higher accuracy it takes a few minutes for the solver to finish.

POSTPROCESSING AND VISUALIZATION

To generate Figure 8-10, follow these steps:

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.
2. On the **General** page, select the solutions at 0.1 s to 1.0 s with intervals of 0.1 s by pressing the Ctrl key and clicking at the appropriate times in the **Solutions to use** list.
3. Click the **Title/Axis** button and enter appropriate title.
4. Click **OK**.
5. Click the **Line/Extrusion** tab, then select Subdomain 1.
6. In the **y-axis data** area, type `c6` in the **Expression** edit field.
7. Set the **x-axis data** to **x**.
8. Click the **Line Settings** button. From the **Line marker** list, select **Cycle**. Select the **Legend** check box, then click **OK**.
9. Click **OK**.

Boat Reactor for Low Pressure Chemical Vapor Deposition

Introduction

Chemical vapor deposition (CVD) is an important step in the process of manufacturing microchips. A common application is the deposition of silicon on wafers at low pressure. Low-pressure reactors are used to get a high diffusivity of the gaseous species, which results in a uniform deposition thickness, because the process becomes limited by the deposition kinetics (Ref. 1 and Ref. 2).

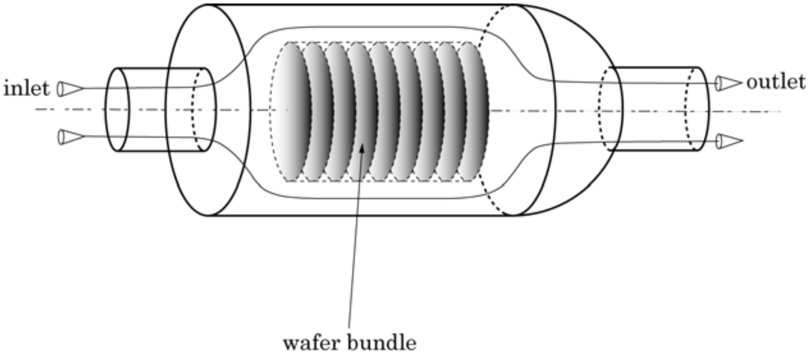


Figure 8-11: Schematic of a boat reactor and the principle of the deposition process.

In this example you model the momentum and mass transport equations coupled to the reaction kinetics for the deposition process. You treat a low-pressure boat reactor, where the goal of the simulation is to describe the rate of deposition as a function of the fluid mechanics and kinetics in the system.

The gas, in this case silane (SiH_4), enters the reactor from the left and reacts on the wafers to form hydrogen and silicon. The remaining mixture leaves the reactor through the outlet on the right. The deposition of silicon on the surface of the wafers depends on the local concentration of silane, which is determined by the operating conditions for the reactor.

You can find more details about this example in *Elements of Chemical Reaction Engineering* by H. Scott Fogler (Ref. 1).

Model Definition

First assume that the density of the gas is constant throughout the reactor. This implies that the reacting gas is either diluted in a carrier gas or that the conversion in the reactor is small. Moreover, only account for the mass transport of the reactant gas, in this case silane, and assume constant temperature in the reactor.

In the wafer bundle subdomain you can neglect convection transport, so that the reacting gas can only be transported through diffusion. To save time and computational memory, also simplify the geometrical description of the wafer bundle by modeling it as an anisotropic medium. To this end, because silane cannot diffuse through the physical wafers, assume that the axial diffusivity in the wafer bundle is zero. Furthermore, correct the diffusivity in the radial direction according to the degree of packing in the bundle. Finally, neglect the influence of the support boat on the transport process that holds the wafer bundle in place. The structure of the boat reactor means that you can reduce the 3D geometry to a 2D axisymmetric model. The modeling domain is shown in Figure 8-12.

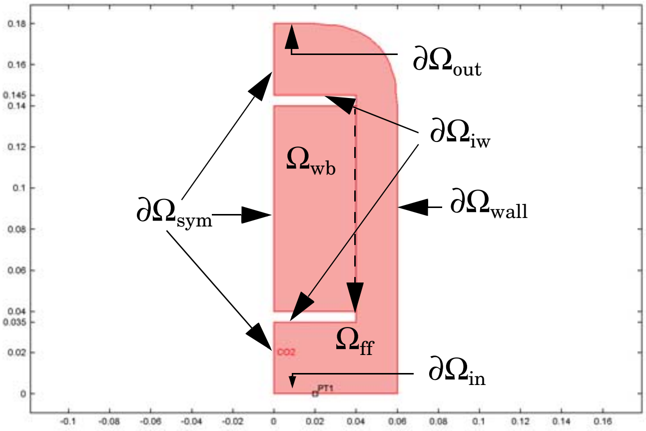


Figure 8-12: The model geometry showing the subdomain and boundary labels.

The chemical reaction you account for in this example is given below:

$$SiH_4(g) \leftrightarrow Si(s) + 2H_2(g) \qquad (8\text{-}18)$$

The rate of this reaction depends on the partial pressure of silane and the temperature in the reactor.

The assumptions mentioned above in combination with the chemical reaction for the deposition process make it possible to define an equation system. The momentum equations and the continuity equations for laminar flow in cylindrical coordinates read

$$\begin{aligned}
&\frac{\partial}{\partial r}\left(-\eta r\frac{\partial u}{\partial r}\right)+\frac{\partial}{\partial z}\left(-\eta r\frac{\partial u}{\partial z}\right)+\rho r\left(u\frac{\partial u}{\partial r}+v\frac{\partial u}{\partial z}\right)+r\frac{\partial p}{\partial r}=0 \text{ in } \Omega_{\text{ff}}\\
&\frac{\partial}{\partial r}\left(-\eta r\frac{\partial v}{\partial r}\right)+\frac{\partial}{\partial z}\left(-\eta r\frac{\partial v}{\partial z}\right)+\rho r\left(u\frac{\partial v}{\partial r}+v\frac{\partial v}{\partial z}\right)+r\frac{\partial p}{\partial z}=0 \text{ in } \Omega_{\text{ff}}\\
&r\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}\right)+v=0 \qquad \text{in } \Omega_{\text{ff}}
\end{aligned} \tag{8-19}$$

Here η (kg/(m·s)) denotes the viscosity; ρ (kg/m^3) is the density of the gas; u and v (m/s) refer to the velocity vector's r- and z-components, respectively; and p (Pa) is the pressure.

The mass transport in the free-fluid subdomain is given by the following equation, expressed in cylindrical coordinates:

$$\frac{\partial}{\partial r}\left(-Dr\frac{\partial c}{\partial r}\right)+\frac{\partial}{\partial z}\left(-Dr\frac{\partial c}{\partial z}\right)+ru\frac{\partial c}{\partial r}+rv\frac{\partial c}{\partial z}=0 \text{ in } \Omega_{\text{ff}} \tag{8-20}$$

Here D denotes the diffusivity (m^2/s) and c is the concentration of silane (mol/m^3). You obtain the corresponding mass transport equation for the wafer bundle subdomain by neglecting transport by convection and adding a reaction-rate term for the dissociation of silane:

$$\frac{\partial}{\partial r}\left(-D_{\text{eff},\,rr}r\frac{\partial c}{\partial r}\right)=-rkS_a c \text{ in } \Omega_{\text{wb}} \tag{8-21}$$

Because you neglect diffusion in the axial direction, the effective diffusivity tensor, D_{eff}, only has an rr component. In the equation above, k (m/s) denotes the rate constant for the reaction, and S_a (m^2/m^3) refers to the specific surface area.

You solve the system of equations defined above by using the proper boundary conditions. For laminar flow, no-slip conditions apply at the reactor-wall surface and between the free channel and the wafer bundle:

$$(u,v)=(0,0) \quad \text{at } \partial\Omega_{\text{wall}},\ \partial\Omega_{\text{iw, ff}},\ \text{and } \partial\Omega_{\text{wb, ff}} \tag{8-22}$$

At the symmetry axis, the radial velocity component vanishes:

$$u = 0 \text{ at } \partial\Omega_{\mathrm{sym}} \tag{8-23}$$

The last three conditions for the momentum equations and continuity equation are

$$\begin{aligned} u &= 0 && \text{at } \partial\Omega_{\mathrm{in}} \\ v &= v_0 && \text{at } \partial\Omega_{\mathrm{in}} \\ p &= p_0 && \text{at } \partial\Omega_{\mathrm{out}} \\ \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} &= \mathbf{0} && \text{at } \partial\Omega_{\mathrm{out}} \end{aligned} \tag{8-24}$$

For the mass transport equations 8-20 and 8-21, the boundary conditions are

$$\left(-D_{i,\,rr}\frac{\partial c}{\partial r}, -D_{i,\,zz}\frac{\partial c}{\partial z}\right) \cdot \mathbf{n} = 0 \text{ at } \partial\Omega_{\mathrm{wall}}, \partial\Omega_{\mathrm{sym}}, \text{ and } \partial\Omega_{\mathrm{iw}} \tag{8-25}$$

where D_i represents the diffusivity in Ω_{ff} or Ω_{wb} depending on to which boundary segment you apply the equation. This equation implies that there is no flux perpendicular to these boundaries. At the inlet, the composition of the gas is known, which yields:

$$c = c_0 \text{ at } \partial\Omega_{\mathrm{in}} \tag{8-26}$$

At the outlet, assume that the transport of species takes place mainly by convection and neglect the concentration gradients perpendicular to this boundary:

$$\left(-D\frac{\partial c}{\partial r}, -D\frac{\partial c}{\partial z}\right) \cdot \mathbf{n} = 0 \text{ at } \partial\Omega_{\mathrm{out}} \tag{8-27}$$

It remains to discuss the material parameters appearing in Equation 8-21: $D_{\mathrm{eff},rr}$, S_{a}, and k. First, calculate the specific surface area (that is, the area per unit volume) of the wafer bundle, S_{a}, by assuming a certain pitch between the wafers; see Figure 8-13.

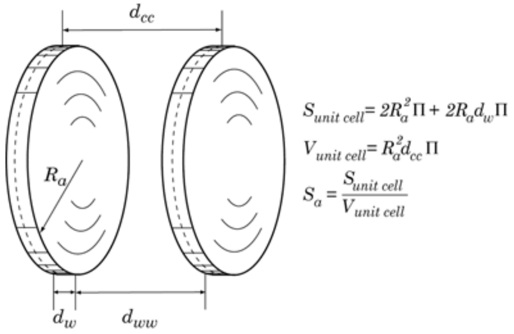


Figure 8-13: Calculation of the specific surface area.

Furthermore, to estimate the effective diffusivity in the radial direction inside the wafer bundle, multiply the diffusivity in the free-fluid subdomain by the ratio of the contact area between the free gas and the wafer bundle to the total lateral surface area of the wafer-bundle subdomain:

$$D_{\mathrm{eff},\,rr} = \left(1 - \frac{d_{\mathrm{w}}}{d_{\mathrm{cc}}}\right) D \quad \text{in } \Omega_{\mathrm{wb}} \tag{8-28}$$

The rate constant, k (m/s), is a function of the partial pressure of silane. At 600 °C and a total system pressure of 25 Pa, Ref. 2 provides the value $k = 8.06 \cdot 10^{-3}$ m/s.

A crucial characteristic of the reactor's performance is the silicon deposition rate, Δ_{Si}, which expresses the growth rate of the silicon layer on the wafers. The amount of silicon deposited on the wafers, expressed in mass per unit area per unit time, is the product of the rate constant, k, the silane concentration, c, and the molar mass of silicon, M_{Si} (kg/mol). Dividing the so obtained quantity by the density of silicon, ρ_{Si} (kg/m^3), gives the deposition rate:

$$\Delta_{\mathrm{Si}} = \frac{kcM_{\mathrm{Si}}}{\rho_{\mathrm{Si}}} \quad (\mathrm{nm/min}) \tag{8-29}$$

In this model, you study the radial and axial distribution of Δ_{Si} inside the wafer bundle.

Results

Figure 8-14 shows the concentration distribution in the boat reactor, indicating that the conversion is quite small.

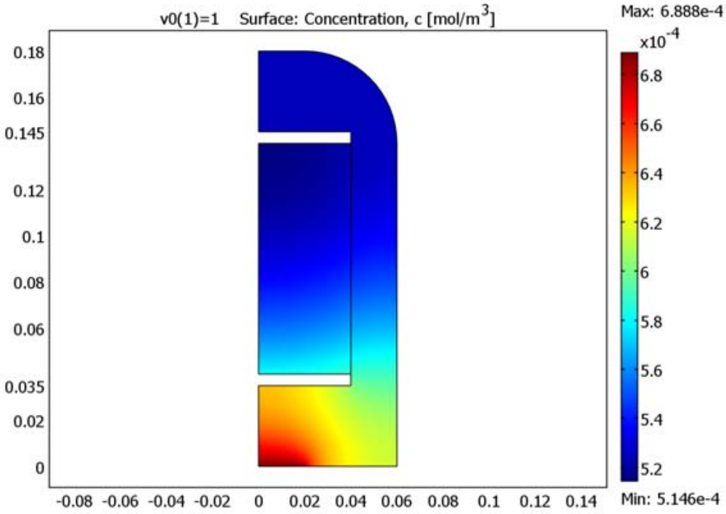


Figure 8-14: Concentration distribution in the reactor.

Figure 8-15 shows the flow distribution in the reactor.

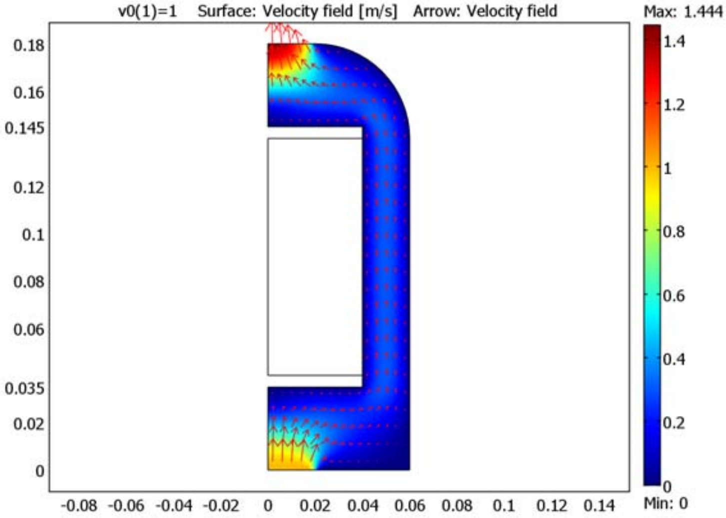


Figure 8-15: Flow distribution in the reactor. The surface color and the arrows both represent the velocity.

The plots in Figure 8-16 display the deposition rate for the inlet velocities 1 m/s (top panel) and 2 m/s (bottom panel).

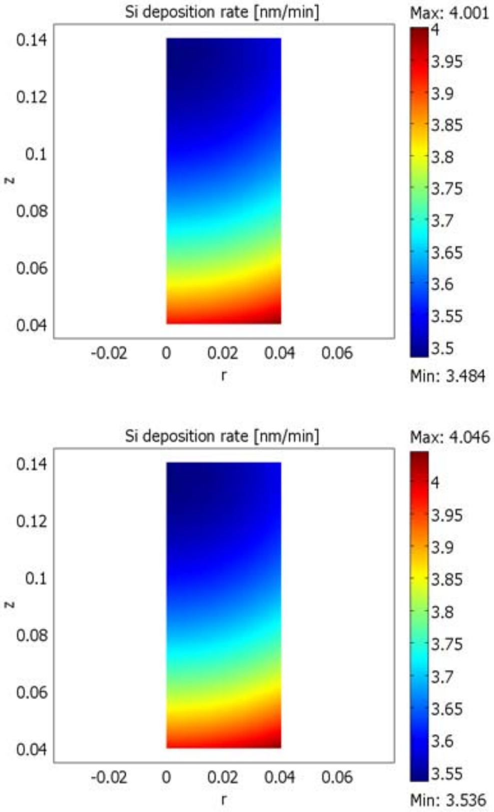


Figure 8-16: The deposition rate in the wafer bundle for the inlet velocities 1 m/s (top) and 2 m/s (bottom).

In both cases, the highest deposition rate is obtained near the reactor inlet and close to the free-fluid channel. The difference in deposition rate between the center and periphery of the wafers is approximately 0.1 nm/min (or roughly 2.5%), and that along the length of the reactor approximately 0.5 nm/min (roughly 12.5%). Thus, as desired, the variations in the deposition rate inside the reactor are rather small.

Moreover, comparing the plots it is evident that the deposition rate changes only marginally when the gas inlet velocity is doubled, showing that convection does not have a major influence on reactors of this type.

References

1. H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 3rd edition, Prentice Hall, 1999.

2. A.T. Voutsas and M. K. Hatalis, "Structure of As-Deposited LPCVD Silicon Films at Low Deposition Temperatures and Pressures," *J. Electrochem. Soc.*, vol. 139, no. 9, pp. 2659–2665, 1992.

Model Library path:
`Chemical_Engineering_Module/Transport_and_Reactions/boat_reactor`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, set **Space dimension** to **Axial symmetry (2D)**.

3 From the **Application Modes** list, select
Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes.

4 Click the **Multiphysics** button and add the application mode to the model by clicking the **Add** button.

5 From the **Application Modes** list, select
Chemical Engineering Module>Mass Transport>Convection and Diffusion.

6 Click the **Add** button to add the application mode to the model.

7 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Axes/Grid Settings**.

2 Specify the axis and grid settings according to the following table:

AXIS		GRID	
r min	`-0.04`	r spacing	`0.02`
r max	`0.1`	Extra r	
z min	`-0.02`	z spacing	`0.02`
z max	`0.2`	Extra z	`0.035 0.145`

3 Click **OK**.

4 From the **Options** menu, select **Constants**.

5 Enter the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
R_a	40[mm]	Wafer radius
d_cc	2.5[mm]	Wafer spacing
d_w	0.5[mm]	Wafer thickness
S_a	2*(R_a^2+R_a*d_w)/ (R_a^2*d_cc)	Specific surface area
p_tot	25[Pa]	Total system pressure
D_amb	5e-5[m^2/s]	SiH4 diffusivity in air at 1 atm
D	D_amb*1.013e5[Pa]/p_tot	Pressure-corrected diffusivity
D_eff	D*(1-d_w/d_cc)	Effective diffusivity in wafer bundle
k	8.06[mm/s]	Rate constant
M_N2	28[g/mol]	Molar mass, N2
M_Si	28[g/mol]	Molar mass, Si
M_SiH4	32[g/mol]	Molar mass, SiH4
R_g	8.314[J/(mol*K)]	Ideal gas constant
T_r	600[degC]	Reactor temperature
rho	p_tot*(0.2*M_SiH4+0.8*M_N2)/ (R_g*T_r)	Gas density
eta	3.1e-5[Pa*s]	Dynamic viscosity
c0	0.2*p_tot/(R_g*T_r)	Inlet concentration, SiH4
v0	1[m/s]	Inlet axial flow velocity
rho_Si	2e3[kg/m^3]	Silicon density
Re	R_a*v0*rho/eta	Reynolds number

Note the value of the Reynolds number in the **Value** column. The small Reynolds number validates the assumption of laminar flow inside the reactor.

6 Choose **Options>Expressions>Scalar Expressions**.

7 Define a constant by the data in the following table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
Delta_Si	c*k*M_Si/rho_Si	Silicon deposition rate

GEOMETRY MODELING

1 Click the **Line** button on the Draw toolbar and draw a line by clicking at the positions (0, 0), (0.06, 0), and (0.06, 0.14) with the left mouse button.
2 Select the **2nd Degree Bézier Curve** button and draw an arc by clicking at the positions (0.06, 0.18) and (0.02, 0.18).
3 Switch back to the **Line** tool and click at the positions (0, 0.18).
4 Click the right mouse button anywhere to create a solid object, CO1.
5 Draw a rectangle, R1, with the lower left corner at (0, 0.035) and upper-right corner at (0.04, 0.04).
6 Draw second rectangle, R2, with the lower left corner at (0,0.04) and upper-right corner at (0.04, 0.14).
7 Draw a third rectangle, R3, with the lower-left corner at (0, 0.14) and upper-right corner at (0.04, 0.145).
8 Click the **Point** button and click at the position (0.02, 0).
9 Click the **Create Composite Object** button in the toolbar and type `CO1+R2-R1-R3` in the **Set formula** edit field.
10 Click **OK** to finalize the geometry.

PHYSICS SETTINGS

Subdomain Settings—Incompressible Navier-Stokes

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.
2 From the **Physics** menu, select **Subdomain Settings**.
3 In the **Subdomain selection** list, select Subdomain 2.
4 Deactivate the Navier-Stokes application mode in Subdomain 2 by clearing the **Active in this domain** check box.
5 Select Subdomain 1. In the ρ edit field type `rho` and in the η edit field type `eta`.
6 Click **OK**.

Boundary Conditions—Incompressible Navier-Stokes

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARIES 1, 7	BOUNDARY 2	BOUNDARY 9	BOUNDARY 12
Boundary type	Symmetry boundary	Inlet	Outlet	Wall
Boundary condition	Axial symmetry	Velocity	Pressure, no viscous stress	No slip
u		0		
v		v0		
p			0	

For the remaining active boundaries (3, 8, 10–15) the default boundary type (wall) and condition (no slip) applies.

3 Click **OK**.

Subdomain Settings—Mass Transport

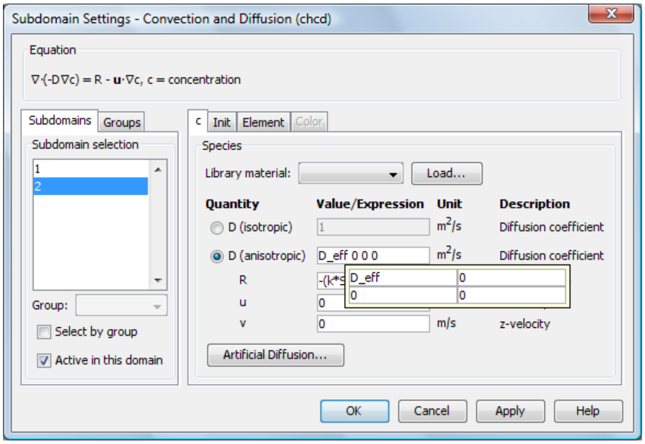
1 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Enter subdomain settings according to the following table:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
D (isotropic)	D	
D (anisotropic)		`[D_eff 0;0 0]`
R	0	`-(k*S_a)*c`
u	u	0
v	v	0

The figure below shows how to enter the anisotropic diffusion coefficients.



Subdomain Settings - Convection and Diffusion (chcd)

Equation

$\nabla\cdot(-D\nabla c) = R - \mathbf{u}\cdot\nabla c$, c = concentration

Subdomain selection: 1, 2 (2 selected)

Group:

☐ Select by group

☑ Active in this domain

Species

Library material:

Quantity	Value/Expression	Unit	Description
○ D (isotropic)	1	m^2/s	Diffusion coefficient
● D (anisotropic)	D_eff 0 0 0	m^2/s	Diffusion coefficient
R	-(k*S		
u	0		
v	0	m/s	z-velocity

D_eff	0
0	0

4 Click **OK**.

Boundary Conditions—Mass Transport

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARIES 1, 4, 7	BOUNDARY 2	BOUNDARY 9
Type	Axial symmetry	Concentration	Convective flux
c		`c0`	

For the remaining boundaries, the default conditions apply.

3 Click **OK**.

MESH GENERATION

This model requires a fairly dense mesh. Therefore, define the maximum mesh edge size for some of the geometry edges.

1. From the **Mesh** menu, select **Free Mesh Parameters**.
2. Go to the **Boundary** page and select Boundaries 2, 9, and 14 from the **Boundary selection** list.
3. In the **Maximum element size** edit field, type `3e-3`.
4. Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1. From the **Solve** menu, select **Solver Parameters**.
2. From the **Solver** list select **Parametric**.
3. In the **Parameter name** edit field, type `v0`.
4. In the **Parameter values** edit field, type `1 1.5 2`.
5. Click **OK**.
6. Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

Generate the plot in Figure 8-14 with the following steps.

1. Click the **Plot Parameters** button on the Main toolbar.
2. In the **Solution to use** area, select **1** from the **Parameter value** list.
3. Click the **Surface** tab. On the **Surface Data** page, type `c` in the **Expression** edit field (alternatively, select **Convection and Diffusion (chcd)>Concentration, c** from the **Predefined quantities** list).
4. Click **Apply**.

   To generate the plot in Figure 8-15, proceed as follows:

5. Return to the **Plot Parameters** dialog box. From the **Predefined quantities** list select **Incompressible Navier-Stokes (chns)>Velocity field**.
6. Click the **Arrow** tab. Select the **Arrow plot** check box.
7. Leave the default selection, **Incompressible Navier-Stokes (chns)>Velocity field (chns)**, in the **Predefined quantities** list. This choice sets the arrows' r-components to `u` and their z-components to `v`.
8. In the **Arrow positioning** area, set the number of **z points** to `25`.
9. In the **Arrow Parameters** area, clear the **Auto** check box and set the **Scale factor** to `2`.

10 Click **OK**.

To create the plots in Figure 8-16, execute the following instructions.

11 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

12 On the **Grid** page, select the **Auto** check box.

13 Click **OK**.

14 From the **Postprocessing** menu, select **Domain Plot Parameters**.

15 On the **General** page, click the **Surface plot** option button.

16 From the **Solutions to use** list, select the parameter value **1** only.

17 Click the **Title/Axis** button. Click the option button next to the **Title** edit field and enter the title `Si deposition rate [nm/min]`. Click **OK** to close the **Title/Axis Settings** dialog box.

18 Back in the **Domain Plot Parameters** dialog box, click the **Surface** tab.

19 From the **Subdomain selection** list, select Subdomain 2.

20 In the **Expression** edit field, enter the deposition rate `Delta_Si`.

21 In the **Unit** edit field, type `nm/min` to get a more suitable unit for the plot.

22 Click **Apply** to generate the upper plot in Figure 8-16.

23 On the **General** page, select the parameter value **2** from the **Solutions to use** list.

24 Click **OK** to generate the lower plot and close the dialog box.

Monolithic Reactor

Introduction

The importance of monolithic reactors[2] has grown rapidly over the last two decades. The most well-known example of a monolithic reactor is the three-way catalytic converter for automobiles. This reactor simultaneously transforms unburned hydrocarbons, carbon monoxide, and nitrogen oxides from the exhaust gases into carbon dioxide, nitrogen, and water.

Catalytic purification of emissions from other sources has also been developed and commercialized in the last decade. An important area of applications is the abatement of volatile organic compounds (VOC) from processes such as spray painting, offset printing, and coating operations. Selective catalytic reduction (SCR) of nitrogen oxides by ammonia is another field where monolithic reactors are used. This technique has been widely applied to purify effluent gases from coal burning boilers and electric power plants.

Yet another challenging application for monolithic reactors is the current development of high-temperature catalytic combustion for heat and power generation. This technology has proven to be a promising alternative to ordinary flame combustion for converting chemical energy into heat or mechanical power with a minimum level of emissions from combustion by-products.

A monolithic reactor consists of thin parallel straight channels of arbitrary shape through which the gas containing the reactants flows. The walls of the channels are coated with a porous ceramic containing the catalyst layer. The transition from reactants to products involves transport of the reactants by convective flow in the channels and molecular diffusion toward the channel walls. Simultaneous diffusion and reactions occur inside the porous washcoat, whereby the products diffuse back into the gas and are transported out from the reactor.

There is obviously a large number of variables in optimizing the reactor performance. Examples of parameters that are important for the general behavior of the reactor are temperature, channel geometry, flow rate, properties of the washcoat, and catalytic activity.

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[2] This model was provided by Dennis Papadias, The Royal Institute of Technology, Stockholm.

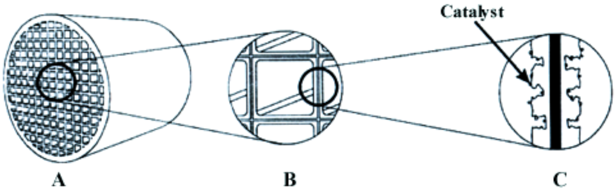


Figure 8-17: A: Monolithic reactor; B: Channel wall; C: Porous ceramic washcoat with catalyst. Figure from Ref. 1.

Model Definition

The following model simulates the catalytic abatement of a volatile organic compound (VOC), in this case a contaminant in a waste gas. For simple geometries the reactor can be described by a 2D model using time as the z-axis. Full 3D modeling is necessary if the channels have irregular shape or if the level of active coating is non-uniform along the monolith channels.

MODEL ASSUMPTIONS

In this model you consider oxidation for one type of VOC. Because the concentrations of contaminants from the waste gases are usually very low, the heat release from the oxidation is negligible. The flow in the monolith channel is laminar. Furthermore, you can neglect the axial diffusion of the reactants because it is small compared to the convective flow.

Assume identical conditions within each channel, so the model of the whole monolith is reduced to one channel. The transversal cross section of the channel is described by a circle surrounded by a square. The area between the circle and the square represents the washcoat of the reactor. Because of symmetry effects, the simulation only includes one eighth of the channel.

BOUNDARY CONDITIONS

The boundary conditions at the channel inlet, $z = 0$, are uniform concentration and a fully developed velocity profile. You can use the Hagen-Poiseuille law to derive the velocity analytically. For a circular tube this gives the parabolic profile

$$V_z = 2U_{\mathrm{m}}(1-x^2-y^2) \tag{8-30}$$

In this equation, V_z describes the velocity profile (m/s) and U_m is the average velocity given in dimensionless coordinates x and y that both run between 0 and 1. For all exterior boundaries, use Neumann boundary conditions for symmetry.

GAS PHASE EQUATION

The equation describing the process for the gas in the monolith channel domain, Ω_1, is

$$U(x, y)\frac{\partial c}{\partial z'} = \frac{\partial}{\partial x'}\left(D\frac{\partial c}{\partial x'}\right) + \frac{\partial}{\partial y'}\left(D\frac{\partial c}{\partial y'}\right) \qquad \Omega_1 \tag{8-31}$$

where $U(x, y)$ is the velocity profile in the monolith channel, D denotes the diffusion coefficient in the free gas (m^2/s), and c refers to the concentration (mol/m^3). This mass transport neglects the contribution of diffusion to the total flux in the axial direction, leading to parabolic equations that are easier to solve.

POROUS CATALYST EQUATIONS

The equations

$$\begin{cases} \frac{\partial}{\partial x'}\left(D_{\text{eff}}\frac{\partial c}{\partial x'}\right) + \frac{\partial}{\partial y'}\left(D_{\text{eff}}\frac{\partial c}{\partial y'}\right) + R = 0 & \Omega_2 \\ R = -ke^{\left(-\frac{E}{R_g T}\right)}c & \Omega_2 \end{cases} \tag{8-32}$$

describe the simultaneous reaction and diffusion in the porous network of the washcoat domain, Ω_2. Treat the washcoat as a homogeneous medium in which the effective diffusion coefficient, D_{eff}, reflects the pore properties. Neglect diffusion in the axial direction also in the porous catalyst. This is justified because concentration differences at the surface of the wash coat are whipped out by convection. Because the concentration of the contaminant species is very low, you can assume the reaction term to be of first order (linear) with respect to the concentration, c. This is expressed in the rate equation where R denotes the reaction rate, k the pre-exponential factor, E the activation energy, T the temperature, and R_g the gas constant. The temperature dependence of the reaction rate is accounted for through the Arrhenius law.

SCALING

Choose the following scaling variables: $V(x, y) = U(x, y)/U_m$, $x = x'/R_c$, $y = y'/R_c$, $z = z'/L$, and $C = c/C_0$, where U_m is the mean inlet velocity, L the reactor length, R_c the radius (or maximum length) of the monolith channel, and C_0 the inlet concentration. Rearranging Equations 8-31 and 8-32 accordingly gives:

$$\begin{cases} V(x,y)K_1\dfrac{\partial C}{\partial z} = \dfrac{\partial}{\partial x}\left(D\dfrac{\partial C}{\partial x}\right) + \dfrac{\partial}{\partial y}\left(D\dfrac{\partial C}{\partial y}\right) & \Omega_1 \\ \dfrac{\partial}{\partial x}\left(D_{\mathrm{eff}}\dfrac{\partial C}{\partial x}\right) + \dfrac{\partial}{\partial y}\left(D_{\mathrm{eff}}\dfrac{\partial C}{\partial y}\right) - K_2C = 0 & \Omega_2 \\ K_1 = \dfrac{U_{\mathrm{m}}R_{\mathrm{c}}{}^2}{L} & \Omega_1 \\ K_2 = ke^{\left(-\frac{E}{R_gT}\right)}R_{\mathrm{c}}{}^2 & \Omega_2 \end{cases} \tag{8-33}$$

In this case, use the following parameter values: $K_1 = 0.39\ \mathrm{cm}^2/\mathrm{s}$, $K_2 = 11.2\ \mathrm{cm}^2/\mathrm{s}$, $D = 0.88\ \mathrm{cm}^2/\mathrm{s}$, and $D_{\mathrm{eff}} = 0.02\ \mathrm{cm}^2/\mathrm{s}$.

Because of the absence of a second derivative in the z direction, it is possible to integrate the system using a time-dependent model with time representing the z-axis. This assumption is an inherent property of the Pseudo modes in the Chemical Engineering Module.

Note that in case of other geometric configurations for the monolith channel, you must compute the velocity profile separately and use the solution in the equation for $V(x,y)$.

Results

Figure 8-18 shows the outlet concentration at time 1, that is, at the outflow of the reactor. Observe that the concentration in the solid phase drops rapidly toward zero close to the monolith wall. This is because the reaction in this model is quite rapid and the reacting gas is mostly consumed near the outer surface. It would therefore be preferable to coat the channels with a smaller amount of washcoat.

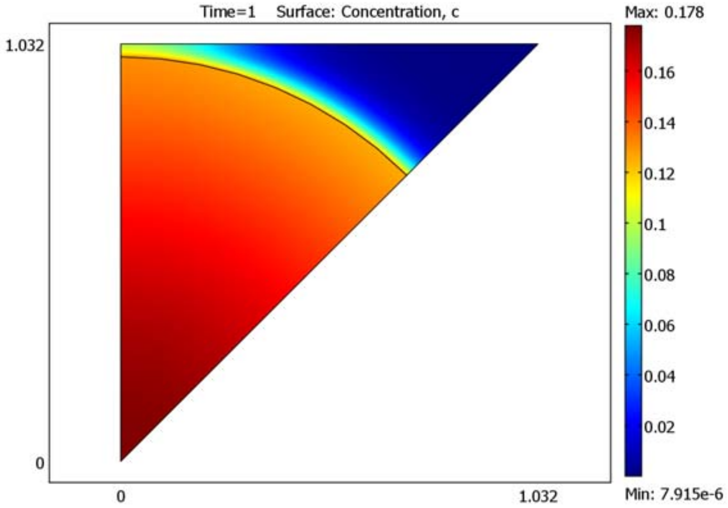


Figure 8-18: Concentration distribution at outlet

Figure 8-19 shows a slice plot along the length of the monolithic reactor and gives an overview of the VOC concentration within the reactor and the catalyst.

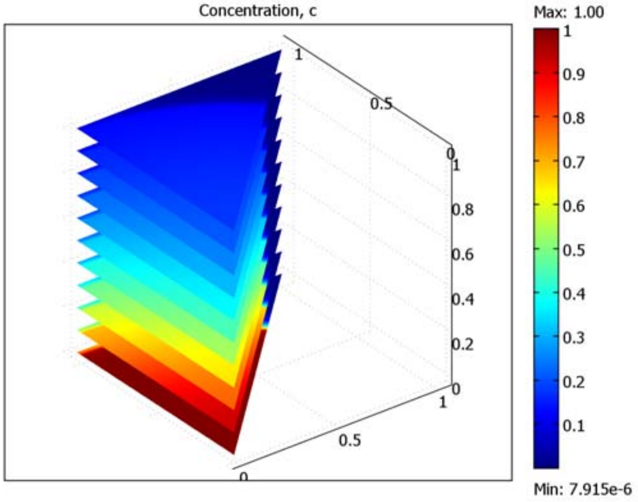


Figure 8-19: Concentration distribution along the length of the reactor.

It is important to investigate the amount of the contaminant gas flowing out from the reactor. The relevant measurable quantity is the bulk (mean) contaminant concentration, which is given by

$$\langle c\rangle = \frac{\int_s Vc\,ds}{\int_s V\,ds}. \qquad (8\text{-}34)$$

Evaluating the integrals over the outlet, the average concentration as a fraction of the inlet concentration turns out to be 0.157. To improve the catalytic purification of the reactor, several parameters can be altered, for example, the length of the reactor, the temperature, or the shape of the channels.

Reference

1. Berg, M., *Catalytic Combustion over High Temperature Stable Metal Oxides*, 1996, Licentiate of engineering thesis, KTH, TRITA-KET R50.

Model Library path: `Chemical_Engineering_Module/Transport_and_Reactions/monolithic_reactor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator,** select **2D** from the **Space dimension** list.
3. From the **Application Modes** list, select **Chemical Engineering Module>Pseudo 3D>Mass Transport>Convection and Diffusion**.
4. Click **OK**.

OPTIONS AND SETTINGS

Axes/Grid Settings

1. From the **Options** menu, select **Axes/Grid Settings**.

2 Specify axis and grid settings according to the following table; when done, click **OK**.

AXIS	X-Y LIMITS	GRID	
x min	`-1.5`	x spacing	`1`
x max	`1.5`	Extra x	`1.032`
y min	`-1.1`	y spacing	`1`
y max	`1.1`	Extra y	`1.032`

Model Settings

Because the model uses dimensionless scaled variables, change the base unit system from the default SI to none:

1. From the **Physics** menu, select **Model Settings**.
2. From the **Base unit system** list, select **None**.
3. Click **OK**.

Constants

1. From the **Options** menu, select **Constants**.
2. Enter the following names, expressions, and descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`D`	`0.88`	`Diffusion coefficient, free gas`
`D_eff`	`0.02`	`Effective diffusion coefficient, catalyst`
`K1`	`0.39`	`Flow-velocity parameter`
`K2`	`11.2`	`Reaction-rate parameter`

GEOMETRY MODELING

1. Click the **Ellipse/Circle (Centered)** button on the Draw toolbar.
2. Right-click on the origin (0, 0), hold down the right mouse-button, and drag the mouse sideways until the circumference snaps to $x = 1$. Release the button.
3. Click the **Line** button. Click the points (0, 0), (1.032, 1.032), and (0, 1.032). Finally, right-click to close the triangle to a solid object.
4. Press Ctrl+A to select all objects.
5. Click the **Create Composite Object** button on the Draw toolbar. In the **Set formula** edit field, type `CO1+CO1*E1`. Click **OK** to form the composite object CO2.
6. Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Specify settings according to the following table:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
D (isotropic)	`D`	`D_eff`
R	`0`	`-K2*c`
u_{dl}	`K1*2*(1-x^2-y^2)`	`0`

3 On the **Init** page, set the initial concentration **c(t$_0$)** to `1` for both subdomains.

4 Click **OK**.

Boundary Conditions

The default boundary conditions (**Insulation/Symmetry**) apply.

MESH GENERATION

You need a finer mesh in Subdomain 2 where the reaction takes place.

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 On the **Subdomain** page, set the **Maximum element size** to `0.1` and `0.015` for Subdomains 1 and 2, respectively.

3 Click **Remesh**.

4 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 Verify that the **Times** edit field entry is `0:0.1:1`.

3 Click **OK** to close the **Solver Parameters** dialog box.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

1 The default plot, Figure 8-18, shows the outlet concentration at time 1, that is, at the reactor outlet.

2. To see the concentration along the whole channel (from $z = 0$ to $z = 1$), click the **Animate** button. You can save the movie by clicking the **Save** button in the movie dialog box.

   To produce a slice plot of the full 3D geometry as depicted in Figure 8-19, use the cross-section plot capabilities of COMSOL Multiphysics:

3. From the **Postprocessing** menu, select **Domain Plot Parameters**.
4. On the **General** page, select all solutions in the **Solutions to use** list.
5. Click the **Surface** tab and select both subdomains in the list.
6. Click **OK**.
7. Experiment with the **Increase Transparency** buttons in the figure window.

   To analyze Equation 8-34, perform the integration from the user interface according to the following procedure:

8. From the **Postprocessing** menu, select **Subdomain Integration**.
9. Select Subdomain 1 and type `c*(1-x^2-y^2)` in the **Expression** edit field.
10. Click **Apply**. The result 0.030976 appears in the message log at the bottom of the user interface.
11. Type `(1-x^2-y^2)` in the **Expression** edit field, then click **OK**. The result is 0.19635.

    The average concentration thus turns out to be 0.157.

Selective Catalytic Reduction of NOx

Introduction

The removal of pollutants from high-temperature gases is often required in combustion processes. In this example, the selective reduction of NOx by ammonia occurs as flue gas passes through a honeycomb reactor. The chemical reactions take place on the surface of a V_2O_5/TiO_2 catalyst that is supported on a ceramic structure.

This example shows how to use the COMSOL Reaction Engineering Lab in concert with the Chemical Engineering Module to readily solve advanced engineering problems. You can start by setting up the reaction kinetics in the Reaction Engineering Lab and then model the chemistry assuming that each of the channels in the monolith behaves as a plug-flow reactor. This gives you a notion about the magnitude of important design parameters such as the residence time and selectivity as a function of temperature. In a second part of the example, you set up a reactor model taking the actual geometry of a monolith channel into account by exporting the reaction model from Reaction Engineering Lab to the Chemical Engineering Module. In the space-dependent model you can solve the mass-balance equations coupled to the momentum balances for free flow and porous media flow.

Note: Solving the first part of this model requires the COMSOL Reaction Engineering Lab.

Model Definition

NO reduction by ammonia can be summarized by the following reaction:

$$4\mathrm{NO} + 4\mathrm{NH}_3 + \mathrm{O}_2 \longrightarrow 4\mathrm{N}_2 + 6\mathrm{H}_2\mathrm{O} \tag{8-35}$$

However, ammonia can at the same time undergo oxidation:

$$4\mathrm{NO} + 4\mathrm{NH}_3 + \mathrm{O}_2 \longrightarrow 4\mathrm{N}_2 + 6\mathrm{H}_2\mathrm{O} \tag{8-36}$$

When optimizing the conversion of NO, you consequently seek to minimize the oxidation reaction while maintaining a reasonable reaction rate for the reduction.

The heterogeneous catalytic conversion of NO to N_2 is described by an Eley-Rideal mechanism. A key reaction step involves the reaction of gas-phase NO with surface-adsorbed NH_3. The following rate equation (mol/(m^3·s)) has been suggested in Ref. 1 for Equation 8-35:

$$r_1 = k_1 c_{\mathrm{NO}} \frac{a c_{\mathrm{NH3}}}{1 + a c_{\mathrm{NH3}}} \tag{8-37}$$

where

$$k_1 = A_1 \exp\left(-\frac{E_1}{R_{\mathrm{g}} T}\right) \tag{8-38}$$

and

$$a = A_0 \exp\left(-\frac{E_0}{R_{\mathrm{g}} T}\right) \tag{8-39}$$

For Equation 8-36, the reaction rate (mol/(m^3·s)) is given by

$$r_2 = k_2 c_{\mathrm{NH3}} \tag{8-40}$$

where

$$k_2 = A_2 \exp\left(-\frac{E_2}{R_{\mathrm{g}} T}\right) \tag{8-41}$$

This example investigates the conversion of NOx through two reactor models. You first set up and solve a plug-flow reactor in the COMSOL Reaction Engineering Lab, and then you solve a space-dependent reactor model using COMSOL Multiphysics.

Assuming steady, the design equation for a plug-flow reactor is given by:

$$\frac{dF_i}{dV} = R_i \tag{8-42}$$

where F_i is the species molar flow rate (mol/s), V represents the reactor volume (m^3), and is R_i the species net reaction rate (mol/(m^3·s)). The molar flow rate is related to the species concentrations, c_i (mol/m^3), through the volumetric flow rate, v (m^3/s):

$$F_i = v c_i \tag{8-43}$$

where the volumetric flow rate is given by the average flow velocity, u (m/s), multiplied by the reactor cross-section A (m^2):

$$v = uA \tag{8-44}$$

The mass balances given by Equation 8-42 are set up and solved in the Reaction Engineering Lab.

The plug-flow model considerably simplifies the reaction conditions compared to actual reactors used in industry. In the extended example, the conversion of NOx occurs in a honeycomb reactor, which consists of packets of thin parallel channels through which the flue gas flows. The ceramic channel walls are coated with a porous catalytic layer, in this case V_2O_5/TiO_2.

The transport and reaction of chemical species can be divided into several steps: First the reactants are transported in the direction of the flow, mainly by convection in the open channels. The reactants diffuse towards the walls and into the porous catalyst where they react on the catalyst surface. Formed products subsequently diffuse out of the porous structure and are transported out of the reactor through the open channels.

The model setup in COMSOL Multiphysics corresponds to a single channel of the honeycomb structure. The model assumes the channel is cylindrical, making it possible to reduce the modeling domain to a 2D geometry with rotational symmetry. The model geometry appears in Figure 8-20.

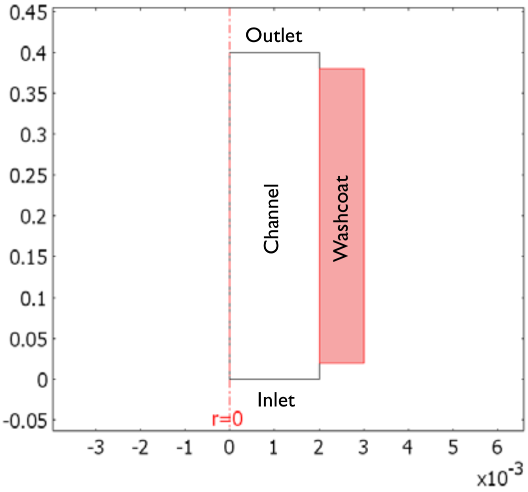


Figure 8-20: Geometry of a reactor-channel model taking axial symmetry into account. Dimensions are in meters (m).

MOMENTUM TRANSPORT

The flow in the free channel is described by the Navier-Stokes equations:

$$\begin{aligned} \nabla\cdot[-\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+p\mathbf{I}] &= -\rho(\mathbf{u}\cdot\nabla)\mathbf{u} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned} \tag{8-45}$$

where ρ denotes density (kg/m^3), $\mathbf{u}$ represents the velocity (m/s), η denotes viscosity (kg/(m· s)), and p equals pressure (Pa). In the porous domain, the Brinkman equations describe the flow:

$$\begin{aligned} \nabla\cdot\left[-\frac{\eta}{\varepsilon_{\mathrm{p}}}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+p\mathbf{I}\right] &= -\frac{\eta}{k}\mathbf{u} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned} \tag{8-46}$$

Here ε_{p} denotes the porosity (dimensionless) and k refers to the permeability (m^2) of the porous medium. As you can see in Equation 8-45 and Equation 8-46, the momentum-balance equations are closely related. The term on the right-hand side of the Navier-Stokes formulation corresponds to momentum transported by convection in free flow. In the Brinkman formulation, this term is replaced by a contribution associated with the drag force experienced by the fluid as it flows through a porous medium. COMSOL Multiphysics effortlessly combines free flow and porous-media flow.

The boundary conditions are

$$\begin{aligned} \mathbf{u}\cdot\mathbf{n} &= v_0 && \text{inlet} \\ \mathbf{u} &= \mathbf{0} && \text{walls} \\ p &= p_{\mathrm{ref}} && \text{outlet} \end{aligned} \tag{8-47}$$

At the outlet viscous stresses are ignored and the pressure is set to 1 atmosphere.

MASS TRANSPORT

The mass-balance equations for the model are the diffusion-convection equations at steady state:

$$-\nabla\cdot(-D_i\nabla c_i+c_i\mathbf{u}) = R_i \tag{8-48}$$

Here D_i denotes the diffusion coefficient (m^2/s), c_i is the species concentration, and $\mathbf{u}$ equals the velocity vector (m/s). The term R_i corresponds to the species' net reaction rate, which is a function of the reaction rates, Equation 8-37 and Equation 8-40, and the reaction stoichiometry.

In the free channel, the inlet conditions are equal to the inlet concentrations:

$$c = c_{\text{in}} \tag{8-49}$$

At the outlet, use the convective flux condition

$$\mathbf{n} \cdot (-D\nabla c) = 0 \tag{8-50}$$

All other boundaries use the insulating or symmetry condition

$$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = 0 \tag{8-51}$$

TRANSPORT PROPERTIES

Setting up momentum and mass balances requires that certain physical properties characteristic of the reacting fluid are determined. For instance, the Navier-Stokes equation (Equation 8-45) and the Brinkman equation (Equation 8-46) both require the fluid viscosity. Furthermore, the mass balances need species specific diffusion coefficients as input.

For reacting gas mixtures, the Reaction Engineering Lab makes use of kinetic gas theory to set up expressions for transport properties such as binary diffusivities, viscosity, and thermal conductivity as functions of temperature, pressure, and composition. In this example, the diffusivities (m^2/s) are calculated using the formula:

$$D = 2.695 \cdot 10^{-3} \cdot \frac{\sqrt{T^3((M_A + M_B)/(2 \cdot 10^3 M_A M_B))}}{p\sigma_A\sigma_B\Omega_D} \tag{8-52}$$

where Ω_D is a collision integral

$$\Omega_D = \mathrm{f}\left(T, \sigma, \frac{\varepsilon}{\mathrm{k}}, \mu\right). \tag{8-53}$$

Furthermore gas viscosity (Ns/m^2) is given by the expression:

$$\eta = 2.699 \cdot 10^{-6} \cdot \frac{\sqrt{T(1 \cdot 10^3 M)}}{\sigma^2\Omega_v} \tag{8-54}$$

where Ω_v is a collision integral

$$\Omega_v = \mathrm{f}\left(T, \sigma, \frac{\varepsilon}{\mathrm{k}}, \mu\right). \tag{8-55}$$

To evaluate Equation 8-52 and Equation 8-54, you need to specify the characteristic length and energy minimum of the Lennard-Jones interaction potential, that is σ (10^{-10} m) and the ε/k (K), respectively. The species dipole moment, μ (Debye), can also be provided. Each species in the reacting gas has a characteristic set of these constants, and you find their values in the literature, in databases, or from experiments. The parameters σ, ε/k, and μ can either be entered manually in the Reaction Engineering Lab GUI, or you can import text files containing the data. In this model you import transport data using the **Import CHEMKIN File** feature.

The structure of a CHEMKIN transport data file is illustrated below:

```
NO     0    97.500    3.620    0.000    0.000    0.000
NH3    0    558.300   2.900    1.470    0.000    0.000
O2     0    106.700   3.470    0.000    0.000    0.000
N2     0    71.400    3.800    0.000    0.000    0.000
H2O    0    809.100   2.640    1.880    0.000    0.000
```

The first column indicates the species name; the second column contains an index describing the geometrical configuration of the molecule; the third column provides the value for ε/k; the fourth column lists the value for σ; the fifth column gives the value of μ; the sixth column indicates polarizability; and the seventh column lists rotational relaxation collision number.

The entries given in columns 1, 3, 4, and 5 are read into the Reaction Engineering Lab when selecting the menu item **File>Import>CHEMKIN Transport Input File**.

Resources for kinetic, thermodynamic, and transport data on the CHEMKIN format are available on the web (see, for instance, www.comsol.com/reaction).

Results

First review the results of the plug-flow model, which you set up and solve in the Reaction Engineering Lab.

Figure 8-21 shows the concentrations of NO and NH_3 as functions of the reactor volume. Reactions take place at 523 K and that the gas enters the reactor with a velocity of 0.3 m/s. The reactor is assumed to be a channel with a length of 0.36 m and a radius of 2 mm. Under these conditions, the simulations show that most of the NO has been converted as the gas leaves the reactor (NO converted > 99%).

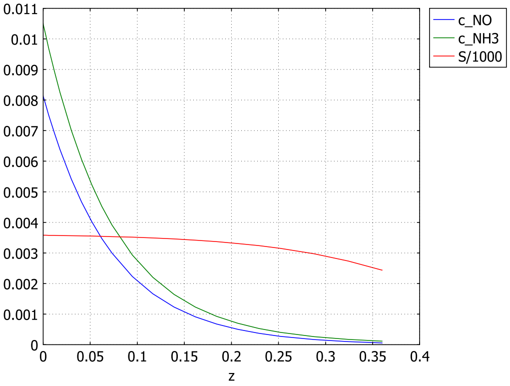


Figure 8-21: Concentrations of NO and NH_3 as functions of axial distance from the reactor inlet. S is the selectivity parameter.

The plot also shows the selectivity parameter, S, giving the ratio of reaction rates according to

$$S = \frac{r_1}{r_2} \tag{8-56}$$

S varies between 3.6 and 2.7 along the reactor length, indicating that the reduction of NO is the dominating reaction pathway.

Figure 8-22 shows the initial reaction rate of NO reduction (r_1) and NH_3 oxidation (r_2) in the temperature interval 450–750 K. Up to approximately 655 K, NH_3 is mainly consumed by the desired reduction reaction, Equation 8-35. At about 670 K the rate of NO reduction reaches a maximum. Above this temperature the desorption of NH_3 from the catalyst surface becomes faster than the reaction of adsorbed NH_3 with gas-phase NO.

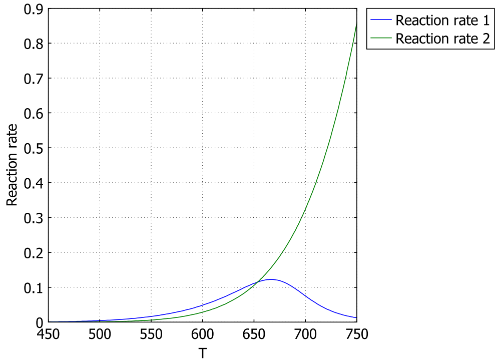


Figure 8-22: Initial rates of NO reduction (Reaction rate 1) and NH_3 oxidation (Reaction rate 2) as functions of temperature for the plug-flow reactor model.

The following results come from the space-dependent reactor model, which you set up and solve in COMSOL Multiphysics. In this case, the chemistry takes place in a channel of a honeycomb reactor.

Figure 8-23 shows the fluid velocity profile, given as a function of radial position at the channel midpoint.

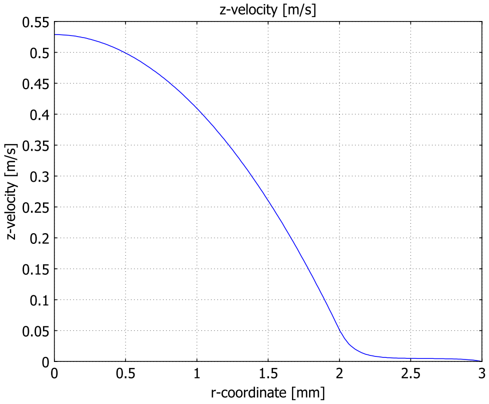


Figure 8-23: Flow velocity as a function of radial position.

Figure 8-24 displays the concentration of NO across the reactor channel. Integrating the boundary flux of NO across the inlet and outlet allows you to calculate the conversion of NO as being 89%.

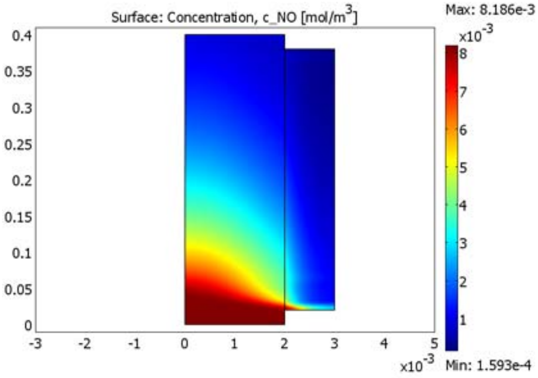


Figure 8-24: Concentration of NO across the space-dependent model domain.

It is easy to extend the model to study the effects of different design parameters such as reaction temperature, inlet velocity, and geometry. It can also easily take into account the effect of material properties such as the permeability of the porous region.

Figure 8-25 compares the results of the plug-flow model and the reactor model including the actual channel geometry. For the channel model, the NO concentration shown is the average concentration evaluated along the section of channel length affected by the catalytic washcoat (0.36 m). The average inlet velocity in the channel model is 0.3 m/s.

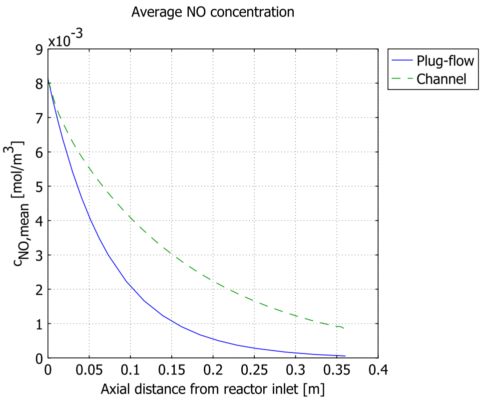


Figure 8-25: Concentration of NO (mol/m^3*) along the reactor channel. The solid line represents data from the plug-flow model and the dashed line represents the mean concentration evaluated from the channel model.*

The assumptions underlying the plug-flow model readily explain the differences in results. In the plug-flow model, reactions are assumed to occur homogeneously throughout the reactor volume. Because the species need not be transported to and from the bulk flow to the reactive washcoat, as is the case in the channel model, the conversion of reactants is, of course, faster.

In summary: This example illustrates the modeling of a heterogeneous catalytic process using the COMSOL Reaction Engineering Lab and the Chemical Engineering Module. The Reaction Engineering Lab helps you set up the chemical kinetics and expressions describing the transport properties of the reacting mixture. In COMSOL Multiphysics you study the reacting flow in a specific reactor geometry.

Reference

1. G. Shaub, D. Unruh, J. Wang, and T. Turek, *Chemical Engineering and Processing*, vol. 42, p. 365, 2003.

The following path gives the location of the Reaction Engineering Lab model:

Model Library path: `Combustion/nox_reduction`

The following path shows the location of the COMSOL Multiphysics model:

Model Library path:

`Chemical_Engineering_Module/Transport_and_Reactions/nox_reduction`

Modeling Using the COMSOL Reaction Engineering Lab

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, go to the **Space dimension** list and select **Axial symmetry (2D)**.
3. Click **OK**.

   The main user interface of COMSOL Multiphysics opens up.
4. From the **File** menu, select **Reaction Engineering Lab**.

   The main user interface of COMSOL Reaction Engineering Lab opens up.
5. Click the **COMSOL Reaction Engineering Lab** window.

OPTIONS AND SETTINGS

1. Click the **Model Settings** button on the Main toolbar.
2. From the **Reactor type** list, select **Plug-flow**.
3. Select the **Calculate thermodynamic properties** check box.
4. Select the **Calculate species transport properties** check box.
5. On the **General** page, type `523` in the **Temperature** edit field.
6. On the **Mass Balance** page, type `v_av*A` in the **Volumetric flow rate** edit field.
7. Click **Close**.

REACTIONS INTERFACE

1. Click the **Reaction Settings** button on the Main toolbar.
2. Make sure the **Reactions** page is active. Create two entries in the **Reaction selection** list by clicking the **New** button twice.

3 Enter the following reaction formulas by first selecting the appropriate row in the **Reaction selection** list and then entering the corresponding text in the **Formula** edit field:

REACTION ID #	REACTION FORMULA
1	`4NO+4NH3+O2=>4N2+6H2O`
2	`4NH3+3O2=>2N2+6H2O`

4 Select the first row in the **Reaction selection** list.

5 Select the **Use Arrhenius expressions** check box.

6 Type `1e6` in the **A** edit field and `60e3` in the **E** edit field.

7 Modify the predefined reaction rate according to Equation 8-37 on page 471 by typing `kf_1*c_NO*a*c_NH3/(1+a*c_NH3)` in the **r** edit field.

You define the expression for `a` later on.

8 Select the second row in the **Reaction selection** list.

9 Select the **Use Arrhenius expressions** check box.

10 Type `6.8e7` in the **A** edit field and `85e3` in the **E** edit field.

11 Modify the predefined reaction rate according to Equation 8-40 on page 471 by typing `kf_2*c_NH3` in the **r** edit field.

SPECIES INTERFACE

1 Click the **Species** tab.

2 Check that the **Species selection** list has the five entries expected from entering the reaction formulas just given.

3 Click the **General** tab. Select the appropriate entry in the **Species selection** list and then enter the corresponding value for the **Molecular weight**:

SPECIES NAME	M [kg/mol]
NO	`30e-3`
NH3	`17e-3`
O2	`32e-3`
N2	`28e-3`
H2O	`18e-3`

4 Select **N2** from the **Species selection** list and choose **Solvent** from the **Type** list.

This selection is appropriate when a species is the main component of a reaction mixture. Setting a species as a **Solvent** removes its mass balance (the concentration is assumed to be constant). Furthermore, the thermodynamic and transport properties of the reacting mixture are based on the properties of the solvent species.

5 Click the **Feed Stream** tab. Select the appropriate entry in the **Species selection** list and then enter the corresponding value for the **Inlet molar flow**:

SPECIES NAME	F_0 [mol/s]
NO	`3.07e-8`
NH3	`3.96e-8`
O2	`6.67e-6`
N2	`7.23e-5`
H2O	`8.78e-6`

6 Select **File>Import>CHEMKIN Transport Input File** and browse to the file `nox_reduction_transport.txt` then click **Import**.

This imports the Lennard-Jones parameters required to set up expressions for the fluid viscosity and species diffusivities.

7 Click the **Transport** page and verify that the σ, ε/k_B, and μ edit fields have been updated with the appropriate parameter values.

As an alternative to reading in the values from file, you can type in the appropriate values in the σ, ε/k_B, and μ edit fields:

SPECIES NAME	σ [m]	ε/k_B [K]	μ [D]
NO	`3.62`	`97.5`	`0`
NH3	`2.90`	`558.3`	`1.47`
O2	`3.47`	`106.7`	`0`
N2	`3.80`	`71.4`	`0`
H2O	`2.64`	`809.1`	`1.88`

8 Click **Close**.

OPTIONS AND SETTINGS

1 Choose **Model>Constants** and type in the following entries:

NAME	EXPRESSION	DESCRIPTION
`A0`	`2.68e-17`	`Frequency factor (1/s)`
`E0`	`-243e3`	`Activation energy (J/mol)`
`rad`	`2e-3`	`Channel radius (m)`
`A`	`pi*rad^2`	`Channel cross section`
`v_av`	`0.3`	`Average gas velocity (m/s)`

2 Click **OK**.

3 Choose **Model>Expressions** and type in the following entries:

NAME	EXPRESSION	DESCRIPTION
`a`	`A0*exp(-E0/(Rg*T))`	`Arrhenius expression`
`S`	`r_1/r_2`	`Selectivity parameter`
`z`	`t/A`	`Axial distance from inlet`

4 Click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Reactor volumes** edit field, type `pi*0.002^2*0.36`, that is, the volume of the monolith channel.

3 Set the **Relative tolerance** to `1e-9` and the **Absolute tolerance** to `1e-10`.

4 Set the **Steady-state relative tolerance** to `1e-12`.

5 Click **OK**.

6 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The concentration transients of all species are plotted by default. Reproduce Figure 8-21 on page 476 and the plug-flow graph of Figure 8-25 on page 479 with the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Remove all entries from the **Quantities to plot** list by clicking the **<<** button.

3 In the **Expression** edit field type `c_NO`, then click the **>** button.

4 In the **x-axis data** area, click first the lower option button and then the **Expression** button. In the **Expression** edit field, type `z`, then click **OK**.

5 From the **Plot in** list, select **New figure**. Click **Apply** to generate the first part of Figure 8-25 in a separate figure window; leave this window open.

6 In the **Expression** edit field type `c_NH3`, then click the **>** button.

7 In the **Expression** edit field type `S/1000`, then click the **>** button.

8 From the **Plot in** list, select **Main axes**, then click **OK** to generate the plot in Figure 8-21.

Now move on to see how temperature affects the initial reaction rates.

OPTIONS AND SETTINGS

1 Click the **Model Settings** button on the Main toolbar.

2 On the **General** page, type `450+300*t` in the **Temperature** edit field.

As you later set the simulation time to 1 second, this imposes a temperature profile increasing linearly from 450 K at $t = 0$ to 750 K at $t = 1$ s.

3 Click **Close**.

SPECIES INTERFACE

1 Click the **Reaction Settings** button on the Main toolbar.

2 Click the **Species** tab.

3 Click the **General** tab.

4 Select **NO** from the **Species selection** list, then select the **Lock concentration/activity** check box.

5 Type `F0_NO/(v_av*A)` in the **Initial concentration** edit field.

Note how you can use the default variable name for the inlet molar flow and divide it by the volumetric flow to create an expression for the initial concentration.

6 Select **NH3** from the **Species selection** list and select the **Lock concentration/activity** check box.

7 Type `F0_NH3/(v_av*A)` in the **Initial concentration** edit field.

8 Click **Close**.

By locking the concentrations of the species affecting the reaction rates r_1 and r_2 you can evaluate the initial rates as functions of temperature.

COMPUTING THE SOLUTION

1. Click the **Solver Parameters** button on the Main toolbar.
2. In the **Reactor volumes** edit field type `1`.
3. Click **OK**.
4. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Reproduce Figure 8-22 on page 477 with the following steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. Remove all entries from the **Quantities to plot** list by clicking the **<<** button.
3. In the **Predefined quantities** list, select Reaction rate 1, then click the **>** button.
4. In the **Predefined quantities** list, select Reaction rate 2, then click the **>** button.
5. Click the **Expression** option button in the **x-axis data** area.
6. Click the **Expression** button and type `T` in the edit field. Click **OK**.
7. Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

Now restore some of the settings in the Reaction Engineering Lab before moving on to export the reaction model to COMSOL Multiphysics.

OPTIONS AND SETTINGS

1. Click the **Model Settings** button on the Main toolbar.
2. Type `523` in the **Temperature** edit field.
3. Click **Close**.

SPECIES INTERFACE

1. Click the **Reaction Settings** button on the Main toolbar.
2. Click the **Species** tab.
3. Select **NO** from the **Species selection** list. Clear the **Lock concentration/activity** check box and type `0` in the **Initial concentration** edit field.
4. Select **NH3** from the **Species selection** list. Clear the **Lock concentration/activity** check box and type `0` in the **Initial concentration** edit field.
5. Click **Close**.

EXPORT SETTINGS

1. Click the **Export to COMSOL Multiphysics** button on the Main toolbar.

2 The **Export to COMSOL Multiphysics** dialog box appears.

3 Go to the **Export mass balance** area, and in the **Application mode** list select **Convection and Diffusion: New**.

4 In the **Group name** edit field type `mass`.

5 Move to the **Export energy balance** area and clear the check box in the upper left corner.

6 Go to the **Export momentum balance** area, and in the **Application mode** list select **Incompressible Navier-Stokes: New**.

7 In the **Group name** edit field type `momentum`.

8 Click the **Export** button at the bottom of the dialog box.

Modeling Using COMSOL Multiphysics

It is now time to investigate the chemistry taking place in a space-dependent model, in this case in a channel of a honeycomb reactor. After drawing the model geometry you use the application modes (predefined balance equations) of the Chemical Engineering Module to set up and solve mass and momentum balances.

Click the **COMSOL Multiphysics** window.

GEOMETRY MODELING

Remember that in the axisymmetry modes, the symmetry axis is at r (or x) = 0, and that the geometry is built to the right of the axis.

1 Press the Shift key and click the **Rectangle/Square** button.

2 Type the following values in the corresponding edit fields for the rectangle dimensions:

SIZE		POSITION	
Width	`2e-3`	r	0
Height	`400e-3`	z	0

3 Click **OK**.

4 Press the Shift key again and click the **Rectangle/Square** button.

5 Type the following values in the corresponding edit fields for the rectangle dimensions:

SIZE		POSITION	
Width	1e-3	r	2e-3
Height	360e-3	z	20e-3

6 Click **OK**.

Now zoom in on this very narrow geometry.

7 Choose **Option>Axes/Grid Settings**.

8 Clear the **Axis equal** check box. In the **r-z limits** area, enter the following settings:

PROPERTY	VALUE
r min	-0.003
r max	0.005
z min	-0.01
z max	0.41

9 Click **OK**.

OPTIONS AND SETTINGS

Constants

1 From the **Options** menu, select **Constants**.

2 Enter the following parameter names and values in the **Constants** dialog box:

NAME	EXPRESSION	DESCRIPTION
v_av	0.3[m/s]	Average inlet velocity
p_ref	101325[Pa]	Pressure
eps_p	0.4	Porosity
k	1e-8[m^2]	Permeability
k_eff	0.25	Effectiveness factor
c_NO_in	8.16e-3[mol/m^3]	Inlet concentration
c_NH3_in	1.05e-2[mol/m^3]	Inlet concentration
c_O2_in	1.77[mol/m^3]	Inlet concentration
c_H2O_in	2.33[mol/m^3]	Inlet concentration

3 Click **OK**.

Projection Coupling Variables

To enable a comparison between the plug-flow and channel models, it is of interest to calculate the NO concentration averaged over the channel cross section as a function of the axial coordinate along the reactor channel. This quantity is given by the integral

$$c_{\mathrm{NO,mean}}(z) = \frac{1}{A}\int_{\Omega} c(\mathbf{x})dA = \frac{2}{R^2}\int_{0}^{R} c_{\mathrm{NO}}(r, z)rdr$$

To make it available for postprocessing, define a projection coupling variable, `co_NO_mean`, according to the following instructions (for a description of projection coupling variables, see the section “Projection Coupling Variables” on page 270 of the *COMSOL Multiphysics User’s Guide*).

1. From the **Options** menu, select **Projection Coupling Variables>Subdomain Variables**.
2. On the **Source** page, select Subdomain 1, then enter the following data on the first row of the table:

NAME	EXPRESSION	INTEGRATION ORDER
`c_NO_mean`	`2/(0.002^2)*r*c_NO`	4

3. Click the **General transformation** option button. In the **Source transformation** area, set **x** to `z` and **y** to `r`.
4. Click the **Destination** tab. From the **Level** list, select **Boundary**.
5. Select Boundary 5, then select the **Use selected boundaries as destination** check box.
6. In the **Destination transformation** area, set **x** to `z`, then click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Navier-Stokes Application Mode

1. From the **Multiphysics** menu, select **Incompressible Navier-Stokes (chns)**.
2. From the **Physics** menu, select **Properties**. From the **Analysis type** list, select **Stationary**. Click **OK**.
3. From the **Physics** menu, select **Subdomain Settings**.
4. Select Subdomains 1 and 2 from the **Subdomain selection** list by pressing Ctrl+A and and clicking in the list.
5. From the **Group** list, select **momentum**.

   Note how the **Density** and **Dynamic viscosity** edit fields are automatically filled in as a result of exporting the group **momentum** from the Reaction Engineering Lab.

6 Click the **Init** tab.

7 Type `p_ref` in the **Pressure** edit field.

8 Go back to the **Physics** tab.

9 Select Subdomain 2 (the porous-medium subdomain) from the **Subdomain selection** list.

10 Select the **Flow in porous media** check box.

11 Type `eps_p` in the **Porosity** edit field and `k` in the **Permeability** edit field.

12 Click **OK**.

Boundary Conditions—Navier-Stokes Application Mode

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the boundary conditions according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	ALL OTHERS
Boundary type	Symmetry boundary	Inlet	Outlet	Wall
Boundary condition	Axial symmetry	Velocity	Pressure, no viscous stress	No slip
u_0		0		
v_0		`v_av*2*(1-s^2)`		
p_0			`p_ref`	

Here you set up a parabolic inlet-velocity profile at the channel inlet. The velocity expression uses the built-in parameterization variable s that is available on boundaries in 2D. The value of *s* runs from 0 to 1 along any given boundary.

3 Click **OK**.

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, select **Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Properties**. From the **Analysis type** list, select **Stationary**. Click **OK**.

3 From the **Physics** menu, select **Subdomain Settings**.

4 Select Subdomains 1 and 2 from the **Subdomain selection list** by pressing Ctrl+A and and clicking in the list.

5 Select **mass** from the **Group** list.

Note how the **Diffusion coefficient** and **Reaction rate** edit fields are automatically filled in as a result of exporting the group **mass** from the Reaction Engineering Lab.

6 Click the **c_NO** tab.

7 Type `u` in the **r-velocity** edit field and `v` in the **z-velocity** edit field.

8 Repeat Steps 6 and 7 for the remaining species (**c_NH3**, **c_O2**, and **c_H2O**) by clicking their respective tabs.

9 Select Subdomain 1 from the **Subdomain selection** list.

10 Click the **c_NO** tab.

11 As no reaction takes place in the gas phase, type `0` in the **Reaction rate** edit field.

12 Repeat Step 11 for the remaining species (**c_NH3**, **c_O2**, and **c_H2O**) by clicking their respective tabs.

13 Select Subdomain 2 from the **Subdomain selection** list.

You must somewhat modify the gas-phase diffusivities exported from the Reaction Engineering Lab to represent the corresponding diffusivities in the porous domain. The effective diffusivity ($D_{i,\mathrm{eff}}$) in a porous material is related to the gas-phase diffusivity (D_i) by

$$D_{i,\,\mathrm{eff}} = \frac{\phi\sigma D_i}{\tau}$$

where, ϕ is the porosity, σ gives the constriction factor, and τ equals the tortuosity. Here, the material properties are grouped into the factor $k_{\mathrm{eff}} = \phi\sigma/\tau$.

14 Click the **c_NO** tab.

15 In the **Diffusion coefficient** edit field, modify the existing expression by typing `k_eff*` at the beginning of the expression, then click **Apply**.

16 Repeat Step 15 for the remaining species (**c_NH3**, **c_O2**, and **c_H2O**) by clicking their respective tabs.

17 Click **OK**.

Boundary Conditions—Convection and Diffusion

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the boundary conditions for each of the species **c_NO**, **c_NH3**, **c_O2**, and **c_H2O** according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	ALL OTHERS
Type	Axial symmetry	Concentration	Convective flux	Insulation/ Symmetry
c_NO_0		`c_NO_in`		
c_NH3_0		`c_NH3_in`		

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	ALL OTHERS
c_O2_0		`c_O2_in`		
c_H2O_0		`c_H2O_in`		

3 Click **OK**.

MESH GENERATION

Because projection coupling variables require simplex mesh elements, you must use a triangular mesh.

1 From the **Mesh** menu, choose **Free Mesh Parameters**.

2 On the **Global** page, select **Extremely fine** from the **Predefined mesh sizes** list.

To fully resolve this model requires a very dense mesh; the above setting results in a model size of roughly 386,000 degrees of freedom. If you want to reduce memory consumption and solution time at the cost of obtaining a solution which is numerically slightly inaccurate, you can select the mesh size **Extra fine** instead.

3 Click the **Advanced** tab. Set the **r-direction scale factor** to `100`. This setting is necessary to obtain a sufficient mesh resolution in the radial direction.

4 Click the **Remesh** button, then click **OK**.

COMPUTING THE SOLUTION

It is not necessary to solve both the momentum and mass balances simultaneously because the fluid flow is independent of the concentration. Therefore, to save time and computer memory, first solve the momentum balances and then solve the mass balances on the existing flow profile.

1 From the **Solve** menu, select **Solver Parameters**.

2 From the **Solver** list, select **Stationary**.

3 Go to the **Advanced** page.

4 In the **Type of scaling** list, select **None**.

5 Click **OK**.

6 From the **Solve** menu, select **Solver Manager**.

7 On the **Solve For** page, select **Incompressible Navier-Stokes** in the **Solve for variables** tree.

8 Click the **Solve** button. The solution time is around 2 minutes.

9 On the **Initial Value** page click the **Store Solution** button.

10 Click the **Stored solution** option button in the **Initial value** area.

11 Return to the **Solve For** page and select **Convection and Diffusion**.

12 Click **OK**.

13 Click the **Solve** button on the Main toolbar. The solution time is roughly 4 minutes.

POSTPROCESSING AND VISUALIZATION

The default plot shows the concentration of NO across the modeling domain, as seen in Figure 8-24 on page 478.

The following steps reproduce Figure 8-23 on page 477:

1. From the **Postprocessing** menu, open the **Cross-Section Plot Parameters** dialog box.
2. On the **General** page, clear the **Display cross-section in main axes** check box.
3. On the **Line/Extrusion** page, select **Incompressible Navier-Stokes (chns)>z-velocity** from the **Predefined quantities** list.
4. In the **x-axis data** area, click first the lower option button and then the **Expression** button to open the **X-Axis Data** dialog box. Type `r` in the **Expression** edit field, then select **mm** from the **Unit** list. Click **OK** to close the dialog box.
5. In the **Cross-Section Plot Parameters** dialog box, go to the **Cross-section line data** area.
6. Type `0` in the **r0** edit field and `0.003` in the **r1** edit field.
7. Type `0.2` in both the **z0** and **z1** edit fields.
8. Click **OK** to close the dialog box and generate the plot.

To finish the plot in Figure 8-25 on page 479, follow these instructions.

1. From the **Postprocessing** menu, open the **Domain Plot Parameters** dialog box.
2. On the **General** page, select the **Keep current plot** check box. From the **Plot in** list, select the figure window in which you plotted the first graph (**Figure 1**, unless you had any open figure windows from previous modeling sessions). If you do not have the COMSOL Reaction Engineering Lab, select **New window** instead.
3. Go to the **Line/Extrusion** page and select Boundary 5. In the **y-axis data** area, type `c_NO_mean` in the **Expression** edit field.
4. Click the **Line Settings** button. From the **Line color** list, select **Color**, then click the **Color** button. In the **Line Color** dialog box, select a green color, then click **OK**. From the **Line style** list, select **Dashed line**, then click **OK** to close the **Line Settings** dialog box.
5. Click **OK** to close the **Domain Plot Parameters** dialog box and generate the plot.

6 Click the **Edit Plot** toolbar button in the figure window, then use the **Edit Plot** dialog box to edit plot title, axis labels, and legends.

To calculate the conversion of NO to N2, perform an integration of the mass flux over the inlet and outlet:

1 From the **Postprocessing** menu, select **Boundary Integration**.

2 Select Boundary 2 (the inlet), and then in the **Predefined quantities** list select **Convection and Diffusion>Normal total flux, c_NO**.

3 Select the check box beside **Compute surface integral (for axisymmetric modes)**.

4 Click **Apply**.

5 Select Boundary 3 (the outlet).

6 Click **OK**.

The values from the flux integrations appear in the message log at the bottom of the user interface. The inlet integration yields $-3.08\cdot10^{-8}$ mol/s, while outlet integration yields $3.5\cdot10^{-9}$ mol/s. The flux is defined as leaving the geometry domain, hence the minus sign at the inlet. The conversion of NO becomes

$$\frac{3.08-0.35}{3.08} = 0.89$$

Porous Reactor with Injection Needle

Introduction

This model treats the flow field and species distribution in an experimental reactor for studies of heterogeneous catalysis. The model exemplifies the coupling of free and porous media flow in fixed bed reactors. The model was inspired by numerical experiments performed by Professor Finlayson's graduate students in chemical engineering at the University of Washington in Seattle.

Model Definition

The reactor consists of a tubular structure with an injection tube whose main axis is perpendicular to the reactor axis. The incoming species in the main and injection tubes react in a fixed porous catalyst bed. The model couples the free fluid and porous media flow through the Navier-Stokes equations and Brinkman's extension of Darcy's law. Because of symmetry, you need only model one half of the reactor; see Figure 8-26.

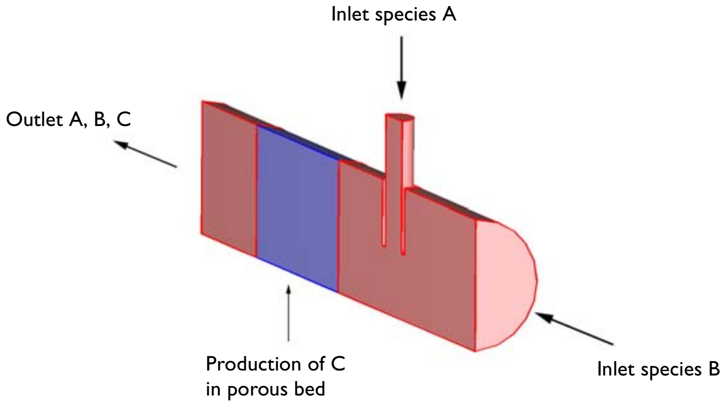


Figure 8-26: The species A and B enter the reactor from the main and injection tubes, respectively, and react in a fixed porous catalyst bed to produce C.

In the porous bed, a reaction takes place that consumes species A and B and produces C:

$$A + B \rightarrow C \tag{8-57}$$

DOMAIN EQUATIONS

The stationary Navier-Stokes equations describe the fluid flow in the free-flow regions:

$$\begin{aligned} \nabla \cdot [-\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p\mathbf{I}] &= -\rho(\mathbf{u} \cdot \nabla)\mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \tag{8-58}$$

In the porous bed, use the Brinkman equations:

$$\begin{aligned} \nabla \cdot \left[-\frac{\eta}{\varepsilon_p}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p\mathbf{I}\right] &= -\frac{\eta}{k}\mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \tag{8-59}$$

In the above equations, η denotes the viscosity of the fluid (Ns/m^2), ε_p is the porosity (dimensionless), **u** the velocity (m/s), ρ the density (kg/m^3), p the pressure (Pa), and κ the permeability (m^2).

Assume that the modeled species are present in low concentrations compared to the solvent gas. This means that you can use a Fickian approach for the diffusion term in the mass transport. Model the mass transport for the three species A, B, and C with the convection-diffusion equation

$$\nabla \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = R_i \tag{8-60}$$

In this equation, c_i denotes the concentration (mol/m^3), D_i the diffusivity (m^2 /s), and R_i the reaction rate for species i (mol/(m^3·s)). Because the reaction takes place in the porous bed only, the reaction term is zero in the free-flow regions. The reaction rates are given by

$$\begin{aligned} R_A &= -k c_A c_B \\ R_B &= -k c_A c_B \\ R_C &= k c_A c_B \end{aligned} \tag{8-61}$$

where k is the reaction rate constant.

BOUNDARY CONDITIONS

At the inlet boundaries, assume fully developed laminar flow. The velocities are then given by

$$\mathbf{n} \cdot \mathbf{u} = u_{\max}\left(1 - \left(\frac{r}{R}\right)^2\right) \tag{8-62}$$

where $\mathbf{n}$ is the boundary normal vector, and r is the distance from the center of the circular cross-section of radius R. The boundary condition for the Navier-Stokes equations at the outlet reads

$$\begin{aligned} \mathbf{t} \cdot \mathbf{u} &= 0 \\ p &= 0 \end{aligned} \tag{8-63}$$

where $\mathbf{t}$ is any tangential vector to the boundary.

In the mass transport, the concentrations at the inlet are fixed:

$$c_i = c_{i0,\,\mathrm{inlet}} \tag{8-64}$$

At the outlet, assume that convection dominates the mass transport:

$$\mathbf{n} \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = \mathbf{n} \cdot c_i \mathbf{u} \tag{8-65}$$

This implies that the gradient of c_i in the direction perpendicular to the outlet boundary is negligible. This is a common assumption for tubular reactors with a high degree of transport by convection in the direction of the main reactor axis. The condition eliminates the need for specifying a concentration or a fixed value for the flux at the outlet boundary. At all other boundaries, insulating conditions apply:

$$\mathbf{n} \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = 0 \tag{8-66}$$

Results

Figure 8-27 shows the flowlines of the velocity field and slices of the modulus of the velocity vector. The flow is almost homogeneous in the porous part of the reactor.

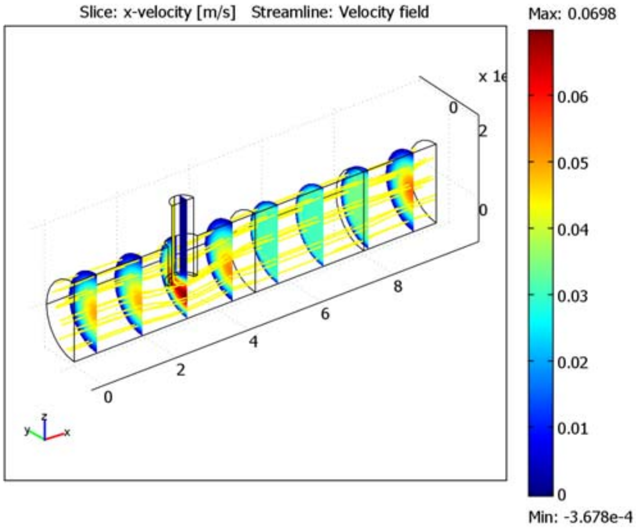


Figure 8-27: Flowlines and slices of the velocity field.

Figure 8-28 shows the pressure drop, which occurs mainly across the porous bed.

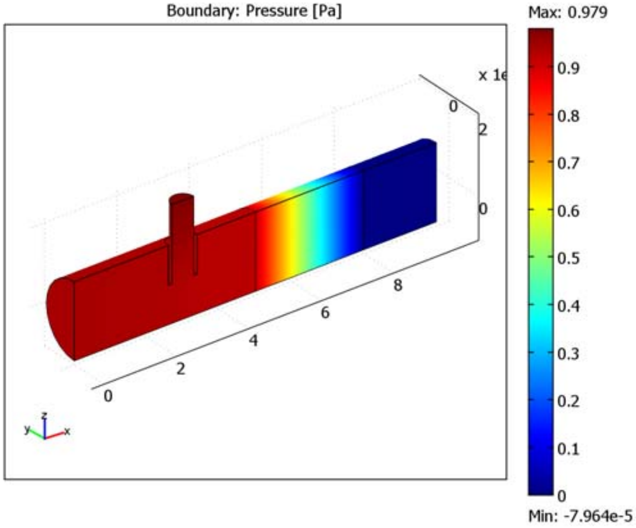


Figure 8-28: The pressure drop across the reactor.

Figure 8-29 and Figure 8-30 show the concentrations of species A and B, respectively.

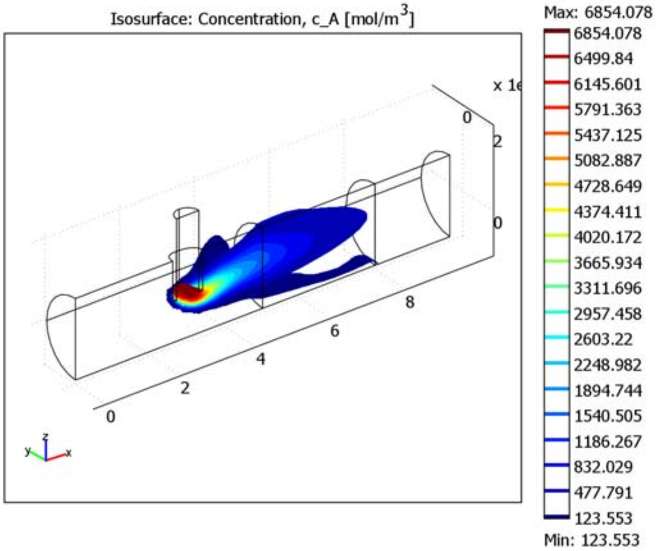


Figure 8-29: Iso-concentration surfaces for species A.

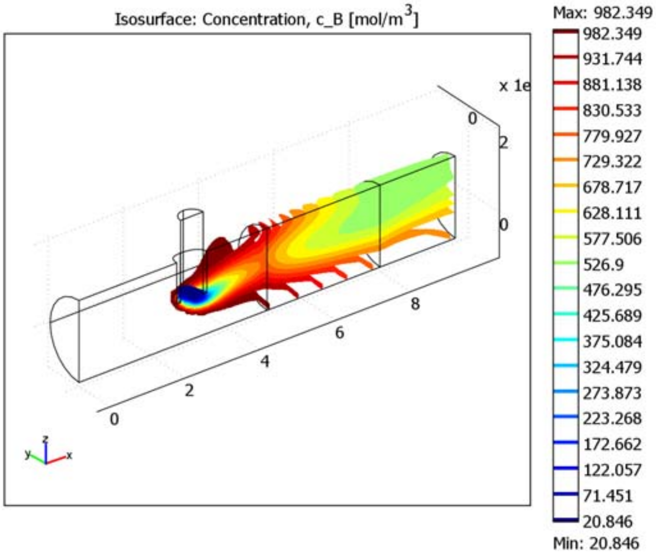


Figure 8-30: Iso-concentration surfaces for species B.

Figure 8-29 shows that the concentration of the injected species A decays very rapidly with the distance from the injection point. This implies that the porous bed is not optimally used. Figure 8-30 shows the iso-concentration surfaces of species B, which is introduced in the main channel of the reactor. The reaction is not uniformly distributed in the catalytic bed and has its maximum close to the radial position of the injection pipe. The low concentration of B at the injection point is due to dilution by the solvent that carries species A.

In summary, the model shows that the injection point is far too close to the porous bed. The reactants are not well mixed and only a fraction of the bed is utilized. A proper design should include a small static mixer after the injection point or a positioning of the injection point further upstream in order to obtain mixing through diffusion.

The following path shows the location of the COMSOL Multiphysics model:

Model Library path:
`Chemical_Engineering_Module/Transport_and_Reactions/porous_reactor`

Modeling Using the Graphical User Interface

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, select **3D** from the **Space dimension** list.
3. Click the **Multiphysics** button.
4. Select the application mode **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes** and click **Add**.
5. Select the application mode **Chemical Engineering Module>Mass Transport>Convection and Diffusion**. In the **Dependent variables** edit field, type `c_A c_B c_C`. Click **Add**.
6. Click **OK**.

OPTIONS AND SETTINGS

1 Enter the following constants in the **Options>Constants** dialog box:

NAME	EXPRESSION	DESCRIPTION
`rho`	`1[kg/m^3]`	`Fluid density`
`eta`	`1e-5[Pa*s]`	`Viscosity`
`epsilon`	`0.4`	`Porosity, catalyst bed`
`kappa`	`1e-9[m^2]`	`Permeability, catalyst bed`
`w_pipe`	`5[cm/s]`	`Maximal inlet velocity, species A`
`r_p`	`0.3[mm]`	`Pipe radius`
`u_tube`	`5[cm/s]`	`Maximal inlet velocity, species B`
`r_t`	`1[mm]`	`Tube radius`
`D_A`	`1e-6[m^2/s]`	`Diffusivity, species A`
`D_B`	`1e-6[m^2/s]`	`Diffusivity, species B`
`D_C`	`1e-6[m^2/s]`	`Diffusivity, species C`
`k`	`0.01[mol*s/m^3]`	`Reaction rate constant`
`c_A0`	`7000[mol/m^3]`	`Inlet concentration of A`
`c_B0`	`1000[mol/m^3]`	`Inlet concentration of B`

2 Click **OK**.

GEOMETRY MODELING

1 Click the **Cylinder** button on the Draw toolbar and enter cylinder properties according to the following table:

PROPERTY	VALUE
Radius	`1e-3`
Height	`1e-2`
Axis base point x	`0`
Axis base point y	`0`
Axis base point z	`0`
Axis direction vector x	`1`
Axis direction vector y	`0`
Axis direction vector z	`0`

2 Click **OK**.

3 Click the **Zoom Extents** button on the Main toolbar.

4 Create three more cylinders according to:

PROPERTY	CYLINDER 2	CYLINDER 3	CYLINDER 4
Radius	`1e-3`	`4e-4`	`3e-4`
Height	`3e-3`	`2e-3`	`2e-3`
Axis base point x	`5e-3`	`3e-3`	`3e-3`
Axis base point y	0	0	0
Axis base point z	0	0	0
Axis direction vector x	1	0	0
Axis direction vector y	0	0	0
Axis direction vector z	0	1	1

5 Click the **Block** button and specify a block with the following properties:

PROPERTY	VALUE 2
Length x	`1e-2`
Length y	`1e-3`
Length z	`3e-3`
Axis base point x	0
Axis base point y	`-1e-3`
Axis base point z	`-1e-3`

6 Click **OK**.

7 Click the **Create Composite Object** button on the Draw toolbar. In the **Set formula** edit field, type `CYL1-CYL3`, then click **Apply**.

8 In the **Set formula** edit field, type `CO1+CYL4`. Clear the **Keep interior boundaries** check box, then click **Apply**.

9 In the **Set formula** edit field, type `CO2+CYL2`. Select the **Keep interior boundaries** check box, then click **Apply**.

10 In the **Set formula** edit field, type `CO1-BLK1`. Make sure that the **Keep interior boundaries** check box is selected, then click **OK**.

PHYSICS SETTINGS

From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (chns)**.

Subdomain Settings—Navier-Stokes

1 Select **Subdomain Settings** from the **Physics** menu.

2 Select Subdomain 2 from the **Subdomain selection** list.

3 Select the **Flow in porous media (Brinkman equations)** check box.

4 Type `rho` in the **Density** edit field, `eta` in the **Dynamic viscosity** edit field, `epsilon` in the **Porosity** edit field, and `kappa` in the **Permeability** edit field.

5 Select Subdomains 1 and 3 from the **Subdomain selection** list.

6 Type `rho` in the **Density** edit field and `eta` in the **Dynamic viscosity** edit field.

7 Click **OK**.

Boundary Settings—Navier-Stokes

To define the boundary conditions in a simple manner, define two expressions at the boundary level.

1 Select **Expressions>Boundary Expressions** from the **Options** menu.

2 Enter boundary expressions according to the following table:

NAME	BOUNDARY 1 /EXPRESSION	BOUNDARY 8 /EXPRESSION
`r_tube`	`sqrt(z^2+y^2)`	
`r_pipe`		`sqrt((x-3e-3)^2+y^2)`

3 Click **OK**.

4 From the **Physics** menu, open the **Boundary Settings** dialog box.

5 Enter boundary conditions according to the table below.

SETTINGS	BOUNDARY 8	BOUNDARY 1	BOUNDARY 19	BOUNDARIES 2, 12, 16	ALL OTHERS
Boundary type	Inlet	Inlet	Outlet	Symmetry boundary	Wall
Boundary condition	Velocity	Velocity	Pressure, no viscous stress		No slip
U_0	`w_pipe*(1-r_pipe^2/r_p^2)`	`u_tube*(1-r_tube^2/r_t^2)`	-	-	-
P_0	-	-	0	-	-

6 Click **OK**.

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select all subdomains in the **Subdomain selection** list by pressing Crtl+A and clicking the list.

4 On each of the pages **c_A**, **c_B**, and **c_C**, in turn, enter the appropriate settings from the following table:

PROPERTY	c_A	c_B	c_C
D (isotropic)	D_A	D_B	D_C
u	u	u	u
v	v	v	v
w	w	w	w

5 Select Subdomain 2 in the **Subdomain selection** list.

6 On each of the pages **c_A**, **c_B**, and **c_C**, in turn, enter the following settings:

PROPERTY	c_A	c_B	c_C
R	-k*c_A*c_B	-k*c_A*c_B	k*c_A*c_B

7 Click **OK**.

Boundary Settings—Convection and Diffusion

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 On the **c_A** page, enter the following boundary conditions for species A:

SETTINGS	BOUNDARY 1	BOUNDARY 8	BOUNDARY 19	ALL OTHERS
Boundary condition	Concentration	Concentration	Convective flux	Insulation/ Symmetry
c_A_0	0	c_A0	-	-

3 On the **c_B** page, enter the following boundary conditions for species B:

SETTINGS	BOUNDARY 1	BOUNDARY 8	BOUNDARY 19	ALL OTHERS
Boundary condition	Concentration	Concentration	Convective flux	Insulation/ Symmetry
c_B_0	c_B0	0	-	-

4 On the **c_C** page, enter the following boundary conditions for species C:

SETTINGS	BOUNDARIES 1, 8	BOUNDARY 19	ALL OTHERS
Boundary condition	Concentration	Convective flux	Insulation/ Symmetry
c_C_0	0	-	-

5 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 Click the **Custom mesh size** option button.

3 In the **Maximum element size** edit field, type `4e-4`.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Because the velocity field is independent of the concentrations, you can compute the velocity field first.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Incompressible Navier-Stokes (chns)**.

3 Click the **Solve** button.

4 Click the **Initial Value** tab. Click the **Store Solution** button.

5 In the **Initial value** area, select the **Stored solution** option button.

6 Click the **Solve For** tab.

7 Select **Convection and Diffusion (chcd)** from the list.

8 Click **OK**.

9 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 8-27, execute the following instructions:

1 Click the **Plot Parameters** button on the main toolbar.

2 On the **General** page, select the **Slice** and **Streamline** check boxes in the **Plot type** area.

3 On the **Slice** page, select **x-velocity** from the **Predefined quantities** list.

4 Set **x levels** to 8.

5 Click the **Streamline** tab.

6 Click the **Line Color** tab.

7 Click the **Uniform color** option button.

8 Click the **Color** button and select yellow. Click **OK**.

9 Set **Line type** to **Tube**, then open the **Tube Radius Parameters** dialog box.

10 Clear the **Auto** check box and set **Radius scale factor** to `0.4`. Click **OK** to close the **Tube radius** dialog box.

11 Click **OK** to generate the figure.

To generate Figure 8-28; proceed as follows:

1 On the **General** page in the **Plot Parameters** dialog box, clear the **Slice** and **Streamline** check boxes in the **Plot type** area.

2 Select the **Boundary** check box.

3 Click the **Boundary** tab.

4 From the **Predefined quantities** list, select **Pressure**.

5 Click **OK**.

Next, generate Figure 8-29 with the following steps:

1 On the **General** page in the **Plot Parameters** dialog box, clear the **Boundary** check box.

2 Select the **Isosurface** check box.

3 Go to the **Isosurface** page.

4 Select **Convection and Diffusion (chcd)>Concentration, c_A** from the **Predefined quantities** list.

5 Type `20` in the **Number of levels** edit field.

6 Click **OK**.

Generate Figure 8-30 in the same way using `c_B` as isosurface data.

Carbon Deposition in Heterogeneous Catalysis

Introduction

Carbon deposition onto the surface of solid catalysts is commonly observed in hydrocarbon processing. Carbon deposits can affect both the activity of catalysts as well as the flow of gas through a catalyst bed.

This example investigates the thermal decomposition of methane into hydrogen and solid carbon. In the first model you look at the isothermal process occurring in an ideal reactor, simulated in the Reaction Engineering Lab. The influence of carbon deposition on catalyst activity is also considered. In the second model, you study the effect that the carbon deposits have on the fluid flow. The second simulation takes place in COMSOL Multiphysics taking both time and space dependencies into account.

Model Definition

CHEMISTRY

Methane decomposes over a Ni/Al_2O_3 catalyst according to the overall chemical reaction:

$$CH_4 \rightleftharpoons C + 2H_2 \tag{8-67}$$

The following reaction rate expression has been reported in the literature (Ref. 1).

$$r = k \cdot \frac{p_{CH4} - \frac{p_{H2}^2}{K_p}}{(1 + k_H \sqrt{p_{H2}})^2} \tag{8-68}$$

where

$$k = \exp\left(20.492 - \frac{104200}{R_g T}\right) \tag{8-69}$$

$$k_{\mathrm{H}} = \exp\left(\frac{163200}{R_g T} - 22.426\right) \tag{8-70}$$

and

$$K_p = 5.088 \cdot 10^5 \cdot \exp\left(-\frac{91200}{R_g T}\right) \tag{8-71}$$

IDEAL REACTOR MODEL

The first model is set up in Reaction Engineering Lab. This treats the isothermal decomposition of methane (Equation 8-67) in a perfectly mixed reactor with constant volume. The species mass balances are summarized by:

$$\frac{dc_i}{dt} = R_i \tag{8-72}$$

The rate term, R_i, takes into account the reaction stoichiometry, ν_i, the reaction rate, r, and the catalyst activity, a:

$$R_i = \nu_i r a \tag{8-73}$$

The mass balances of the reacting species are then:

$$\frac{dc_{\mathrm{CH4}}}{dt} = -ra \tag{8-74}$$

$$\frac{dc_{\mathrm{C}}}{dt} = ra \tag{8-75}$$

$$\frac{dc_{\mathrm{H2}}}{dt} = 2ra \tag{8-76}$$

The time dependency of the catalytic activity is expressed by the ODE:

$$\frac{da}{dt} = -k_a r^2 c_{\mathrm{C}} a \tag{8-77}$$

where

$$k_a = \exp\left(\frac{135600}{R_g T} - 32.007\right) \tag{8-78}$$

Solving the mass balances provides the evolution of the species concentrations over time. The fact that carbon is in the solid phase is taken into account by removing its effect on gas phase physical properties. The pressure in the reactor is a function of only the methane and hydrogen concentrations:

$$p = R_g T(c_{CH4} + c_{H2}) \tag{8-79}$$

SPACE- AND TIME-DEPENDENT MODEL

The second model is solved in COMSOL Multiphysics and takes both fluid flow and the chemical reaction into account.

The flow reactor is set up in 2D, as illustrated below:

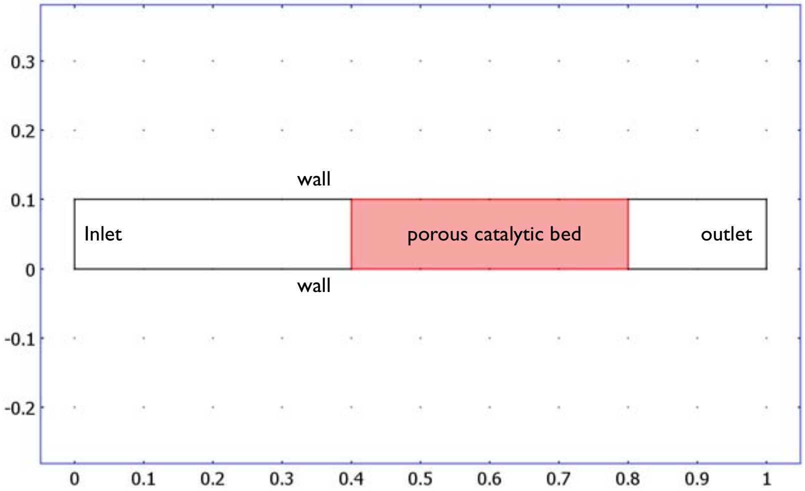


Figure 8-31: A flow reactor is set up in 2D. Methane enters from the left and reacts in the porous catalytic bed in the mid-section of the geometry.

Methane first flows through a free section of the reactor, and then encounters a porous catalytic bed where the decomposition reaction takes place.

Momentum Balances

The flow in the free channel section is described by the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot [-\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p\mathbf{I}] = -\rho(\mathbf{u} \cdot \nabla)\mathbf{u} \tag{8-80}$$

$$\nabla \cdot \mathbf{u} = 0$$

where ρ denotes density (kg/m^3), $\mathbf{u}$ represents the velocity (m/s), η denotes viscosity (kg/(m· s)), and p equals pressure (Pa). In the porous domain, the Brinkman equations govern the flow:

$$\frac{\rho}{\varepsilon_p}\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \left[-\frac{\eta}{\varepsilon_p}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p\mathbf{I}\right] = -\frac{\eta}{k}\mathbf{u} \qquad (8\text{-}81)$$
$$\nabla \cdot \mathbf{u} = 0$$

where ε_p is the porosity and k denotes permeability (m^2) of the porous media. As you can see in Equation 8-80 and Equation 8-81, the momentum-balance equations are closely related. The term on the right-hand side of the Navier-Stokes formulation corresponds to momentum transported by convection in free flow. In the Brinkman formulation, this term is replaced by a contribution associated with the drag force experienced by the fluid as it flows through a porous medium. COMSOL Multiphysics automatically combines free and porous-media flow to solve the equations simultaneously.

The boundary conditions for the flow are:

$$\begin{aligned} \mathbf{u} \cdot \mathbf{n} &= u_0 && \text{inlet} \\ \mathbf{u} &= \mathbf{0} && \text{walls} \\ p &= 0 && \text{outlet} \end{aligned} \qquad (8\text{-}82)$$

Mass transport in the reactor is described by the diffusion-convection equations:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = R_i \qquad (8\text{-}83)$$

where D_i denotes the diffusion coefficient (m^2/s) and c_i is the species concentration. The term R_i corresponds to the species' net reaction rates.

In the free channel, the inlet conditions are equal to the inlet concentrations

$$c = c_{\mathrm{in}} \qquad (8\text{-}84)$$

At the outlet, you use the convective flux condition

$$\mathbf{n} \cdot (-D\nabla c) = 0 \qquad (8\text{-}85)$$

All other boundaries use the insulating or symmetry condition

$$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = 0 \qquad (8\text{-}86)$$

Balance for Void Fraction

The void fraction of the catalytic bed decreases as carbon is deposited. This in turn affects the flow through the reactor. A balance for the void fraction, or porosity, of the bed is given by:

$$\frac{d\varepsilon}{dt} = -\frac{\varepsilon r}{M_c \rho_{\mathrm{soot}}} \tag{8-87}$$

This equation can be implemented in the PDE, General Form application mode of COMSOL Multiphysics, resulting in porosity distribution across the catalytic bed as a function of time. The initial porosity of the bed is assumed to be $\varepsilon = 0.4$.

The porosity is related to the permeability of the porous domain by the expression (Ref. 2):

$$k = k_0 \left(\frac{\varepsilon}{\varepsilon_0}\right)^{3.55} \tag{8-88}$$

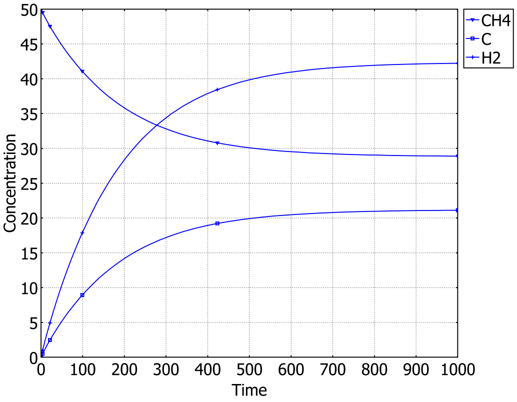
In this way, the porosity balance couples the mass and momentum balances describing the reacting system.

Results

IDEAL REACTOR MODEL

The upper graph of Figure 8-32 shows the concentration transients of methane, hydrogen and deposited carbon, as methane decomposes over a Ni/Al_2O_3 catalyst.

The lower graph is a plot of the reactor pressure. Deactivation of the catalyst is not taken into account at this point.



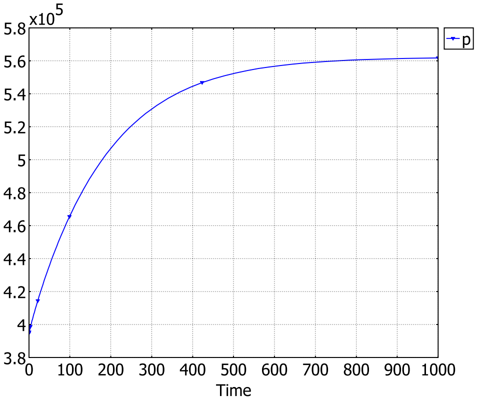


Figure 8-32: Upper graph: concentration transients of methane decomposition over a Ni/Al_2O_3 *catalyst. Lower graph: reactor pressure. Deactivation of the catalyst is not considered.*

Taking catalyst deactivation into account (Equation 8-77) produces the results shown in Figure 8-33. Under the simulated conditions a moderate drop in activity is noted (upper graph), leading to a largely unaffected overall process, as can be seen by comparing with the concentration transients of the previous model (lower graph).

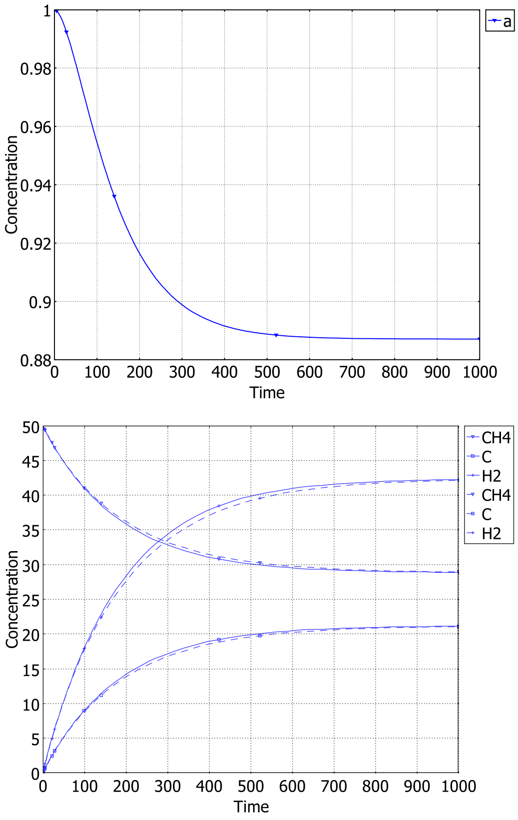


Figure 8-33: Upper graph: catalyst activity drops off as carbon deposits at the catalyst surface. Lower graph: concentration transients of methane, hydrogen and deposited carbon with no deactivation present (solid lines) and with deactivation taken into account (dashed lines).

SPACE- AND TIME-DEPENDENT MODEL

The following results concern a space- and time-dependent model simulated in COMSOL Multiphysics. Methane decomposition occurs in a porous region where solid catalyst particles are packed. Figure 8-34 shows the velocity field across the reactor prior to carbon deposition. The 2D plot shows that the velocity profile is parabolic in the free channel sections and close to constant in the porous domain. The line plot in the bottom graph in Figure 8-34 shows the velocity along the reactor centerline.

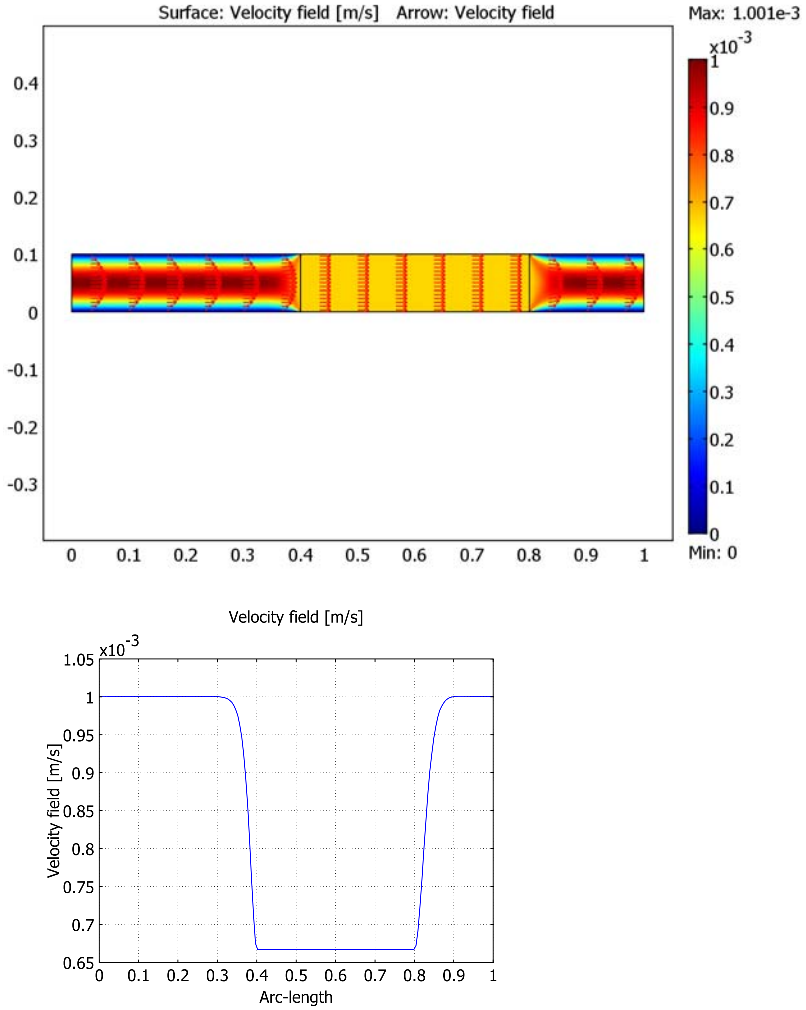


Figure 8-34: Upper graph: velocity flow field in the 2D reactor domain. Lower graph: the gas velocity plotted along the reactor centerline.

Reactions take place in the packed catalytic bed located in the mid section of the reactor. Figure 8-35 shows the concentration profiles along the centerline of the bed.

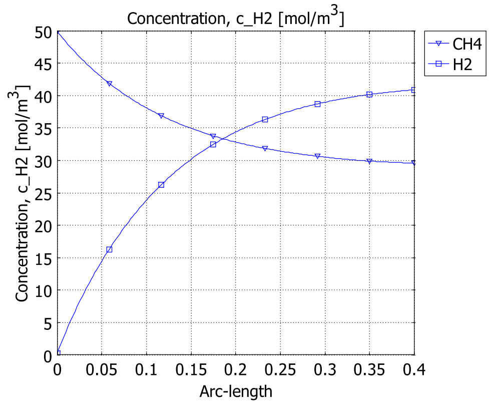


Figure 8-35: Methane and hydrogen concentrations as a function of the bed position.

The methane and hydrogen concentrations are equal after passing approximately 0.18 m into the bed. Figure 8-34 shows that the velocity in the bed is near $0.67 \cdot 10^{-3}$ m/s, equaling a residence time of 270 s. This result agrees with the findings from the ideal reactor simulation, shown in Figure 8-32.

Now, consider the effects as methane is constantly supplied to the reactor for 1000 seconds. The initial permeability is a constant $1 \cdot 10^{-9}$ m^2 across the bed. Note how the permeability at the front end of the bed changes by four orders of magnitude during the first 1000 s of carbon deposition.

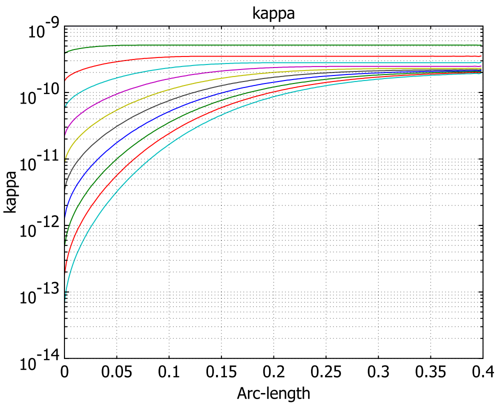


Figure 8-36: Permeability of the packed catalytic bed as the decomposition of methane proceeds for 1000 s. The time interval between each line is 100 s.

As carbon deposits in the reacting bed, the pressure distribution across the reactor is affected. Figure 8-37 shows a small, linear pressure drop as unreacting gas passes through a clean catalyst bed.

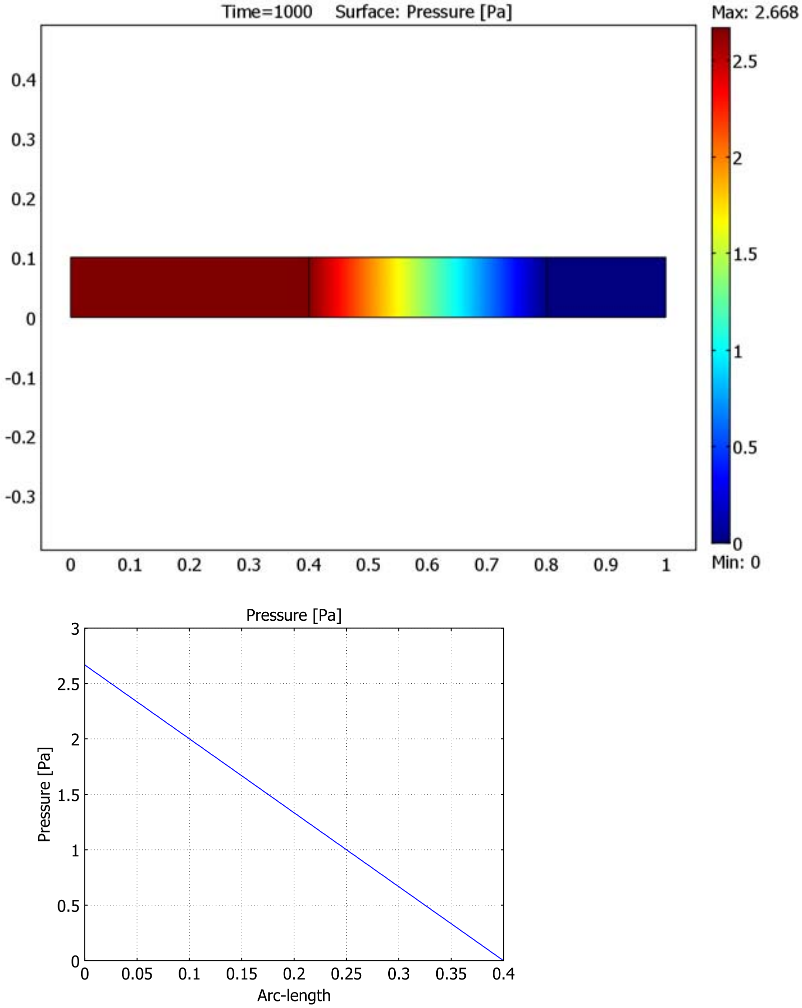


Figure 8-37: Distribution of pressure as an unreacting gas passes a clean catalyst bed. Upper graph: pressure distribution across the 2D reactor domain. Lower graph: pressure drop along the packed catalyst bed.

Figure 8-38 shows the pressure distribution across the reactor after methane decomposition has occurred for 1000 s. The pressure drop is notably greater and occurs across the first 10 cm of the bed.

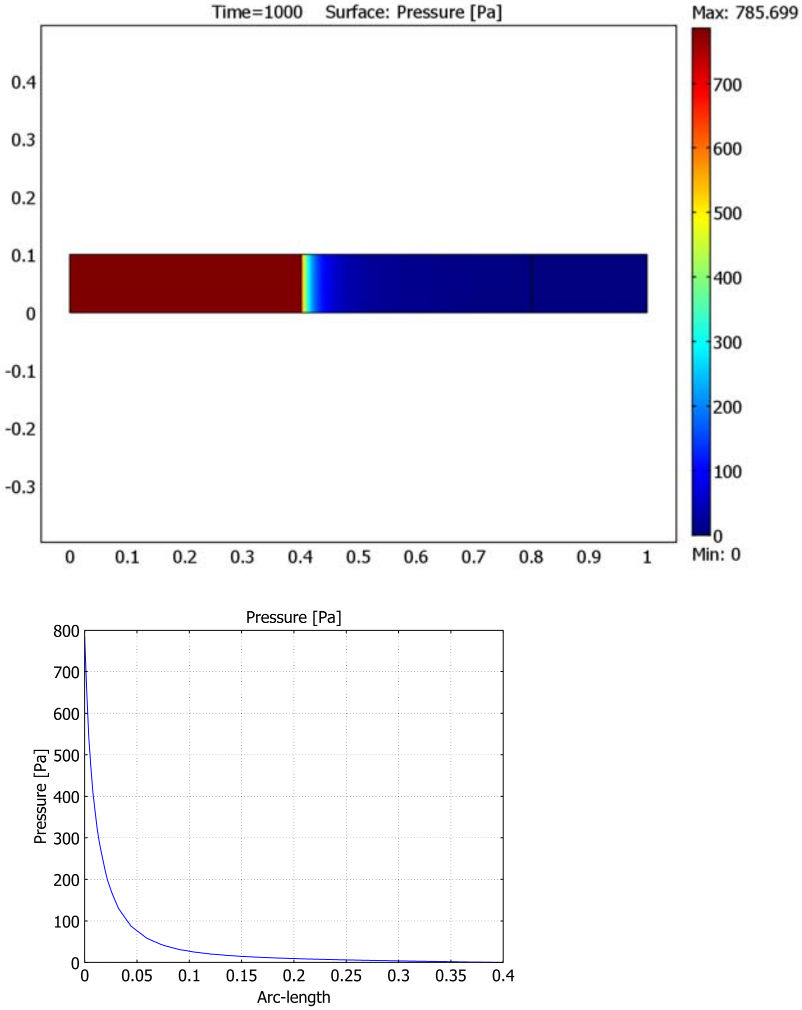


Figure 8-38: Distribution of pressure when methane decomposition has been allowed to occur for 1000 s. Upper graph: pressure distribution across the 2D reactor domain. Lower graph: pressure drop along the packed catalyst bed.

References

1. S.G. Zavarukhin and G.G. Kuvshinov, *J. Appl. Catal. A*, vol. 272, p. 219, 2004.

2. E.A. Borisova and P.M. Adler, *Phys. Rev. E*, vol. 71, p. 016311-1, 2005.

The following path shows the location of the Reaction Engineering Lab model:

Model Library path: `Process_Chemistry/carbon_deposition`

The following path shows the location of the COMSOL Multiphysics model:

Model Library path: `Reaction_Engineering_Lab/Process_Chemistry/carbon_deposition`

Modeling Using the COMSOL Reaction Engineering Lab

MODEL NAVIGATOR

1. Start COMSOL Reaction Engineering Lab.
2. Click **New** in the **Model Navigator** window.

REACTIONS INTERFACE

1. Click the **Reaction Settings** button on the Main toolbar.
2. Make sure the **Reactions** page is active. Create a new entry in the **Reaction selection** list by clicking the **New** button.
3. Type `CH4=>C+2H2` in the **Formula** edit field.
4. Modify the predefined reaction rate according to Equation 8-68 by typing the following in the **r** edit field: `c_a*k*(p_CH4-p_H2^2/Kp)/(1+kh*sqrt(p_H2))^2`.

   You will define the parameters and constants for the rate expression later on.

SPECIES INTERFACE

1. Click the **Species** tab.
2. Create a new entry in the **Species selection** list by clicking the **New** button.

3 Type `a` in the **Formula** edit field.

When a new species is created a mass balance equation is set up along with it, in this case:

$$\frac{dc_a}{dt} = R_a$$

The left hand side is defined internally in the software and the right hand side corresponds to the expression given in the **R** edit field.

Note also that you can remove the effect of catalyst activity from your model by selecting the **Lock concentration/activity** check box. This removes the species mass balance and sets the concentration of the species to the value entered in the **Initial concentration** edit field.

4 Proceed to define the equation for the catalyst activity (Equation 8-77) by selecting species **a** from the **Species selection** list and typing `-ka*r_1^2*c_C*c_a` in the **R** edit field.

5 Select the appropriate entry from the **Species selection** list and then enter the corresponding value for the **Initial concentration**:

SPECIES NAME	c0
CH4	50
a	1

6 Click **Close**.

OPTIONS AND SETTINGS

1 Click the **Model Settings** button on the Main toolbar.

2 On the **General** page type `950` in the **Temperature** edit field.

3 In the **p** edit field, modify the predefined expression for the pressure to: `Rg*T*(c_CH4+c_H2)`.

The predefined expression for the pressure in the reactor is:

$$p = R_g T \sum c_i$$

You remove the contributions from the carbon species and the activity parameter, as they do not contribute to the gas phase pressure.

4 Click **Close**.

5 Select the menu item **Model>Expressions**.

6 Enter the following expressions by typing them in. Alternatively, click the **Import Variables From File** button and browse to the file: `carbon_deposition_expressions.txt`:

NAME	EXPRESSION	DESCRIPTION
`k`	`2.31e-5*exp(20.492-104200/Rg/T)`	`Arrhenius expression`
`Kp`	`5.088e5*exp(-91200/Rg/T)`	`Arrhenius expression`
`kh`	`exp(163200/Rg/T-22.426)`	`Arrhenius expression`
`ka`	`43240*exp(135600/Rg/T-32.077)`	`Arrhenius expression`
`p_CH4`	`c_CH4*Rg*T/100000`	`CH4 pressure (bar)`
`p_H2`	`c_H2*Rg*T/100000+eps`	`H2 pressure (bar)`

7 Click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 Type `1000` in the **Times** edit field.

3 Click **OK**.

4 Compute the solution by clicking the **Solve Problem** button on the Main toolbar.

EXPORT SETTINGS

You will now export the reaction model from Reaction Engineering Lab to COMSOL Multiphysics, and see how the chemistry of methane decomposition behaves in a time and space dependent system. The COMSOL Multiphysics model assumes that the catalyst activity is constant. The deposition of carbon, however, affects reactor performance because the deposits affect the permeability of the porous section of the reactor.

1 Click the **Reaction Settings** button on the Main toolbar.

2 Go to the **Species** page.

3 Select the **a** from the **Species selection** list and select the **Lock concentration/activity** check box.

The activity is assumed to be constant and equal to one.

4. Select the species **C** from the **Species selection** list and then select the **Lock concentration/activity** check box.

   The purpose of this setting is to avoid the automatic set up of a mass balance equation for the species C in COMSOL Multiphysics. The effect of the carbon deposition rate will be taken into account by a balance equation for the reactor bed void fraction (Equation 8-87), that will be set up after the export.
5. Click **Close**.
6. Click the **Export to COMSOL Multiphysics** button on the Main toolbar.
7. Select **2D** from the **Space dimension** list and click **OK**.
8. The **Export to COMSOL Multiphysics** dialog box appears.
9. Go to the **Export mass balance** area, and in the **Application mode** list select **Convection and Diffusion: New**.
10. In the **Group name** edit field type `reactions`.
11. Move to the **Export energy balance** area and clear the check box in the upper left corner.
12. Move to the **Export momentum balance** area and clear the check box in the upper left corner.
13. Click the **Export** button at the bottom of the dialog box.

Modeling Using COMSOL Multiphysics

Click the **COMSOL Multiphysics** window.

MODEL NAVIGATOR

1. Select the menu item **Multiphyiscs>Model Navigator**.
2. In the **Application Modes** tree, select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes**.
3. Click the **Add** button.
4. In the **Application Modes** tree, select **COMSOL Multiphysics>PDE Modes>PDE, General Form**.
5. Type `por` in the **Dependent variables** edit field, then click the **Add** button.
6. Click the **OK** button.

GEOMETRY MODELING

1. Press the Shift key and click the **Rectangle/Square** button.

2 Type the following values in the corresponding edit fields for the rectangle dimensions.

SIZE		**POSITION**	
Width	1	x	0
Height	`0.1`	y	0

3 Click **OK**.

4 Press the Shift key again and click the **Rectangle/Square** button.

5 Type the following values in the corresponding edit fields for the rectangle dimensions

SIZE		**POSITION**	
Width	`0.4`	x	`0.4`
Height	`0.1`	y	0

6 Click **OK**.

7 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings—Navier-Stokes Application Mode

1 Select **Incompressible Navier-Stokes (chns)** from the **Multiphysics** menu.

2 Select **Subdomain Settings** from the **Physics** menu.

3 Select all subdomains by pressing Ctrl+A and clicking the **Subdomain selection** list.

4 Type `1` in the **Density** edit field.

5 Type `1e-5` in the **Dynamic viscosity** edit field.

6 Select Subdomain 2 (the porous media subdomain) from the **Subdomain selection** list.

7 Select the **Flow in porous media (Brinkman equations)** check box.

8 Type `por` in the **Porosity** edit field.

9 Type `kappa` in the **Permeability** edit field.

10 Click **OK**.

Boundary Conditions—Navier-Stokes Application Mode

1 Select **Boundary Settings** from the **Physics** menu.

2 Enter the boundary settings according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 5,6	BOUNDARY 10	ALL OTHERS
Boundary type	Inlet	Wall	Outlet	Wall
Boundary condition	Laminar inflow	Slip	Pressure	No slip
U_0	`u_in`			
p_0			0	

3 Click **OK**.

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu select **Convection and Diffusion (chcd)**.

2 From the **Physics** menu select **Subdomain Settings**.

3 From the **Subdomain selection** list, select Subdomain 2.

4 Select **reactions** from the **Group** list.

Note how the **Reaction rate** edit fields are automatically filled in as a result of exporting the group **reactions** from the Reaction Engineering Lab.

5 Select all subdomains by pressing Ctrl+A and clicking the **Subdomain selection** list.

6 On page **c_CH4** type `u` in the **x-velocity** edit field and `v` in the **y-velocity** edit field.

7 Go to page **c_H2** and type `u` in the **x-velocity** edit field and `v` in the **y-velocity** edit field.

8 Click **Apply**.

9 Click the **Init** page and type `50` in the **c_CH4(t_0)** edit field.

10 Click **Apply**.

11 Type expressions into the **Diffusion coefficient** edit field according to the following table:

SUBDOMAIN	PAGE / C_CH4	PAGE / C_H2
1	D_CH4	D_H2
2	k_eff*D_CH4	k_eff*D_H2
3	D_CH4	D_H2

12 Click **OK**.

Boundary Conditions—Convection and Diffusion

1 From the **Physics** menu select **Boundary Settings**.

2 Enter the boundary conditions for the species **c_CH4** and **c_H2** according to the following table:

SETTINGS	BOUNDARY 1	BOUNDARY 10	ALL OTHER
Boundary condition	Concentration	Convective flux	Insulation/Symmetry
c_CH4_0	`cCH4_in`		
c_H2_0	`cH2_in`		

3 Click **OK**.

Subdomain Settings—PDE, General Form

1 From the **Multiphysics** menu select **PDE, General Form (g)**.

2 From the **Physics** menu select **Subdomain Settings**.

3 Select 1 and 3 in the **Subdomain selection** list and clear the **Active in this domain** check box.

4 Select 2 in the **Subdomain selection** list.

5 Type `0` in the two **Flux vector** edit fields.

6 Type `-por*r_1_rxn_chcd/M_C/rho_soot` in the **Source term** edit field.

The above settings have reduced the general form PDE

$$e_a\frac{\partial^2\varphi}{\partial t^2}+d_a\frac{\partial\varphi}{\partial t}+\nabla\cdot\Gamma = F$$

to the form of the void fraction balance (Equation 8-87)

$$d_a\frac{\partial\varphi}{\partial t} = F = -\frac{\varepsilon r}{M_c\rho_{\text{soot}}}$$

7 Go to the **Init** page.

8 Type `por0` in the **por(t$_0$)** edit field.

9 Click **OK**.

Boundary Conditions—PDE, General Form

1 From the **Physics** menu select **Boundary Settings**.

2 Select Boundaries 4, 5, 6 and 7 and select the **Neumann boundary condition** option button.

3 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu select **Constants**.

2 Enter the following parameter names and values in the **Constants** dialog box, either by typing them in, or by clicking the **Import Variables From File** button and browsing to the file: `carbon_deposition_constants.txt`, followed by clicking **Open**.

NAME	EXPRESSION	DESCRIPTION
`u_in`	`0.667e-3`	`average inlet velocity`
`cCH4_in`	`50`	`inlet concentration`
`cH2_in`	`0`	`inlet concentration`
`kappa0`	`1e-9`	`permeability of clean catalyst`
`por0`	`0.4`	`porosity of clean catalyst bed`
`rho_soot`	`4e3`	`density of soot deposits`
`M_C`	`12.011e-3`	`molar weight of carbon`
`D_CH4`	`1e-6`	`diffusion coefficient`
`D_H2`	`4e-6`	`diffusion coefficient`
`k_eff`	`0.1`	`effectiveness factor`

3 Click **OK**.

4 From the **Options** menu select **Expressions>Scalar Expressions**.

5 Enter the following parameter names and expressions, then click **OK**.

NAME	EXPRESSION	DESCRIPTION
`kappa`	`kappa0*(por/por0)^3.55`	`permeability`

MESH GENERATION

1 From the **Mesh** menu choose **Free Mesh Parameters**.

2 Click the **Boundary** tab.

3 Select the appropriate entries in the **Boundary selection** list and enter the following mesh settings:

BOUNDARY	MAXIMUM ELEMENT SIZE
2-9	5e-3

4 Click the **Remesh** button and then the **OK** button.

COMPUTING THE SOLUTION

Start by computing a flow field where chemical reactions are disregarded. This is to have a good starting guess for the flow when solving the coupled problem.

1. From the **Solve** menu select **Solver Parameters**.
2. Select **Stationary** from the **Solver** list.
3. Click **OK**.
4. From the **Solve** menu select **Solver Manager**.
5. On the **Solve For** page, select **Incompressible Navier-Stokes (chns)** in the **Solve for variables** tree.
6. Click the **OK** button.
7. Click the **Solve** button on the Main toolbar.

The following steps produce a plot of the flow field:

1. From the **Postprocessing** menu open the **Plot Parameters** dialog box.
2. Go to the **Surface** page.
3. Select **Incompressible Navier-Stokes (chns)>Velocity field** from the **Predefined quantities** list.
4. Go to the **Arrow** page and select the **Arrow plot** check box.
5. Select **Incompressible Navier-Stokes (chns)>Velocity field** from the **Predefined quantities** list.
6. Click **OK**.

Proceed to solve the time-dependent problem, which takes the chemical reactions and carbon deposition into account.

1. From the **Solve** menu select **Solver Parameters**.
2. Select **Time dependent** from the **Solver** list.
3. Type `0:100:1000` in the **Times** edit field.
4. Click **OK**.
5. From the **Solve** menu select **Solver Manager**.
6. On the **Initial Value** page click the **Store Solution** button.
7. Click the **Stored solution** option button in the **Values of variables not solved for and linearization point** area.

8 Return to the **Solve For** page and select **Convection and Diffusion (chcd)** and **PDE, General Form (g)** from the **Solve for variables** tree, by pressing Ctrl and clicking the entries.

9 Click **OK**.

10 Click the **Solve** button on the Main toolbar.

Plot gas phase concentrations of methane and hydrogen in the reactive bed:

1 From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box.

2 On the **General** page, select **1000** from the **Solutions to use** list.

3 Select the **Keep current plot** check box.

4 Go to the **Line/Extrusion** page.

5 Select **Convection and Diffusion (chcd)>Concentration, c_CH4** from the **Predefined quantities** list.

6 Enter the following parameters in the **Cross-section line data** area:

EDIT FIELD	VALUE
x0	`0.4`
y0	`0.05`
x1	`0.8`
y1	`0.05`

7 Click **Apply**.

8 Select **Convection and Diffusion (chcd)>Concentration, c_H2** from the **Predefined quantities** list.

9 Click **OK**.

In the last simulation of this example, look at how the flow is affected by the deposition of soot in the porous bed.

1 From the **Solve** menu select **Solver Manager**.

2 On the **Initial Value** page click the **Store Solution** button.

3 In the **Store Solution** window, click **OK** to store all solutions.

4 Click the **Stored solution** option button in the **Values of variables not solved for and linearization point** area.

5 Select **All** from the **Solution at time** list.

6 On to the **Solve For** page, select **Incompressible Navier-Stokes (chns)** in the **Solve for variables** tree.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar.

To plot the permeability in the porous bed as a function of time follow these steps:

1 From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box.

2 On the **General** page, press Ctrl+A and click the **Solutions to use** list.

3 Select **New figure** from the **Plot in** list.

4 Go to the **Line/Extrusion** page.

5 Type `kappa` in the **Expression** edit field.

6 Click **OK**.

7 In the **Figure** window, click the **y log** button.

Finally, plot the reactor pressure after 1000 seconds.

1 From the **Postprocessing** menu open the **Plot Parameters** dialog box.

2 Go to the **General** page and select **1000** from the **Solutions at time** list.

3 Clear the **Arrow** check box.

4 Go to the **Surface** page.

5 Select **Incompressible Navier-Stokes (chns)>Pressure** from the **Predefined quantities** list.

6 Click **OK**.

9

Electrochemical Cells and Electrochemical Engineering

This chapter contains examples of mass transport and balances coupled to momentum transport and electric fields, where the systems are affected by electrochemical reaction kinetics. COMSOL Multiphysics is well suited for these types of processes for two reasons:

- *Its ability to model multiphysics applications easily and quickly.* Often you need to model mass transport to a description of the electric potential field and sometimes fluid flow, both in free and porous media. Other models might also require energy transport. The reaction kinetics are often functions of concentration (mass transport), temperature (energy transport), pressure (momentum transport), and electric potential (Ohm's law).
- *Its ability to handle equation-based modeling.* Electrochemical kinetics involve arduous equations that you can quickly enter into COMSOL Multiphysics. Furthermore, these systems often include large aspect ratios so the ability to quickly add scaling and corrections to diffusion coefficients and other material properties becomes important.

Current Distribution in a Chlor-Alkali Membrane Cell

Introduction

The chlor-alkali membrane process is one of the largest processes in industrial electrolysis with production of roughly 40 million metric tons of both chlorine and caustic soda per year (Ref. 1). Chlorine's largest use is in the production of vinyl chloride monomer, which in turn is used for the production of poly vinyl chloride (PVC). Among the applications of PVC are as electrical insulator in cables and as a material for pipes, carpets, raincoats, and many other products. The production of chlorine implies a simultaneous production of caustic soda (alkali), which is widely used in the chemical industry for alkalization and neutralization of acidic streams. Caustic soda is also used in alkaline batteries.

The traditional process for manufacturing chlorine and caustic soda is the mercury-cell process. This technology has been partly replaced by the diaphragm process, and in later years the membrane process has been the dominating process in retrofits and for new plants. The purpose of the diaphragm or membrane is to separate the products chlorine and caustic soda, which otherwise would react to produce hypochlorite and hydrochloric acid. Chlorine and caustic soda are produced at the anode and cathode, respectively. Figure 9-1 shows a diagram of the process.

Current density in membrane-cell technology has increased dramatically during the last decade as the membranes themselves have improved. This results in lower investment costs for greater production. However, the increase in current density implies an increase in power consumption if nothing is done to dampen the voltage increase. Advances in cell design by increased internal convection, decreased ohmic losses, and better membranes have allowed for large increases in current density with small increases in cell voltage. One of the important parameters in the design of modern membrane cells is the current-density distribution on the electrode surfaces. It is important, from the viewpoint of catalyst lifetime and minimization of losses, that the current density on the electrode frontal surfaces is as uniform as possible.

This example describes the current-density distribution in a realistic structure for the anodes and cathodes in a membrane cell. This discussion limits the model to one unit cell of the entire cell. This unit cell appears on the right side in Figure 9-1.

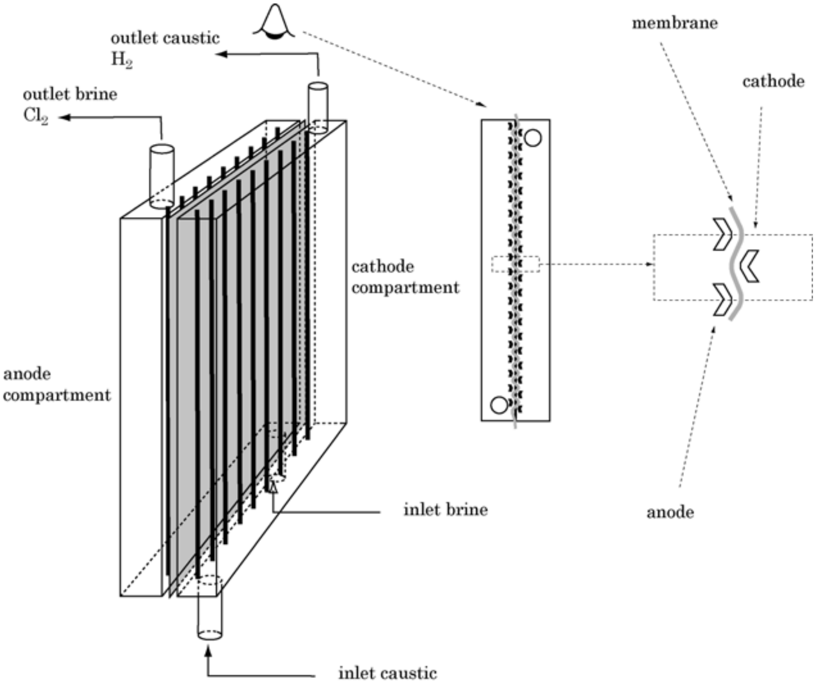


Figure 9-1: Drawing of the unit cell.

The anode and cathode ribs are separated by the membrane, which is a cation-selective membrane. It is forced to adapt its shape to fit within the inter-electrode distance. The membrane prevents mixing between brine and chlorine on the anode side with the caustic soda and hydrogen on the cathode side.

A detailed description of the process of chlor-alkali electrolysis is available in Ref. 1.

Model Definition

This example models the current and potential distribution in a unit cell in the membrane cell sketched in Figure 9-1. This model is a secondary current-distribution model (see Ref. 2), which implies that you take into account the dependence of the electron transfer on the local potential, and that you assume constant composition in the subdomains. The electron transfer reactions at the anode and cathode surfaces are:

$$\begin{aligned} &2\mathrm{Cl}^- = \mathrm{Cl}_2(g) + 2e^- && \text{at the anode} \\ &2\mathrm{H}_2\mathrm{O} + 2e^- = 2\mathrm{OH}^- + \mathrm{H}_2(g) && \text{at the cathode} \end{aligned} \qquad (9\text{-}1)$$

The domain in the model is half of the unit cell shown in Figure 9-1, as explained in Figure 9-2.

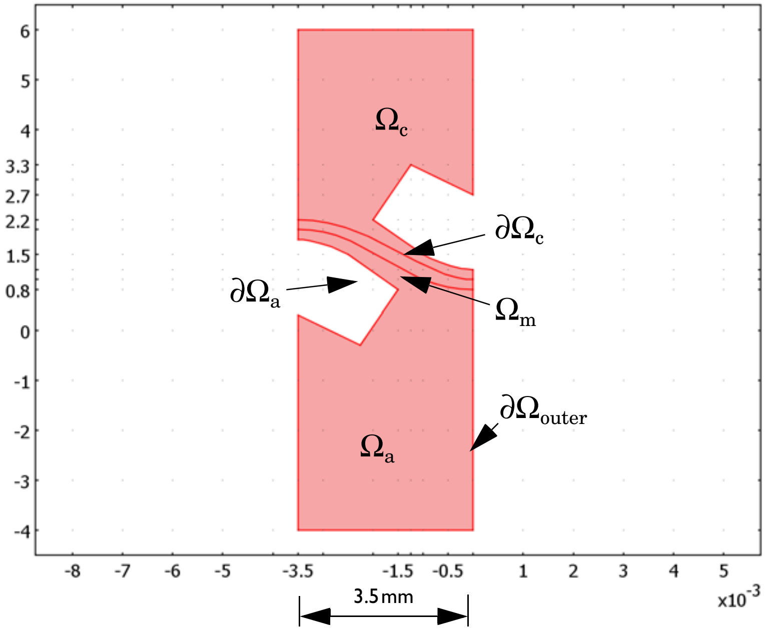


Figure 9-2: The modeling geometry with subdomain and boundary labels.

The chemical reactions show that there is gas evolution in both the anodic and cathodic compartments, creating a vigorous internal convection in the respective compartments. This makes it possible to simplify the model by neglecting the concentration gradients in the anolyte and catholyte. The simplification implies that the transport of ionic current inside the cell takes place exclusively through migration, that is, the electric field induces a flux of ions. For this reason you do not need to model the complex problem of internal free convection of the two-phase flow in order to get an estimation of the current-density distribution in the cell.

The equation that gives the transport of charged species in the electrolyte is

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_i F c_i \nabla \phi + c_i \mathbf{u} \tag{9-2}$$

where $\mathbf{N}_i$ denotes the transport vector (mol/(m^2·s)), c_i denotes the concentration in the electrolyte (mol/m^3), z_i represents the charge number for the ionic species, u_i indicates the mobility of the charged species (mol·m^2/(J·s)), F is Faraday's constant (C/mol), ϕ equals the potential in the electrolyte (V), and $\mathbf{u}$ is the velocity (m/s). If you neglect transport by diffusion in the electrolyte, the result is

$$\mathbf{N}_i = -z_i u_i F c_i \nabla \phi + c_i \mathbf{u} . \tag{9-3}$$

You can obtain the current-density vector from the transport of charged species through Faraday's law:

$$\mathbf{i} = -F \sum z_i \mathbf{N}_i . \tag{9-4}$$

In an electrochemical system, the potential gradients are fairly moderate, which implies that no separation of charges takes place in the electrolyte. This means that the electroneutrality condition is valid in the bulk of the electrolyte:

$$\sum z_i c_i = 0 . \tag{9-5}$$

Combining Equation 9-5 with Equation 9-3 and Equation 9-4 leads to

$$\mathbf{i} = -F \sum -z_i^2 u_i F c_i \nabla \phi , \tag{9-6}$$

which you can rewrite to get Ohm's law for electrolytes

$$\mathbf{i} = -\kappa \nabla \phi \tag{9-7}$$

where κ is the conductivity of the electrolyte (S/m). You can now set up a balance of current in the three subdomains at steady state:

$$\nabla \cdot \mathbf{i} = 0 . \tag{9-8}$$

This gives for the three subdomains

$$\begin{aligned} \nabla \cdot (-\kappa_\mathrm{a} \nabla \phi) &= 0 \quad \text{in} \ \ \Omega_\mathrm{a} \\ \nabla \cdot (-\kappa_\mathrm{m} \nabla \phi) &= 0 \quad \text{in} \ \ \Omega_\mathrm{m} \\ \nabla \cdot (-\kappa_\mathrm{c} \nabla \phi) &= 0 \quad \text{in} \ \ \Omega_\mathrm{c} \end{aligned} \tag{9-9}$$

The indices denote the anode, the membrane, and the cathode, respectively. You solve these equations with the proper boundary conditions. The anode reaction is very fast, and small changes in potential provide large changes in current density. This implies that you can assume a constant potential at the anode's surface that gives an error in potential of approximately 20 mV at that surface (Ref. 3).

For the cathodic reaction, you must account for the potential distribution around the electrode surface to get a proper current-density distribution. From the earlier discussion you can formulate the following boundary conditions:

$$\begin{aligned} &\phi = \phi_{\mathrm{a}} && \text{at } \partial\Omega_{\mathrm{a}} \\ &\mathbf{i}\cdot\mathbf{n} = -i_0 \exp\left(\frac{\alpha F}{R_{\mathrm{g}}T}\phi\right) && \text{at } \partial\Omega_{\mathrm{c}} \\ &\mathbf{i}\cdot\mathbf{n} = 0 && \text{at } \partial\Omega_{\mathrm{outer}} \end{aligned} \tag{9-10}$$

Here i_0 denotes the exchange current density (A/m^2) for the cathodic reaction, α represents the transfer coefficient, R_{g} equals the gas constant (J/(mol·K)), and T is the temperature (K). The last equation implies that you have no current flow out of the domain at the outer walls of the unit cell.

Now solve the problem for the potential in the electrolyte and the current distribution in the electrolyte and at the electrode surfaces.

Results

Figure 9-3 shows the potential in the anode and cathode compartments as well as in the membrane electrolyte. From this plot note that the largest ohmic losses arise in the membrane, as expected from its low conductivity.

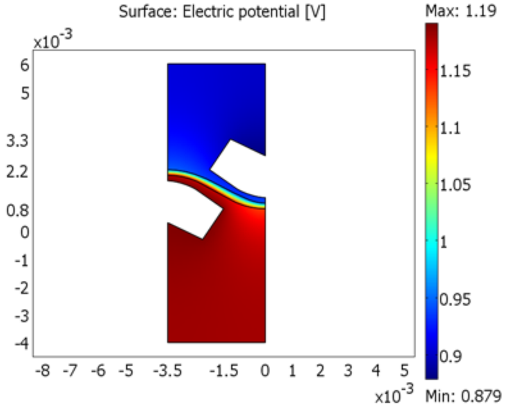


Figure 9-3: Potential profile in the three subdomains.

An arrow plot of the current-density vector shows how the distribution is more uniform on the cathode than on the anode surface.

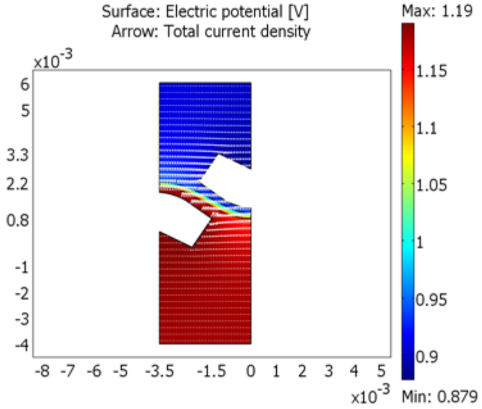


Figure 9-4: Current-density vectors in the three subdomains.

The modulus of the current-density vector illustrates “hot spots” in the electrolyte where the current density is large. These hot spots arise at the electrode edges where catalyst can be lost due to accelerated wear.

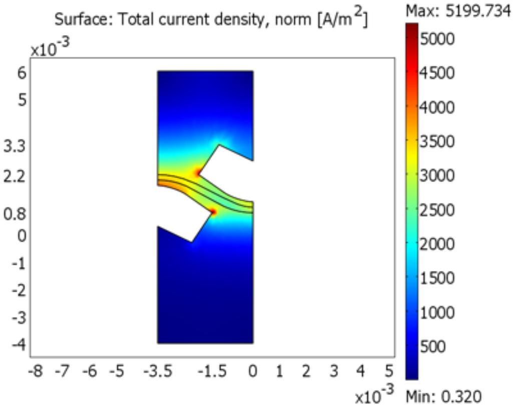


Figure 9-5: Current density magnitude.

References

1. H. S. Burney, “Past Present and Future of the Chlor-Alkali Industry,” *Chlor-Alkali and Chlorate Technology: R.B. Macmullin Memorial Symposium*, Proc Electrochemical Society, vol. 99-21, 1999.

2. J. S. Newman, *Electrochemical Systems*, 2nd ed., Prentice Hall, 1991.

3. P. Bosander, P. Byrne, E. Fontes, and O. Parhammar, “Current Distribution on a Membrane Cell Anode,” *Chlor-Alkali and Chlorate Technology: R.B. Macmullin Memorial Symposium*, Proc Electrochemical Society, vol. 99-21, 1999.

Model Library path: `Chemical_Engineering_Module/Electrochemical_Engineering/chlor_alkali`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the list of application modes select **COMSOL Multiphysics> Electromagnetics>Conductive Media DC**.

3 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Axes/Grid Settings**.

2 Enter the following settings; when done, click **OK**.

AXIS		GRID	
x min	`-4e-3`	x spacing	`1e-3`
x max	`1e-3`	Extra x	`-3.5e-3 -1.5e-3 -1.25e-3 -0.5e-3`
y min	`-4.5e-3`	y spacing	`1e-3`
y max	`6.5e-3`	Extra y	`0.8e-3 1.2e-3 1.5e-3 2.2e-3 2.7e-3 3.3e-3`

3 From the **Options** menu, select **Constants**.

4 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`K_a`	`50[S/m]`	`Conductivity, anode`
`K_c`	`100[S/m]`	`Conductivity, cathode`
`K_m`	`3[S/m]`	`Conductivity, membrane`
`phi0`	`1.19[V]`	`Anode potential`
`i0`	`1[mA/m]`	`Exchange current density`
`alpha`	`0.5`	`Transfer coefficient`
`F`	`96485[C/mol]`	`Faraday's constant`
`Rg`	`8.314[J/(mol*K)]`	`Ideal gas constant`
`T`	`90[degC]`	`Temperature`

GEOMETRY MODELING

1 Click the **3rd Degree Bézier Curve** button on the Draw toolbar.

2 Draw a Bézier curve by clicking on the points (–0.0035, 0.0022), (–0.002, 0.0022), (–0.0015, 0.001), and (0, 0.001).

3 Continue by clicking the **Line** button and drawing a line between the points (0, 0.001) and (0, 0.0008).

4 Draw a second **3rd Degree Bézier Curve** by clicking on the points (0, 0.0008), (–0.0015, 0.0008), (–0.002, 0.002), and (–0.0035, 0.002).

5 Right-click to create a solid object, CO1.

6 Double-click on the solid object to open the **Object Properties** dialog box.

7 From the **Curve selection** list, select **4**. Replace the value on the third row of the **x** column to `-0.0010`.

8 Click **OK**.

At this stage you have the membrane geometry. Continue by drawing the cathode:

1 Click the **2nd Degree Bézier Curve** button on the Draw toolbar.

2 Draw an arc by clicking on the points (0, 0.0012), (–0.0005, 0.0012), and (–0.001, 0.0015).

3 Continue by clicking the **Line** button and drawing lines between the points (–0.001, 0.0015), (–0.002, 0.0022), (–0.00125, 0.0033), and (0, 0.0027).

4 Right-click to create a solid object, CO2.

You have now created the cathode; use this object to create the anode:

1 Select the solid object CO2 and from the **Edit** menu select **Copy**.

2 Select **Edit>Paste**. Click **OK**.

3 Rotate the solid object CO3 by clicking the **Rotate** button on the Draw toolbar. In the resulting dialog box, enter `180` in the **Rotation angle** edit field, `-0.00175` in the **x Center point** edit field, and `0.0015` in the **y Center point** edit field.

4 Click **OK**.

5 Draw a rectangle **R1** with lower left corner at (-0.0035, -0.004) and upper right corner at (0, 0.006) (width=0.0035, height= 0.01).

6 In the **Draw** menu, select **Create Composite Object** and type `R1+CO1-CO2-CO3` in the **Set formula** edit field.

7 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Enter PDE coefficients for each Subdomain according to the following table:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2	SUBDOMAIN 3
σ	`K_a`	`K_m`	`K_c`

3 Click the **Init** tab so you can specify initial conditions.

4 Specify the initial conditions in the respective subdomains according to the following table:

SETTING	SUBDOMAIN 1	SUBDOMAIN 2	SUBDOMAIN 3
$V(t_0)$	`phi0`	`0.85*phi0`	`0.77*phi0`

This helps the solver reach convergence because the nonlinear solver uses the initial conditions as a first guess.

5 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary coefficients according to the following table:

SETTINGS	BOUNDARIES 3, 8, 9, 17	BOUNDARIES 10–12, 18	BOUNDARIES 1, 2, 4–7, 13–16
Boundary condition	`Electric potential`	`Inward current flow`	`Electric insulation`
V_0	`phi0`	`0`	
J_n		`-i0*exp(V*alpha*F/(Rg*T))`	

3 Click **OK**.

MESH GENERATION

Initialize the mesh by clicking the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 9-4, perform the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Arrow** page, select the **Arrow plot** check box.

3 On the **Subdomain Data** page, verify that the selection in the **Predefined quantities** list is **Conductive Media DC (dc)>Total current density**.

4 Click the **Color** button. Select white as the arrow color, then click **OK**.

5 In the **Arrow positioning** area, type 40 in the **Number of points** edit fields for **x points** and **y points**.

6 In the **Arrow parameters** area, clear the **Auto** check box for **Scale factor** and type `1.5` in the associated edit field.

7 Click **Apply** to generate the plot.

To reproduce the plot in Figure 9-5, proceed as follows:

8 Still on the **Arrow** page, clear the **Arrow plot** check box.

9 Click the **Surface** tab.

10 On the **Subdomain Data** page, select **Conductive Media DC (dc)>Total current density, norm** from the **Predefined quantities** list.

11 Click **OK**.

Fuel Cell Cathode

Introduction

The development of fuel cells has accelerated during the last decade. The field of fuel cells for traction applications has experienced the largest boost in development due to efforts by car manufacturers. Despite funding being more limited for stationary applications, those types of fuel cells have also gained from the general development and have proven to give excellent performance in small-scale applications.

A fuel cell is a continuous electrochemical reactor that converts chemical energy to electric energy. It does so by physically separating the oxidation of hydrogen and reduction of oxygen at separate electrodes, the anode and cathode. Separation occurs through an ion-conducting electrolyte.

The fuel cell presented in this example is a high-temperature model for stationary applications. Fuel cells are named after their electrolyte medium, and this case deals with the molten carbonate fuel cell (MCFC). This cell operates at 650 °C where the fuel, which can be either hydrogen or natural gas, is oxidized at the anode. Oxygen is used as the oxidant, being reduced at the cathode together with carbon dioxide.

The cathode is the electrode that gives the largest contribution to energy losses in the cell, that is, it has the largest overvoltage. The overvoltage consists of ohmic overvoltages in the electrolyte and catalyst, activation overvoltage for the electron transfer reaction, and concentration overvoltage due to mass transfer resistance in the porous electrode.

This example demonstrates the applicability of multiphysics analysis in limiting the definition of variables to certain subdomains. You solve a model for the porous oxygen reducing cathode, in the fuel cell, and the electrolyte between the anode and cathode. The electrolyte is defined in the porous electrode and in the free electrolyte, while the solid phase is present only in the porous electrode subdomain.

The potential difference between the liquid and solid phases is proportional to the distribution of the electron transfer reaction in the electrode, the property under study.

Model Definition

The porous fuel cell cathode consists of three different phases: the solid catalyst, the electrolyte that transfers into the porous phase through the action of capillary forces, and the gas phase in the large pores of the electrode (Figure 9-6). This exercise individually treats these three phases as homogeneous, defined over the whole electrode. Furthermore, the liquid phase is defined in the free electrolyte between the anode and cathode.

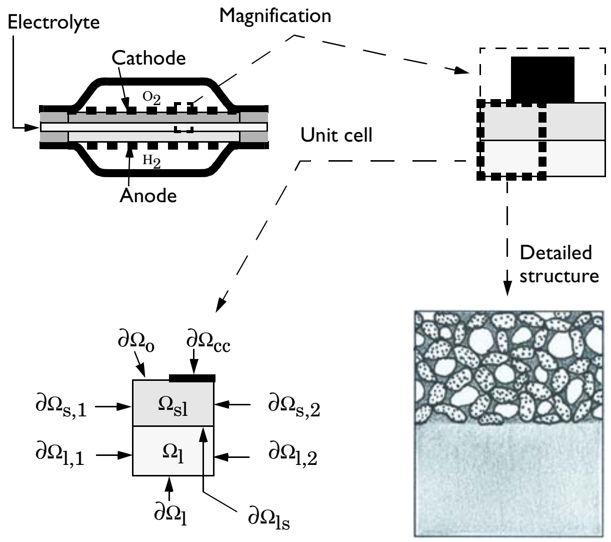


Figure 9-6: Depiction of the unit cell model geometry and labels from the original cell design of an MCFC. This exercise looks at a half-cell that is made up of an electrolyte and an agglomerate structure for the cathode.

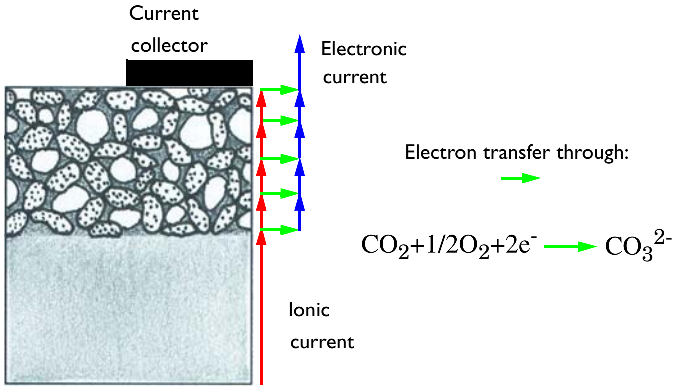


Figure 9-7: Process for electric current transport. Ionic current transforms to electron current gradually through the thickness of the cathode.

The electron transfer reaction, shown in Figure 9-7, transfers the current from ionic conduction in the electrolyte to electronic conduction in the solid catalyst. The solid catalyst makes electronic contact with the current collector, which is the perforated plate on the top of the cathode. The perforations are required to allow gas to be supplied to the electrode.

The catalyst agglomerates are sketched as dotted particles in Figure 9-7, the electrolyte is shaded gray, while the gas-filled macropores are white. Oxygen must first dissolve into the electrolyte in the porous cathode to further react on the catalyst particles that make up the agglomerates.

You can see that there is a mass-transfer resistance in the electrolyte surrounding as well as inside the catalyst agglomerates. These agglomerates consist of tightly packed smaller catalyst particles with electrolyte in the remaining space between them. The mass-transport resistance is considered in the homogenization of the system by a function that is linearly dependent on the oxygen concentration in the gas phase. This function has previously been found to give good approximations of mass-transfer resistance in agglomerates contained in the cathode (Ref. 1).

Assume that gas in the porous electrode is transported by diffusion, and that current is conducted through the migration of ions in the molten carbonate electrolyte and electronic conduction in the catalyst. The model is based on a mass transport for oxygen in the gas phase and charge balances in the solid-catalyst and liquid-electrolyte phases.

Furthermore, by assuming that the concentration and potential gradients through the depth of the cell are small in comparison with the local gradients, you can state that symmetry is obtained perpendicular to the page in the previous figure. This assumption simplifies the problem from a 3D to a 2D model.

The model equations in the subdomains are:

$$\begin{aligned}
&\nabla \cdot (-D_{\mathrm{eff}} \nabla c) + k_{\mathrm{o}} c(\phi_{\mathrm{s}} - \phi_{\mathrm{l}}) = 0 && \text{in } \Omega_{\mathrm{sl}} \\
&\nabla \cdot (-\kappa_{\mathrm{s,\,eff}} \nabla \phi_{\mathrm{s}}) + k c(\phi_{\mathrm{s}} - \phi_{\mathrm{l}}) = 0 && \text{in } \Omega_{\mathrm{sl}} \\
&\nabla \cdot (-\kappa_{\mathrm{l,\,eff}} \nabla \phi_{\mathrm{l}}) - k c(\phi_{\mathrm{s}} - \phi_{\mathrm{l}}) = 0 && \text{in } \Omega_{\mathrm{sl}} \\
&\nabla \cdot (-\kappa_{\mathrm{l,\,free}} \nabla \phi_{\mathrm{l}}) = 0 && \text{in } \Omega_{\mathrm{l}}
\end{aligned} \qquad (9\text{-}11)$$

In these equations, D_{eff} denotes the effective diffusion coefficient in the gas phase inside the porous electrode (m^2/s), c equals the concentration in the gas inside the electrode ($\mathrm{mol/m}^3$), and k is the effective exchange current density (S/mol). The potential in the catalyst is denoted by ϕ_{s} (V), while in the liquid phase it is denoted by

ϕ_l . The effective conductivities are denoted by $\kappa_{s,\mathrm{eff}}$ and $\kappa_{l,\mathrm{eff}}$ in the catalyst and liquid phases (S/m), respectively. The conductivity in the free electrolyte is denoted by $\kappa_{\mathrm{l,free}}$. Finally, $k_0 = k/(2F)$, where F is Faraday's constant (96,485 C/mol). All parameters are given in SI units. Overall, you now have a system of four coupled equations to solve in the domain.

To obtain the boundary conditions required to solve this problem, assume symmetry for the lateral boundaries of the unit cell, that is, assume that the solution is identical for any unit cell of the cathode.

$$\begin{aligned}
(-D_{\mathrm{eff}}\nabla c)\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{s},1} \text{ and } \partial\Omega_{\mathrm{s},2}\\
(-\kappa_{\mathrm{s,eff}}\nabla\phi_{\mathrm{s}})\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{s},1} \text{ and } \partial\Omega_{\mathrm{s},2}\\
(-\kappa_{\mathrm{l,eff}}\nabla\phi_{\mathrm{l}})\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{s},1} \text{ and } \partial\Omega_{\mathrm{s},2}
\end{aligned} \tag{9-12}$$

The only defined variable in the free electrolyte is the potential in the liquid phase:

$$(-\kappa_{\mathrm{l,free}}\nabla\phi_{\mathrm{l}})\cdot\mathbf{n} = 0 \qquad \text{at } \partial\Omega_{\mathrm{l},1} \text{ and } \partial\Omega_{\mathrm{l},2}\,.$$

At the position of the perforation in the collector plate, assume current is insulated for transferring from the catalyst or liquid phases. Furthermore, assume that the concentration of oxygen in the gas stream is known. This gives the following boundary conditions:

$$\begin{aligned}
c &= c_0 \quad \text{at } \partial\Omega_{\mathrm{o}}\\
(-\kappa_{\mathrm{s,eff}}\nabla\phi_{\mathrm{s}})\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{o}}\\
(-\kappa_{\mathrm{l,eff}}\nabla\phi_{\mathrm{l}})\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{o}}
\end{aligned} \tag{9-13}$$

Further, gas is unable to be transported to or from the electrode at the position of the current collector:

$$(-D_{\mathrm{eff}}\nabla c)\cdot\mathbf{n} = 0 \qquad \text{at } \partial\Omega_{\mathrm{cc}}\,. \tag{9-14}$$

At the position of the current collector, you can arbitrarily set the potential in the solid catalyst to zero (because potential is relative). Furthermore, you know that no current is transferred from the liquid phase to the current collector because a catalyst is needed for this to happen. Therefore

$$\begin{aligned}
\phi_{\mathrm{s}} &= 0 \quad \text{at } \partial\Omega_{\mathrm{cc}}\\
(-\kappa_{\mathrm{l,eff}}\nabla\phi_{\mathrm{l}})\cdot\mathbf{n} &= 0 \quad \text{at } \partial\Omega_{\mathrm{cc}}
\end{aligned} \tag{9-15}$$

Next assume that the potential is known for the boundary facing the anode, which means that the total overvoltage is given at the position of this boundary. Therefore, total overpotential comes from the difference between the potentials of the current collector and the liquid phase at this boundary,

$$\phi_l = \phi_{l,o} \qquad \text{at } \partial\Omega_l. \tag{9-16}$$

In addition, you need the boundary conditions for the concentration of oxygen in the gas phase and potential in the solid catalyst. The model neglects the transport of oxygen from the gas phase to the electrolyte. Furthermore, assume that the transport of current from the catalyst to the free electrolyte is negligible because this direct contact surface is minimal:

$$\begin{gathered}(-D_{\text{eff}}\nabla c)\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{ls} \\ (-\kappa_{s,\text{eff}}\nabla\phi_s)\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{ls}\end{gathered} \tag{9-17}$$

Results

Figure 9-8 shows the electron-transfer reaction rate. The reaction rate is greater in the regions near the free electrolyte and the current collector. The low effective electrolyte conductivity inside the porous electrode forces current to be transferred from the electrolyte to the catalyst phase at the electrode's lower boundary. Furthermore, the relatively low conductivity of the solid phase favors reactions taking place on the electrode's right side, where the current collector is positioned. The oxygen concentration is fairly uniform and does not affect the reaction-rate distribution. The average current density is approximately 1600 A/m^2.

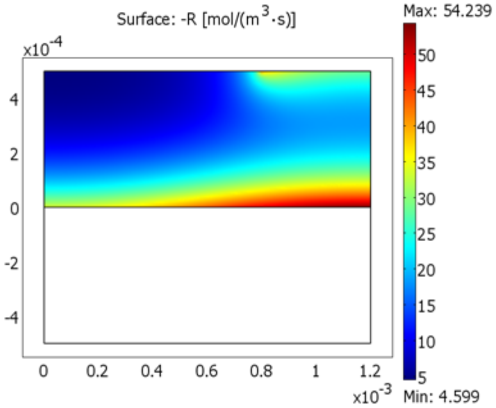


Figure 9-8: Electron-transfer reaction-rate distribution.

Figure 9-9 shows the potential distribution in the electrolyte. Note the large difference in conductivity between the electrolyte in the porous electrode and the free electrolyte due to the large difference in the potential gradient in the two subdomains.

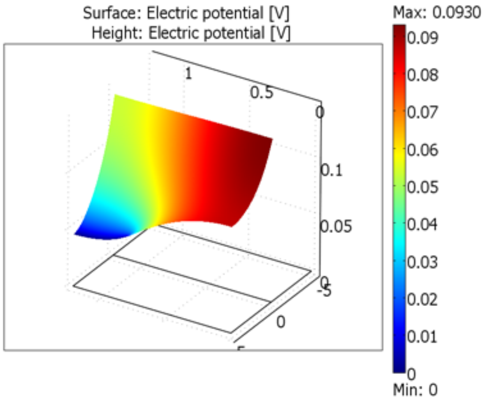


Figure 9-9: Ionic potential distribution in the fluid electrolyte.

Reference

1. E. Fontes, C. Lagergren, G. Lindbergh, and D. Simonsson, “Influence of Gas Phase Mass Transfer Limitations on Molten Carbonate Fuel Cell Cathodes,” *Jour. Applied Electrochemistry*, vol. 27, pp. 1149–1156, 1997.

Model Library path:

`Chemical_Engineering_Module/Electrochemical_Engineering/mcfc`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. From the **Space dimension** list, select **2D**. Click the **Multiphysics** button.
3. From the list of application modes select **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**.
4. In the **Dependent variables** edit field, type `phi_e`, and in the **Application mode name** edit field, type `electrolyte`. Click **Add**.
5. Again select the **COMSOL Multiphysics>Electromagnetics>Conductive Media DC** application mode.
6. In the **Dependent variables** edit field, type `phi_c`, and in the **Application mode name** edit field, type `catalyst`. Click **Add**.
7. In the list of application modes select **Chemical Engineering Module>Mass Transport>Diffusion>Steady-state analysis**.
8. In the **Application mode name** edit field, type `oxygen`.
9. Click **Add**, then click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, select **Constants**.

2 Enter the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`kappa_c`	`20[S/m]`	`Effective conductivity, catalyst`
`kappa_e`	`5[S/m]`	`Effective conductivity, electrolyte in cathode`
`kappa_e_free`	`142[S/m]`	`Conductivity, free electrolyte`
`k`	`6.7e7[S/mol]`	`Effective exchange current density`
`D_eff`	`2.8e-5[m^2/s]`	`Effective oxygen diffusion coefficient, cathode`
`F`	`96485[C/mol]`	`Faraday's constant`
`k_o`	`k/(2*F)`	`Effective rate constant`
`phi_e0`	`0.15[V]`	`Electrolyte potential, electrolyte-anode interface`
`c0`	`1.98[mol/m^3]`	`Oxygen concentration, upper cathode boundary`

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar.

2 Enter properties according to the following table; when done, click **OK** to create the rectangle R1.

Size	Width	`1.2e-3`
	Height	`0.5e-3`
Position	Base	Corner
	x	`0`
	y	`0`

3 Click the **Zoom Extents** button on the Main toolbar.

4 By repeating Steps 1–2, create a second rectangle, R2, with the same properties except for the **y** position, which you set to `-0.5e-3`.

5 Click the **Zoom Extents** button on the Main toolbar.

6 Shift-click the **Point** button on the Draw toolbar.

7 In the **Coordinates** area of the **Point** dialog box, set **x** to `0.8e-3` and **y** to `0.5e-3`.

8 Click **OK**.

PHYSICS SETTINGS

Subdomain Expressions

1 From the **Options** menu, select **Expressions>Subdomain Expressions**.

2 Select Subdomain 2.

3 Enter the following expressions for the electron-transfer reaction rate and the electronic current density, respectively (the software automatically fills in the unit column):

NAME	EXPRESSION	UNIT
R	`k_o*c*(phi_c-phi_e)`	$mol/(m^3 \cdot s)$
Q	`k*c*(phi_c-phi_e)`	A/m^3

4 Click **OK**.

Subdomain Settings—Electrolyte Charge Balance

1 From the **Multiphysics** menu, select **1 Conductive Media DC (electrolyte)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Specify settings according to the following table; when done, click **OK**.

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
σ	`kappa_e_free`	`kappa_e`
Q_j	`0`	`Q`

Boundary Conditions—Electrolyte Charge Balance

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	ALL OTHERS
Type	Electric potential	Electric insulation
V_0	`phi_e0`	

Subdomain Settings—Catalyst Charge Balance

1 From the **Multiphysics** menu, select **2 Conductive Media DC (catalyst)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1. Clear the **Active in this subdomain** check box to deactivate the charge-balance equations for the catalyst in the electrolyte domain.

4 Select Subdomain 2.

5 Specify PDE properties according to the following table; when done, click **OK**.

PROPERTY	VALUE
σ	`kappa_c`
Q	`-Q`

Boundary Conditions—Catalyst Charge Balance

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 6	BOUNDARIES 3–5, 8
Type	Ground	Electric insulation

Subdomain Settings—Oxygen Mass Transport

1 From the **Multiphysics** menu, select **3 Diffusion (oxygen)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1. Clear the **Active in this subdomain** check box to deactivate the mass transport equation for oxygen in the electrolyte domain.

4 Select Subdomain 2.

5 Specify PDE properties according to the following table; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	`D_eff`
R	`R`

Boundary Conditions—Mass Transport

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 5	BOUNDARIES 3, 4, 6, 8
Type	Concentration	Insulation/Symmetry
c_0	`c0`	

MESH GENERATION

The model requires a fairly dense mesh. Click the **Refine Mesh** button on the Main toolbar to generate a refined mesh.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot of the reaction-rate distribution displayed in Figure 9-8 on page 546, follow these steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. Go to the **Surface** page.
3. Type `-R` in the **Expression** edit field on the **Surface Data** page, then click **Apply**.

   Finally, to visualize the electrolyte potential, as in Figure 9-9, do as follows:
4. On the **Surface Data** page, type `phi_c` in the **Expression** edit field.
5. Click the **Height Data** tab.
6. Select the **Height data** check box and type `phi_e` in the **Expression** edit field.
7. Click **OK**.

Electrochemical Treatment of Tumors

Introduction

The electrochemical treatment of tumors implies that diseased tissue is treated with direct current through the use of metallic electrodes inserted in the tumor. When tissue is electrolyzed, two competing reactions take place at the anode: oxygen evolution and chlorine production. The oxygen-evolution reaction also produces H^+ ions, which lower the pH close to the anode. It should be stressed that chlorine production also leads to lowered pH through the hydrolysis of chlorine. One effect of low pH is the permanent destruction of hemoglobin in the tissue, which results in destruction of tumor tissue.

$$\begin{aligned} 2\mathrm{Cl}^- &= \mathrm{Cl}_2(\mathrm{g}) + 2e^- && \text{at the anode} \\ 2\mathrm{H}_2\mathrm{O} &= 4\mathrm{H}^+ + \mathrm{O}_2(\mathrm{g}) + 4e^- && \text{at the anode} \end{aligned} \tag{9-18}$$

One challenge in developing this method of cancer treatment is in predicting the doses required for tumor destruction. One possible tool for dose planning is by modeling the reactions that take place close to the electrodes.

This example presents a first simple model for the development of dose-planning methods. More advanced models for dose planning, including secondary effects of chlorine, are found in Ref. 1, which also presents and solves models for the cathode.

Model Definition

This model uses the Nernst-Planck application mode to predict the transport and reaction in the electrolysis of tumor tissue in a liver. A needle electrode is placed in the tumor, and transport is assumed to take place radially to and from this electrode. Because you can assume rotational symmetry, the computational domain reduces to a line (r_a, r_r) where r_a is 1 mm and r_r is 6 cm (see Figure 9-10).

The species you consider in the model are the protons, chloride, and sodium. At the surface of the anode you account for the chlorine and oxygen evolution reactions; see Equation 9-18.

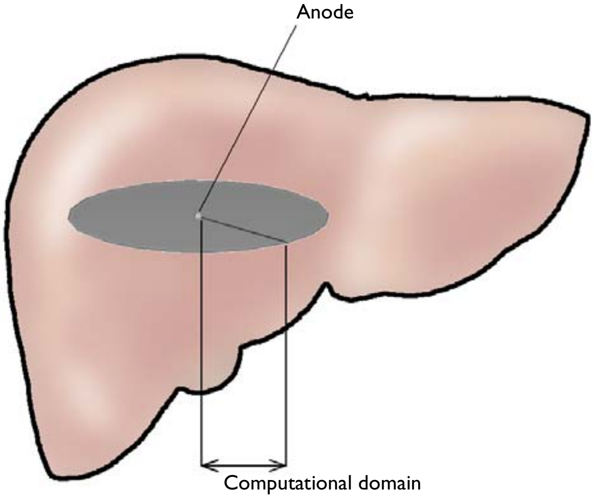


Figure 9-10: Diagram of the cylindrical modeling domain inside a tumor.

This simplified model considers only a 1D model of the transport between two points, that is, between the two electrodes. The material balance for the species i is given by

$$\frac{\partial c_i}{\partial t} = D_i \Delta c_i + z_i u_{\mathrm{m}i} F \nabla (c_i \nabla V) + R_i \tag{9-19}$$

where c_i is the concentration (mol/m^3), D_i give the diffusivities (m^2/s), z_i equals the charge, $u_{\mathrm{m}i}$ represents the mobility ((mol·m^2)/(J· s)), and R_i is the production term for species i (mol/(m^3·s)), F denotes Faraday's constant (C/mol), and V is the potential (V). The mobility, $u_{\mathrm{m}i}$, can be expressed in terms of D_i, R, and T as

$$u_{\mathrm{m}i} = \frac{D_i}{RT}. \tag{9-20}$$

The conservation of electric charge is obtained through the divergence of the current density:

$$\nabla \cdot \left(\sum_{i=1}^{N} z_i^2 F u_{\mathrm{m}i} c_i \nabla V \right) + \sum_{i=1}^{N} z_i D_i \Delta c_i = 0. \tag{9-21}$$

At the electrode surface ($r = r_a$) you specify the fluxes for the ionic species that are included in the electrode reactions, H^+ and Cl^-. For the inert ionic species, Na^+, the transport through the electrode surface equals zero. The expressions for molar fluxes at the boundary for the reacting species are

$$\mathbf{N}_i \cdot \mathbf{n} = \frac{\nu_{ij} j_j}{n_j F} \tag{9-22}$$

where $\mathbf{N}_i$ is the flux, ν_{ij} represents the stoichiometric coefficient for the ionic species i in reaction j, and n_j is the number of electrons in reaction j.

Introducing dimensionless pressure, $P = p/p_b$, and concentration, $C = c/c_b$, (where b denotes the reference concentration), you can express the current densities for the two reactions. For the oxygen evolution reaction it is

$$j_{\mathrm{I}} = j_{\mathrm{I},0} \left\{ e^{-\frac{F(V + E_{\mathrm{eq,I}c})}{2RT}} - (P_{\mathrm{O}_2})^{1/4} C_{\mathrm{H}^+} e^{\frac{F(V + E_{\mathrm{eq,I}})}{2RT}} \right\}: \tag{9-23}$$

where $j_{\mathrm{I}0,}$ is the exchange current density ($\mathrm{A/m^2}$) and $E_{\mathrm{eq,I}}$ is the standard electrode potential (V). The chlorine evolution reaction is given by the expression

$$j_{\mathrm{II}} = j_{\mathrm{II},0} \left\{ c_{\mathrm{Cl}^-} e^{-\frac{F(V + E_{\mathrm{eq,II}})}{2RT}} - (P_{\mathrm{Cl}_2})^{1/2} e^{\frac{F(V + E_{\mathrm{eq,II}})}{2RT}} \right\}. \tag{9-24}$$

Using the input values $n_{\mathrm{I}} = n_{\mathrm{I}} = 1$, $\nu_{\mathrm{H,I}} = 1$, and $\nu_{\mathrm{Cl,I}} = -1$, gives the fluxes at the electrode surface:

$$N_{\mathrm{H}} \cdot \mathbf{n} = \frac{j_{\mathrm{I}}}{F} \tag{9-25}$$

$$N_{\mathrm{Cl}} \cdot \mathbf{n} = -\frac{j_{\mathrm{II}}}{F}. \tag{9-26}$$

At the exterior boundary, assume the concentration is constant, $c_i = c_{i0}$, and set the potential to

$$V_0(t) = -\left(0.4977 + 0.2567 \cdot \ln\left(100 + \frac{t}{1\ \mathrm{s}}\right)\right)\ \mathrm{V} \tag{9-27}$$

where t denotes time.

The initial concentration is constant: $c_i = c_{i0}$. You obtain the initial potential profile from the solution of the domain equations and boundary conditions at $t = 0$, yielding

$$V(t=0) = V_{ra0} + \frac{j_{ra0} r_a}{\kappa_0} \log\frac{r_a}{r} \tag{9-28}$$

where V_{ra0} is the potential satisfying $j_{\mathrm{I}} + j_{\mathrm{II}} = j_0$ and κ_0 is the conductivity at $t = 0$.

The input data is listed in this table:

TABLE 9-1: INPUT DATA

PARAMETER	VALUE	DESCRIPTION
D_{Na}	$1.33 \cdot 10^{-9}\ \mathrm{m^2/s}$	Diffusion coefficient, Na^+
D_{H}	$9.31 \cdot 10^{-9}\ \mathrm{m^2/s}$	Diffusion coefficient, H^+
D_{Cl}	$2.03 \cdot 10^{-9}\ \mathrm{m^2/s}$	Diffusion coefficient, Cl^-
$c_{\mathrm{Na},0}$	0.16 mol/liter	Inlet concentration, Na^+
$c_{\mathrm{H},0}$	10^{-7} mol/liter	Inlet concentration, H^+
$c_{\mathrm{Cl},0}$	0.16 mol/liter	Inlet concentration, Cl^-
j_0	$100\ \mathrm{A/m^2}$	Initial current density
$j_{\mathrm{I},0}$	$10^{-6}\ \mathrm{A/m^2}$	Exchange current density, reaction I
$j_{\mathrm{II},0}$	$10\ \mathrm{A/m^2}$	Exchange current density, reaction II
$V_{ra,0}$	-1.4787 V	Initial anode potential
$E_{\mathrm{eq,I}}$	1.23 V	Equilibrium potential, reaction I
$E_{\mathrm{eq,II}}$	1.36 V	Equilibrium potential, reaction II
T	298 K	Temperature
p_{O2}	1 atm	
p_{Cl2}	1 atm	

Results

The plot in Figure 9-11 shows the pH for different time steps. You can see that values below pH 2 are reached after 2160 seconds. At this pH, tumor destruction starts to occur very rapidly according to the experimental and theoretical findings in Ref. 1.

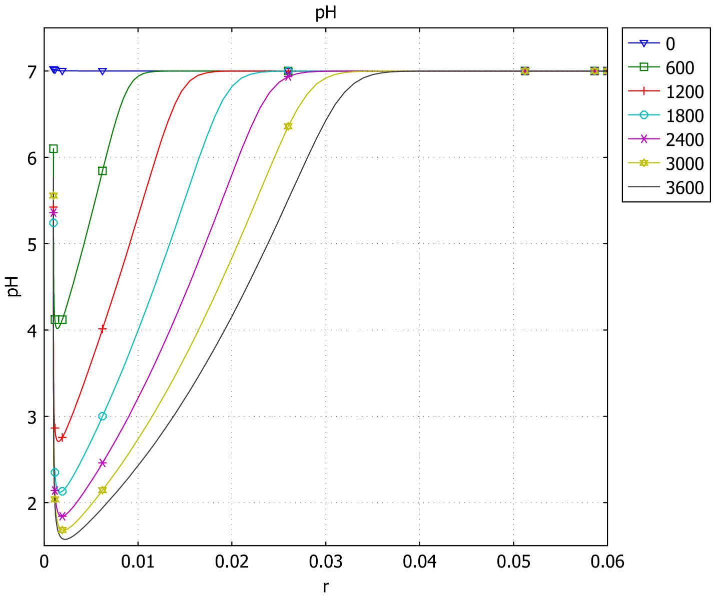


Figure 9-11: pH-profiles at different time steps during the treatment.

The corresponding H^+ profile in Figure 9-12 shows that the concentration maximum is not at the anode surface.

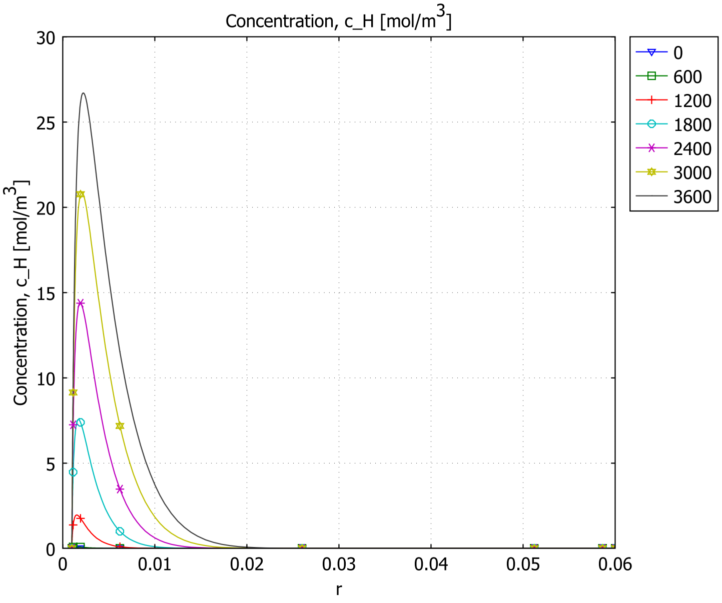


Figure 9-12: Proton concentration in the domain at different time steps.

This result arises because the current density is not constant over time. At high current densities, large amounts of protons are produced and this front moves inwards in the domain as the current density is lowered

The corresponding plot for chloride (Figure 9-13) shows a continuous decrease of chloride concentration close to the anode surface. This in turn decreases the production of chlorine and increases oxygen evolution.

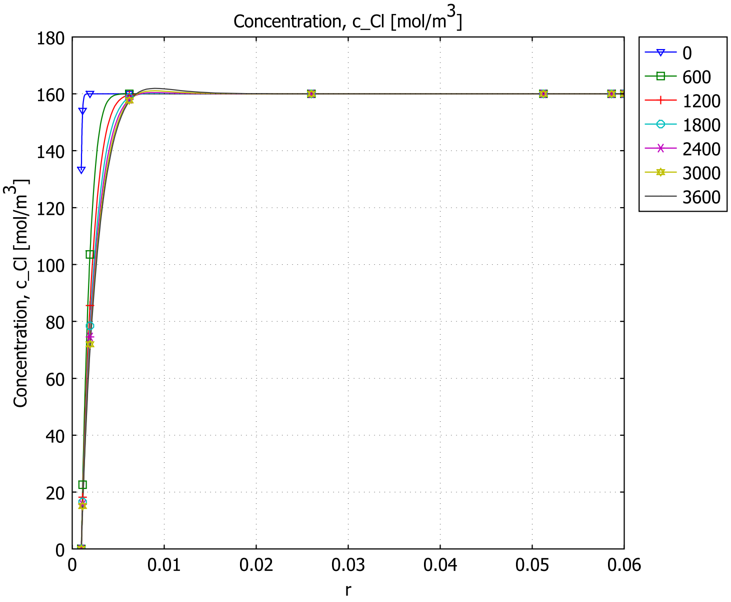


Figure 9-13: Chloride concentration at different time steps.

The current-density plot in Figure 9-14 shows that the total current decreases rapidly as the concentration overvoltage for chlorine formation increases, due to lowered chloride concentration at the anode surface. The potential is then increased, which results in an increase in total current through increased oxygen evolution.

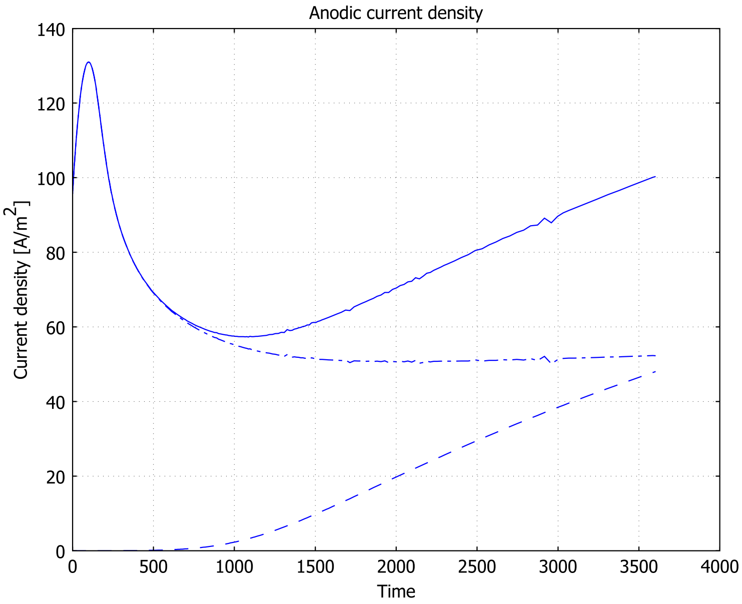


Figure 9-14: Total current density and current density for the competing reactions on the anode surface. Oxygen evolution is the lowest graph.

Reference

1. E. Nilsson, *Modelling of the Electrochemical Treatment of Tumors*, doctoral thesis, Dept. Chemical Engineering and Technology, Royal Inst. of Technology, Stockholm, Sweden, 2000.

Model Library path:

`Chemical_Engineering_Module/Electrochemical_Engineering/tumor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **Axial symmetry (1D)** from the **Space dimension** list.

3 Select the application mode **Chemical Engineering Module>Mass Transport>Nernst-Planck>Transient analysis**.

4 In the **Dependent variables** edit field, type `V c_Na c_H c_Cl`. Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**. Define the following constants:

NAME	EXPRESSION	DESCRIPTION
`r_a`	`1[mm]`	`Anode radius`
`D_Na`	`1.33e-9[m^2/s]`	`Diffusivity, Na`
`D_H`	`9.31e-9[m^2/s]`	`Diffusivity, H`
`D_Cl`	`2.03e-9[m^2/s]`	`Diffusivity, Cl`
`T`	`298[K]`	`Temperature`
`R`	`8.314[J/(mol*K)]`	`Gas constant`
`F`	`96485[C/mol]`	`Faraday's constant`
`u_Na`	`D_Na/(R*T)`	`Mobility, Na`
`u_H`	`D_H/(R*T)`	`Mobility, H`
`u_Cl`	`D_Cl/(R*T)`	`Mobility, Cl`
`c_Na0`	`0.16[mol/liter]`	`Initial concentration, Na`
`c_H0`	`1e-7[mol/liter]`	`Initial concentration, H`
`c_Cl0`	`0.16[mol/liter]`	`Initial concentration, Cl`
`z_Na`	`1`	`Charge number, Na`
`z_H`	`1`	`Charge number, H`
`z_Cl`	`-1`	`Charge number, Cl`
`j_tot0`	`100[A/m^2]`	`Initial total current density`
`j_I0`	`1e-6[A/m^2]`	`Exchange current density, reaction I`
`j_II0`	`10[A/m^2]`	`Exchange current density, reaction II`
`V_ra0`	`-1.4787[V]`	`Initial anode potential`
`E_eqI`	`1.23[V]`	`Equilibrium potential, reaction I`

NAME	EXPRESSION	DESCRIPTION
`E_eqII`	`1.36[V]`	`Equilibrium potential, reaction II`
`kappa0`	`F^2*(u_Na*c_Na0+u_H*c_H0+u_Cl*c_Cl0)`	`Initial Conductivity`

2 Click **OK**.

3 From the **Options** menu, select **Expressions>Scalar Expressions**.

4 Define the following variables (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`j_I`	`j_I0*(exp(-F*(V+E_eqI)/(2*R*T))-c_H/c_H0*exp(F*(V+E_eqI)/(2*R*T)))`	`Current exchange density, reaction I`
`j_II`	`j_II0*(c_Cl/c_Cl0*exp(-F*(V+E_eqII)/(2*R*T))-exp(F*(V+E_eqII)/(2*R*T)))`	`Current exchange density, reaction II`
`V0`	`-(0.4977+0.2567*log(100+t/1[s]))`	`Inlet potential`
`pH`	`-log10(c_H/1[mol/liter])`	`pH value in tissue`

GEOMETRY MODELING

1 Choose **Draw>Specify Objects>Line**.

2 In the **r** edit field, type `1e-3 6e-2`. Click **OK**.

3 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.

2 Select Subdomain 1. On the appropriate pages, set the subdomain properties according to this table:

PROPERTY	cNa	cH	cCl
D	`D_Na`	`D_H`	`D_Cl`
u_m	`u_Na`	`u_H`	`u_Cl`
z	`z_Na`	`z_H`	`z_Cl`

3 Click the **Init** tab. Set the initial conditions for the voltage profile and the concentrations as follows:

VARIABLE	VALUE
$V(t_0)$	`V_ra0+j_tot0*r_a*log(r_a/r)/kappa0`
$c\_H(t_0)$	`c_H0`
$c\_Cl(t_0)$	`c_Cl0`

4 On the **Element** page, select **Lagrange - Quartic** from the **Predefined elements** list.

5 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 On the pages **Current/Potential**, **cH**, and **cCl**, specify boundary conditions according to the following table:

BOUNDARY	**Current/Potential**		**c_H**		**c_Cl**	
1	Current inflow		Flux		Flux	
	i_0	`j_I+j_II`	N_0	`j_I/F`	N_0	`-j_II/F`
2	Potential		Concentration		Concentration	
	V_0	`V0`	c_0	`c_H0`	c_0	`c_Cl0`

3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Custom mesh size** button. On the **Global** page, set the **Maximum element size** to `5e-3`.

3 Click the **Boundary** tab.

4 Select Boundary 1. Type `1e-5` in the **Maximum element size** edit field.

5 Select Boundary 2. Type `1e-4` in the **Maximum element size** edit field.

6 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Times** edit field, type `0 3600`.

3 Set the **Relative tolerance** to `1e-5` and the **Absolute tolerance** to `1e-6`.

4 On the **Time Stepping** page, select **Time steps from solver** from the **Times to store in output** list. Click **OK**.

5 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

You can use the software's cross-section plotting features to plot the pH in the tissue surrounding the anode, as in Figure 9-11.

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 On the **General** page, select **Interpolated times** from the **Select via** list and type `0:600:3600` in the **Times** edit field.

3 Click the **Line/Extrusion** tab. Type `pH` in the **Expression** edit field to plot the pH value.

4 Click the **Line Settings** button. Select the **Legend** check box, then click **OK**.

5 Click **Apply** to generate the plot.

Similarly, you generate Figure 9-12 and Figure 9-13 by plotting the predefined quantities `c_H` and `c_Cl` instead of the pH expression.

To visualize the current contributions on the anode from the reactions (Figure 9-14), follow these steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 On the **General** page, select **Stored output times** from the **Select via** list. Now all output times in the **Solution at time** list should automatically be selected.

3 From the **Plot in** list, select **New Figure**.

4 Click the **Title/Axis** button. Type `Anodic current density` in the **Title** edit field and `Current density [A/m<sup>2</sup>]` in the **Second axis label** edit field. Click **OK**.

5 Select the **Keep current plot** check box.

6 Click the **Point** tab. Select Point 1.

7 First plot the total current density by typing `j_I+j_II` in the **Expression** edit field.

8 Click **Apply** to generate the first plot.

9 Change the **Expression** to `j_I`. Click the **Line Settings** button. From the **Line style** list, select **Dashed line**, then click **OK**.

10 Click **Apply** to generate the second graph.

11 Change the **Expression** to `j_II`. Click the **Line Settings** button. From the **Line style** list, select **Dash-dot line**, then click **OK**.

12 Click **OK** to close the **Domain Plot Parameters** window and generate the third graph.

Mass Transport and Electrochemical Reaction in a Fuel Cell Cathode

Introduction

One of the most important—and most difficult—parameters to model in a fuel cell is the mass transport through backing and reactive layers. Gas concentrations are often quite large and are significantly affected by the reactions that take place. This makes Fickian diffusion an inappropriate assumption for modeling the mass transport.

Figure 9-15 shows an example 3D geometry of a cathode from a fuel cell with perforated current collectors. It is often seen in self-breathing cathodes or in small experimental cells. Due to the perforation layout, a 3D model is needed in the study of the mass transport, current, and reaction distributions.

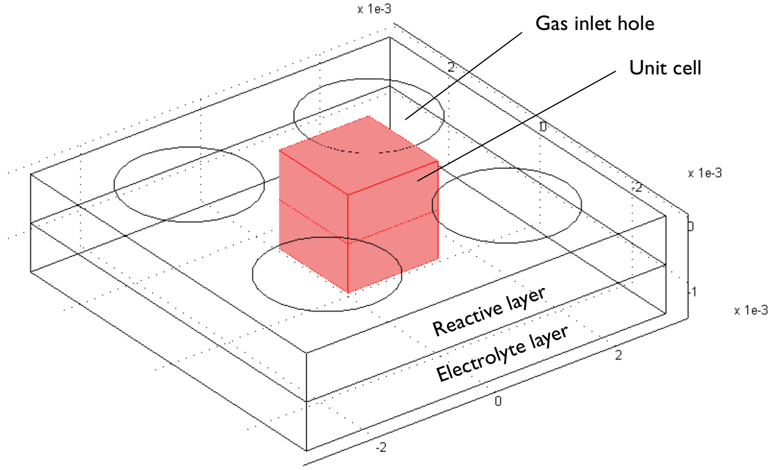


Figure 9-15: A fuel cell cathode with a perforated current collector.

This model investigates such a geometry and the mass transport that occurs through Maxwell-Stefan diffusivity. It couples this mass transport to a generic, Tafel-like electrochemical kinetics in the reaction term at a cathode.

Model Definition

Figure 9-16 shows details for a unit cell from Figure 9-15. The circular hole in the collector is where the gas enters the modeling domain, where the composition is known. The upper rectangular domain is the reaction-zone electrode. It is a porous structure that contains the feed-gas mixture, an electronically conducting material covered with an electrocatalyst, and an electrolyte. The lower domain corresponds to a free electrolyte ionically interconnecting the two electrodes of the fuel cell. No reaction takes place in this domain. Neither are there pores to allow gas to flow or material for electronic current—current is conducted ionically.

The reaction zone is 75 µm thick, as is the electrolyte layer. The unit cell is 1.5×1.5 mm in surface, and the gas inlet hole has a radius of 1.0 mm.

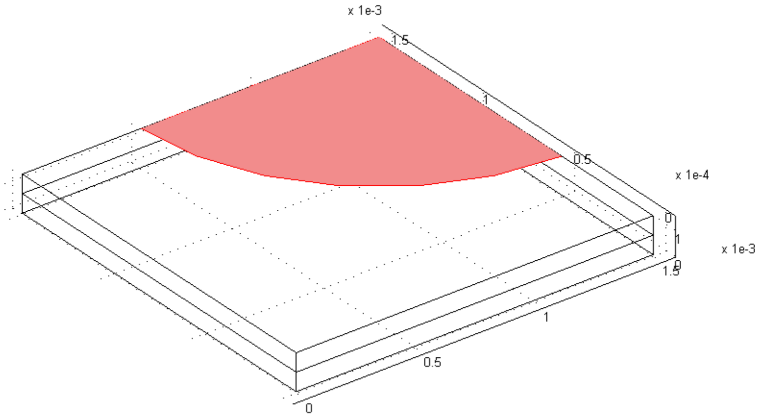


Figure 9-16: The modeled fuel cell cathode unit cell. The marked zone is the surface of the cathode that is open to the feed gas inlet, while the rest of the top surface sits flush against the current collector. The top modeling subdomain is the porous cathode, while the bottom subdomain is the free electrolyte.

The ionic current balance in the cathode is

$$-\nabla(-\kappa_{l,\,\mathrm{eff}}\nabla\phi_l) = -S_\mathrm{a}i_\mathrm{ct} \tag{9-29}$$

where $\kappa_{l,\mathrm{eff}}$ is the effective electrolyte conductivity (S/m), ϕ_l is the electrolyte potential (V), S_a is the surface area ($\mathrm{m}^2/\mathrm{m}^3$), and i_ct equals the local charge transfer current density ($\mathrm{A/m}^2$). The ionic current balance in the free electrolyte between the anode and cathode is

$$-\nabla(-\kappa_l \nabla\phi_l) = 0 \tag{9-30}$$

where κ_l is the conductivity of the free electrolyte (S/m). The electronic charge balance is defined only in the electrode subdomain and is given by the equation

$$-\nabla(-(\kappa_{s,\,\mathrm{eff}} \nabla\phi_s)) = S_{\mathrm{a}} i_{\mathrm{ct}} \tag{9-31}$$

where $\kappa_{s,\mathrm{eff}}$ is the effective conductivity in the solid phase (S/m), and ϕ_s is the solid phase potential (V).

The transport of masses are given by the Maxwell-Stefan equations for oxygen (Species 1) and water (Species 2) in the gas phase. They are defined only in the electrode subdomain. The final equation is the sum of all fluxes, which equals the convective term. This equation gives the mass balance for nitrogen (Species 3). The fluxes are given through

$$\mathbf{n}_i = \left\{ -\rho w_i \sum_{j=1}^{3} \frac{MD_{ij}}{M_j}\left(\nabla w_j + \frac{\tilde{w}_j}{M}\nabla M\right) + w_i \rho \mathbf{u} \right\} \tag{9-32}$$

where $\mathbf{n}_i$ denotes the mass flux of component i, ρ is the density of the mixture (kg/m^3), w_i is the mass fraction of species i, M and M_j are the mole masses of the mixture and species j (kg/mol), respectively, and $\mathbf{u}$ is the velocity (m/s). The material balance for oxygen is

$$-(\nabla \cdot \mathbf{n}_1) = -\frac{i_{\mathrm{ct}} S_a M_1}{4F}, \tag{9-33}$$

and for water vapor it is

$$-(\nabla \cdot \mathbf{n}_2) = 0, \tag{9-34}$$

again assuming that the air is saturated so that the reaction produces no water vapor. The total mass flux gives the velocity vector:

$$\mathbf{u} = \left(\sum_{i=1}^{3} \mathbf{n}_i\right)\left(\sum_{i=1}^{3} \rho_i\right)^{-1}. \tag{9-35}$$

The velocity vector is coupled to Darcy's law accordingly:

$$\mathbf{u} = -\frac{k_p}{\mu}\nabla p \tag{9-36}$$

where k_p is the permeability (m^2), μ is the viscosity (Pa·s), and p is the pressure (Pa). The continuity equation for the gas flow mixture is the sum of the continuity for the three involved species, which in two dimension yields

$$-\nabla\left(-\rho\frac{k_p}{\mu}\nabla p\right) = -\frac{i_{\mathrm{ct}}S_a M_1}{4F}\,. \tag{9-37}$$

The local charge transfer current density couples the current balances with the mass balances, according to

$$i_{\mathrm{ct}} = i_0\left\{\exp\left[\frac{0.5F(\phi_s - \phi_l - \Delta\phi_{\mathrm{eq}})}{RT}\right] - \frac{c_{\mathrm{O2}}}{c_{\mathrm{O2,ref}}}\exp\left[-\frac{0.5F(\phi_s - \phi_l - \Delta\phi_{\mathrm{eq}})}{RT}\right]\right\} \tag{9-38}$$

where $\Delta\phi_{\mathrm{eq}}$ is the equilibrium potential difference (V), F is Faraday's constant (As/mol), R is the gas constant (J/(mol·K)), T is the temperature (K), and c_{O2} is the concentration of oxygen (mol/m^3).

The boundary conditions for the ionic current balances are insulating at all boundaries:

$$-\mathbf{n}\cdot(-(\kappa_{l,\,\mathrm{eff}}\nabla\phi_l)) = 0 \tag{9-39}$$

except for the lowest boundary for the free electrolyte subdomain. The condition at this boundary sets the ionic potential:

$$\phi_l = \phi_{l,\,0}\,. \tag{9-40}$$

The boundaries for the electronic current balance are those that encompass the electrode subdomain. The boundary conditions are all insulating except for the current collector boundary where the potential is set:

$$\phi_s = V_{\mathrm{cell}}\,. \tag{9-41}$$

The boundary conditions for the material balances are also those that encompass the electrode subdomain and are all insulating except for the gas-channel boundary. The insulating condition gives

$$\mathbf{n}\cdot\mathbf{n}_i = 0 \tag{9-42}$$

while the condition at the gas-channel boundary are given by the composition of the inlet gas

$$w_i = w_{i,0}\,. \tag{9-43}$$

For the momentum transport through Darcy's law all boundaries are insulating:

$$\mathbf{n}\cdot\left(-\frac{k_p}{\mu}\nabla p\right) = 0 \tag{9-44}$$

except for the gas-channel boundary, where the pressure is set:

$$p = p_{\mathrm{atm}}\,. \tag{9-45}$$

The input data to the model appear in Table 9-2 except for the electrolyte conductivity in the free electrolyte domain, which you set to 5 S/m.

TABLE 9-2: MODEL PARAMETERS

i_0	S_a	T	V_{cell}	$\Delta\phi_{\mathrm{eq}}$	$\phi_{1,0}$	$k_{1,\mathrm{eff}}$	$k_{s,\mathrm{eff}}$	ε
As/mol	1/m	K	V	V	V	S/m	S/m	
10^{-3}	10^{9}	353	0	0	0.19	1	10^{3}	0.4
D_{12}	D_{23}	D_{13}	$w_{1,0}$	$w_{2,0}$	$w_{3,0}$	k_p	μ	p_{atm}
m^2/s	m^2/s	m^2/s				m^2	Pa·s	Pa
$2.75\cdot10^{-5}$	$3.5\cdot10^{-5}$	$3.5\cdot10^{-5}$	0.145	0.476	0.379	10^{-13}	10^{-5}	10^{5}

Results and Discussion

Figure 9-17 shows the oxygen concentration at a total potential drop over the modeled domain of 190 mV. The figure shows that concentration variations are small along the thickness of the cathode for this relatively small current density, while they are substantially larger along the electrode's width.

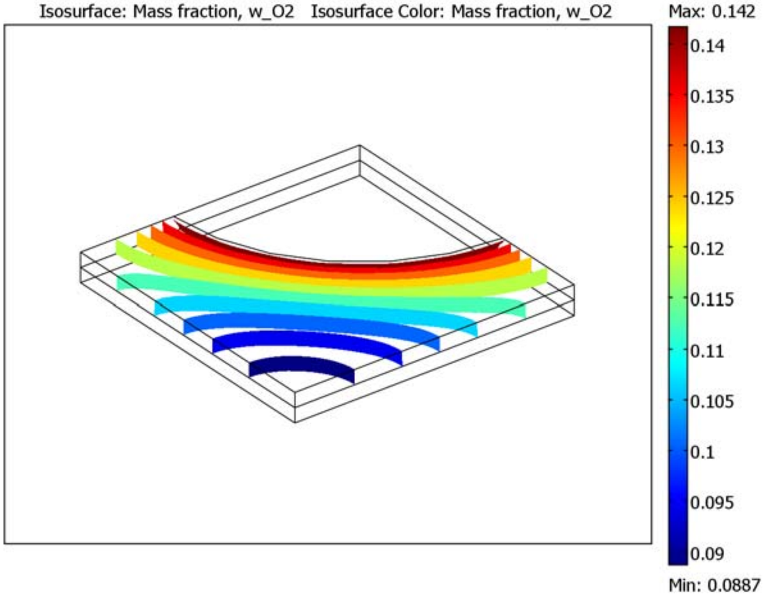


Figure 9-17: Isosurfaces of the weight fraction of oxygen at a total potential drop over the modeled domain of 190 mV.

Figure 9-18 shows the gas velocity in the porous cathode. There is a significant velocity peak at the edge of the inlet orifice. This is caused by the contributions of the reactive layer underneath the current collector because in this region the convective flux dominates the mass transport. Thus it is important to model the velocity field properly.

In this case, the combination of circular orifice and square unit cell eliminates the possibility of approximating the geometry with a rotational symmetric model.

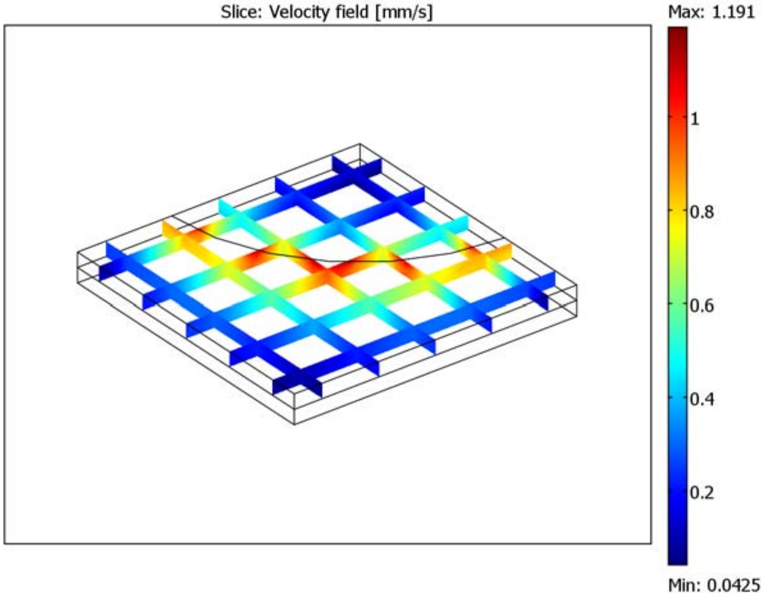


Figure 9-18: Velocity field for the gas phase in the cathode's porous reactive layer.

The electrochemical reaction rate, represented by the local current density, is related to both the local overvoltage and oxygen concentration. Figure 9-19 depicts the local overvoltage, which is rather even throughout the cathode. This is caused by the high electronic conductivity in the porous material. Another observation is that the maximum overvoltage is –180 mV. This means that there is a voltage loss of 100 mV in the electrolyte layer.

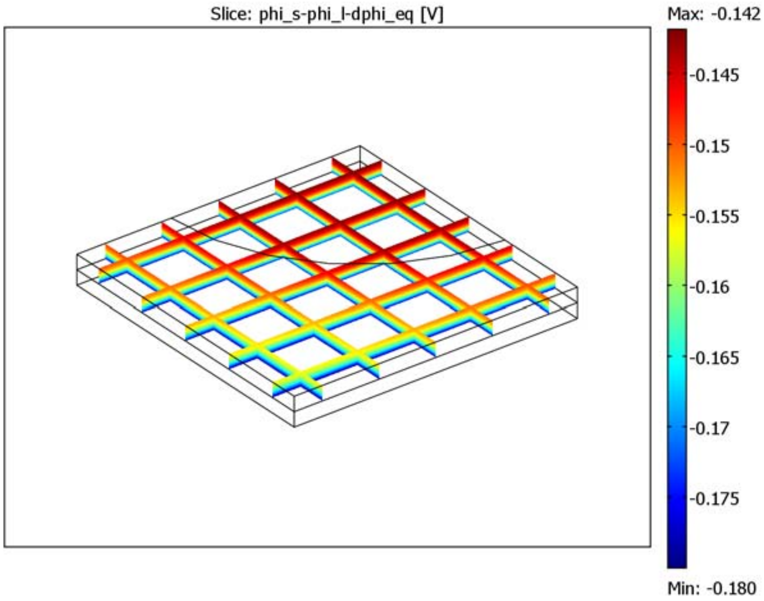


Figure 9-19: Local overvoltage in the cathode reactive layer.

Although the local overvoltage distribution is rather even, the concentration of oxygen is not. This means that the reaction rate is nonuniform in the reactive layer. One way to study the distribution of the reaction rate is to plot the ionic current density at the bottom boundary of the free electrolyte. Figure 9-20 shows such a plot.

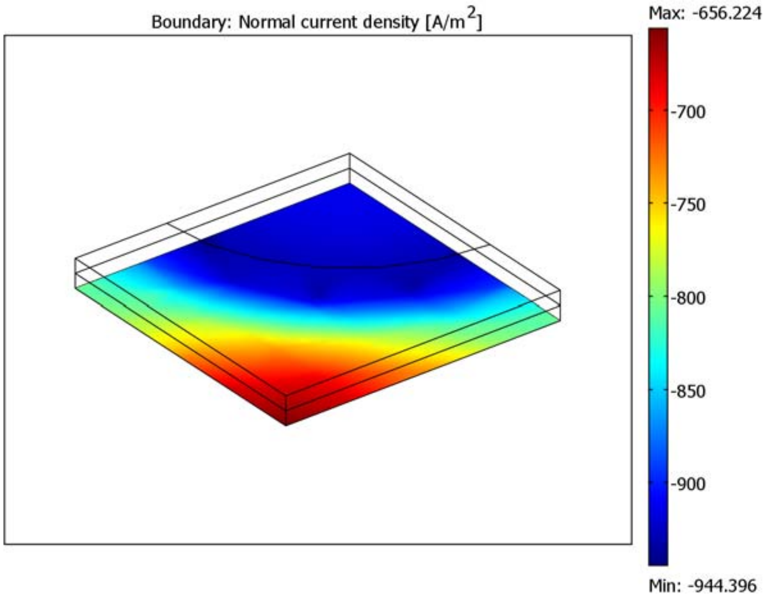


Figure 9-20: Current density perpendicular to the lower, free electrolyte boundary.

The current-density distribution shows that the variations are rather large. The rate of reaction and the current production are higher beneath the orifice and decrease as the distance to the gas inlet increases. This means that the mass transport of reactant dictates the electrode's efficiency in this design and at these particular conditions.

Model Library path:

`Chemical Engineering Module/Electrochemical Engineering/fc_cathode`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, set the **Space dimension** to **2D**. Click **OK**.

GEOMETRY MODELING

1 Create a rectangle by selecting **Draw>Specify Objects>Square**. Type `1.5e-3` in the **Width** edit field, then click **OK**.

2 Click the **Zoom Extents** button on the Main toolbar.

3 To add a 3D geometry, open the **Model Navigator** from the **Multiphysics** menu, click the **Add Geometry** button, select **3D** from the **Space dimension** list, and click **OK** twice.

4 Return to the 2D geometry by clicking the **Geom1** tab.

5 To extrude the rectangle to the 3D geometry, open the **Draw>Extrude** dialog box. Type `0.75e-4 1.5e-4` in the **Distance** edit field, then click **OK**.

6 Return to **Geom1** and create a circle by selecting **Draw>Specify Objects>Circle**. Type `1e-3` in the **Radius** edit field and type `1.5e-3` in both the **x** and the **y** edit field in the **Position** area, then click **OK**.

7 Select both the rectangle and the circle (press Ctrl while you click the objects) and click the **Intersection** button on the Draw toolbar.

8 Choose **Draw>Work-Plane Settings**, type `1.5e-4` in the **z** edit field for the *xy*-plane, and click **OK**.

9 To embed the intersection object to the top surface of the 3D object in **Geom2**, select **Draw>Embed** and click **OK**.

MODEL NAVIGATOR

1 From the **Multiphysics** menu, open the **Model Navigator**.

2 Select **COMSOL Multiphysics>Electromagnetics>Conducive Media DC** from the list of application modes. Type `phi_l` in the **Dependent variables** edit field and type `ionic` in the **Application mode name** edit field. Click **Add**.

3 Repeat step 2 using the variable name `phi_s` and the application mode name `electronic`.

4 Select **Chemical Engineering Module>Mass Transport> Maxwell-Stefan Diffusion and Convection**. Type `w_O2 w_H2O w_N2` in the **Dependent variables** edit field, then click **Add**.

5 Select **Chemical Engineering Module>Momentum Transport>Porous Media Flow> Darcy's Law**, then click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constant expressions (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
F	96485[C/mol]	Faraday's constant
i0	1e-3[A/m^2]	Exchange current density
Rg	8.314[J/(mol*K)]	Gas constant
S	1e9[1/m]	Specific area
T	353[K]	Temperature
V_cell	0[V]	Potential, current collector
dphi_eq	0[V]	Equilibrium potential difference
phi0	0.19[V]	Ionic potential, electrolyte layer bottom boundary
k_l_eff	1[S/m]	Effective conductivity, electrolyte
k_s_eff	1e3[S/m]	Effective conductivity, solid phase
k_l	5[S/m]	Conductivity, free electrolyte
e_por	0.4	Porosity
c_o2ref	3.6641[mol/m^3]	Reference concentration, O2
k_d	3.16e-8[Pa*m^2/s]	Empirical MS diffusivity expression prefactor
p_atm	1.013e5[Pa]	Ambient pressure
v_o2	16.6e-6	Molar diffusion volume, O2 (m^3/mol)
v_h2o	12.7e-6	Molar diffusion volume, H2O (m^3/mol)
v_n2	17.9e-6	Molar diffusion volume, N2 (m^3/mol)
Mo2	32[g/mol]	Molar mass, O2
Mn2	28[g/mol]	Molar mass, N2
M_h2o	18[g/mol]	Molar mass, H2O
D_o2n2	k_d*(T[1/K])^1.75/(p_atm*(v_o2^(1/3)+v_n2^(1/3))^2)*(1[kg/mol]/M_o2+1[kg/mol]/M_n2)^0.5	Maxwell-Stefan diffusivity
D_o2n_eff	D_o2n2*(e_por^1.5)	Effective MS diffusivity
D_o2h2o	k_d*(T[1/K])^1.75/(p_atm*(v_o2^(1/3)+v_h2o^(1/3))^2)*(1[kg/mol]/M_o2+1[kg/mol]/M_h2o)^0.5	Maxwell-Stefan diffusivity
D_o2h2oeff	D_o2h2o*(e_por^1.5)	Effective MS diffusivity

NAME	EXPRESSION	DESCRIPTION
`D_n2h2o`	`k_d*(T[1/K])^1.75/(p_atm*(v_h2o^(1/3)+v_n2^(1/3))^2)*(1[kg/mol]/M_h2o+1[kg/mol]/M_n2)^0.5`	`Maxwell-Stefan diffusivity`
`D_n2h2oeff`	`D_n2h2o*(e_por^1.5)`	`Effective MS diffusivity`
`m_o2ref`	`0.1446`	`Inlet mass fraction, O2`
`mn2`	`0.4761`	`Inlet mass fraction, N2`
`m_h2oref`	`0.3793`	`Inlet mass fraction, H2O`
`perm`	`1e-13[m^2]`	`Permeability`
`eta`	`3e-5[Pa*s]`	`Viscosity`

3 Click **OK**.

4 From the **Options** menu, select **Visualization/Selection Settings**.

5 Select the **Geometry labels** check box, then click **OK**.

PHYSICS SETTINGS

1 With **Geom2** active, specify expressions according to the following table using the **Options>Expressions>Scalar Expressions** dialog box; when finished, click **OK**.

NAME	EXPRESSION
`x1mf`	`(w_O2/M_o2)/(w_O2/M_o2+w_H2O/M_h2o+w_N2/M_n2)`
`i_ct`	`i0*(exp((0.5*F*((phi_s-phi_l)-dphi_eq))/(Rg*T))-x1mf*c_tot/c_o2ref*exp((-0.5*F*((phi_s-phi_l)-dphi_eq))/(Rg*T)))`
`rho`	`c_tot*(x_w_O2_chms*M_o2+x_w_H2O_chms*M_h2o+x_w_N2_chms*M_n2)`
`c_tot`	`p_atm/(Rg*T)`

Subdomain Settings—Conductive Media DC (ionic)

1 In the **Multiphysics** menu, select the **Conductive media DC (ionic)** application mode.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1 and type `k_l` in the σ edit field.

4 Select Subdomain 2 and type `k_l_eff` and `S*i_ct` in the σ and $\mathbf{Q_j}$ edit fields, respectively.

5 Select both subdomains, click the **Init** tab, and type `phi0` in the **Electric potential** edit field. Click **OK**.

Boundary Settings—Conductive Media DC (ionic)

1 From the **Physics** menu, select **Boundary Settings**.

2 Select all boundaries (select any of the boundaries, then press Ctrl+A to select all), then choose **Electric insulation** from the **Boundary condition** list.

3 Select Boundary 3, choose **Electric potential** from the list, and type `phi0` in the **Electric potential** edit field. Click **OK**.

Subdomain Settings—Conductive Media DC (electronic)

1 In the **Multiphysics** menu, select **Conductive media DC (electronic)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then clear the **Active in this domain** check box to disable the application mode.

4 Select Subdomain 2. Type `k_s_eff` and `-S*i_ct` in the σ and $\mathbf{Q_j}$ edit fields, respectively.

5 Click the **Init** tab. Type `V_cell` in the **Electric potential** edit field, then click **OK**.

Boundary Settings—Conductive Media DC (electronic)

1 From the **Physics** menu, select **Boundary Settings**.

2 Select all boundaries. Choose **Electric insulation** from the **Boundary condition** list.

3 Select Boundary 7. Choose **Electric potential** from the list, and type `V_cell` in the **Electric potential** edit field. Click **OK**.

Subdomain Settings—Maxwell-Stefan Diffusion and Convection (chms)

1 In the **Multiphysics** menu, select **Maxwell-Stefan Diffusion and Convection (chms)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then clear the **Active in this domain** check box.

4 Select Subdomain 2. Type `rho`, `p_atm`, `T`, `u_chdl`, `v_chdl`, and `w_chdl` in the edit fields for **Density**, **Pressure**, **Temperature**, **x-velocity**, **y-velocity**, and **z-velocity**, respectively.

5 Click the **Edit** button for $\mathbf{D_{ij}}$ and type `D_o2h2oeff`, `D_o2n2eff`, `D_n2h2oeff`, in the matrix in Row 1, Column 2 as well as in (1, 3) and in (2, 3). Click **OK**.

6 On the **w_O2** page, type `M_o2` and `S*i_ct*M_o2/(4*F)` in the **M** and **R** edit fields, respectively.

7 On the **w_H2O** page, type `M_h2o` in the **M** edit field.

8 On the **w_N2** page, type `M_n2` in the **M** edit field.

9 On the **Init** page, type `m_o2ref` and `m_h2oref` in the **Mass fraction** edit fields for **w_O2** and **w_H2O**, respectively. Click **OK**.

Boundary Conditions—Maxwell-Stefan Diffusion and Convection (chms)

1. Open the **Boundary Settings** dialog box and select Boundary 10.
2. On the **w_O2** page select **Mass fraction** from the **Boundary condition** list, then type `m_o2ref` in the $\mathbf{w\_O2_0}$ edit field.
3. On the **w_H2O** page select **Mass fraction** from the **Boundary condition** list, then type `m_h2oref` in the $\mathbf{w\_H2O_0}$ edit field. Click **OK**.

Subdomain Settings–Darcy's Law (chdl)

1. Select the **Darcy's Law (chdl)** application mode in the **Multiphysics** menu.
2. Open the **Subdomain Settings** dialog box, select Subdomain 1, and clear the **Active in this domain** check box.
3. Select Subdomain 2. Type `rho`, `perm`, `eta`, and `S*i_ct*M_o2/(4*F)` in the edit fields for **Density**, **Permeability**, **Dynamic viscosity**, and **Source term**, respectively.
4. On the **Init** page type `p_atm` in the **Pressure** edit field. Click **OK**.

Boundary Settings—Darcy's Law (chdl)

1. Open the **Boundary Settings** dialog box.
2. Select Boundary 10 and choose **Inflow/Outflow** from the **Boundary condition** list.
3. Type `(perm/eta)*(p_atm-p)/1[mm]` in the **Inward velocity** edit field, then click **OK**. Here the pressure gradient in the normal direction, $\partial p/\partial n$, is approximated by $\Delta p/\Delta x = (p - p_{\mathrm{atm}})/1\ \mathrm{mm}$.

MESH

1. From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.
2. On the **Global** page, select **Extra Coarse** from the **Predefined mesh sizes** list.
3. On the **Subdomain** page, select Subdomain 2. In the **Maximum element size** edit field, type `2e-4`.
4. On the **Edge** page, select Edge 14. In the **Maximum element size** edit field, type `1e-4`.
5. On the **Advanced** page, type `5` in the **z-direction scale factor** edit field.
6. Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to compute the solution. The calculations require approximately 600 MB of free memory and take roughly 30 seconds (on an Intel Pentium Mobile M 1.6 GHz laptop).

POSTPROCESSING AND VISUALIZATION

To generate Figure 9-17, follow these steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, clear the **Slice** check box and select the **Isosurface** check box.
3. On the **Isosurface** page, select **Maxwell-Stefan Diffusion and Convection(chms)>Mass fraction, w_O2** from the **Predefined quantities** list, and type `10` in the **Number of levels** edit field.
4. Click **Apply** to generate the plot.

   To reproduce the plot in Figure 9-18, proceed as follows:

5. On the **General** page, clear the **Isosurface** check box and select the **Slice** check box.
6. On the **Slice** page, select **Darcy's Law(chdl)>Velocity field** from the **Predefined quantities** list. Type `5` in both the **x levels** and **y levels** edit fields. From the **Unit** list, select **mm/s**.
7. Click **Apply**.
8. To generate Figure 9-19, type `phi_s-phi_l-dphi_eq` in the **Expression** edit field while still on the **Slice** page. Click **Apply**.

Finally, create Figure 9-20.

Suppress all boundaries except Boundary 3:

9. From the **Options** menu, select **Suppress>Suppress Boundaries**.
10. Select Boundary 3, then click **Apply**. Click the **Invert Suppression** button, then click **OK**.
11. In the **Plot Parameters** dialog box, go to the **General** page.
12. Clear the **Slice** check box and select the **Boundary** check box.
13. On the **Boundary** page, select **Conductive Media DC(ionic)>Current density outflow** from the **Predefined quantities** list.
14. Click **OK**.

Proton Exchange Membrane Fuel Cell

Introduction

This example demonstrates the multiphysics modeling of a proton exchange membrane (PEM) fuel cell with an interdigitated flow field design. The model uses current balances, mass transport equations (Maxwell-Stefan diffusion for reactant, water and nitrogen gas), and momentum transport (gas flow) to simulate a PEM fuel cell's behavior.

One main candidate for clean high-efficiency power production in future cars is the PEM fuel cell. In a fuel cell-powered engine, the fuel is converted to electric energy through electrochemical reactions instead of combustion. An electric motor, which generally operates at a very high efficiency, powers the vehicle. The efficiency limitations (approximately 40%) of the Carnot cycle are overcome in this way, and the theoretical efficiency is substantially higher than that for combustion engines. Thus, a fuel cell-powered car can run for longer distances with the same amount of fuel compared to a conventional car. Carbon dioxide emissions are consequently lowered, because smaller amounts of fuel are consumed for the same distance traveled. In addition, the low temperatures in the process practically eliminate the production of NO_x and SO_x.

Figure 9-21 depicts the working principle of the PEM fuel cell. Oxidation of hydrogen and the reduction of oxygen takes place at the anode and cathode, respectively:

$$\begin{aligned} &\mathrm{H_2} \Rightarrow 2\mathrm{H}^+ + 2e^- && \text{at the anode} \\ &\mathrm{O_2} + 4\mathrm{H}^+ + 4e^- \Rightarrow 2\mathrm{H_2O} && \text{at the cathode.} \end{aligned} \tag{9-46}$$

Electrons are released to an outer circuit at the anode, and they are received through the same circuit at the cathode. The electronic current is transported to and from the electrodes through the gas backing to the current collector and then to the outer electrical circuit. There is also an ionic current of protons running from the anode to the cathode through the electrolyte. Fuel cells are named after their electrolyte medium. In the PEM fuel cell, a polymeric proton exchange membrane serves as the electrolyte medium.

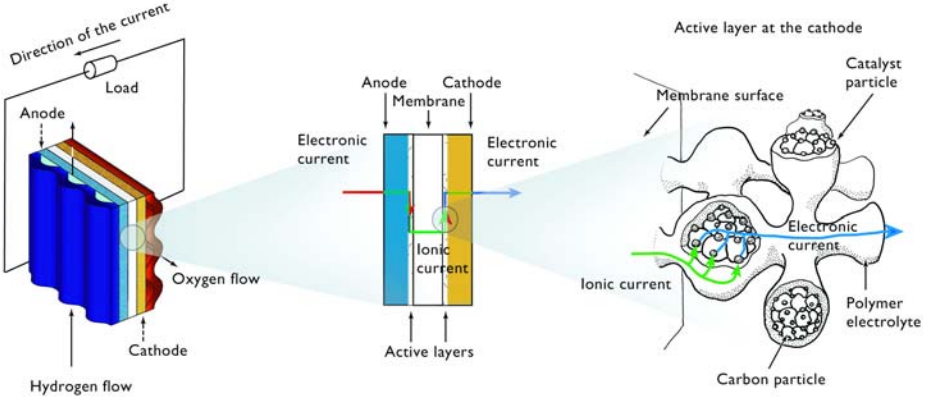


Figure 9-21: Working principle of a PEM fuel cell.

The PEM fuel cell electrodes are of the gas diffusion type. They consist of a supporting carbon structure with gas-filled pores (denoted gas backing) and a porous active layer that also contains the polymer electrolyte. The electrochemical reactions take place in the active layer, which contains a platinum catalyst. The gas diffusion electrodes are designed to maximize the specific area available for the reaction, maximize the distribution of reactant (that is, achieve a low gas-transport resistance), and minimize the resistance for the proton transport to and from the active sites at the electrodes.

Mathematical modeling is an important tool in the development of fuel cells. A combination of modeling and experiments has shown to lower costs and accelerate the pace of building prototypes and understanding these new systems. A number of models, each with a different focus and degree of complexity, have been presented in the literature (see References 1–4).

Model Definition

The modeled section of the fuel cell consists of three domains: an anode (Ω_a), a proton exchange membrane (Ω_m), and a cathode (Ω_c) as indicated in Figure 9-22. Each of the porous electrodes is in contact with an interdigitated gas distributor, which has an inlet channel ($\partial\Omega_{a,inlet}$), a current collector ($\partial\Omega_{a,cc}$), and an outlet channel ($\partial\Omega_{a,outlet}$). The same notation is used for the cathode side.

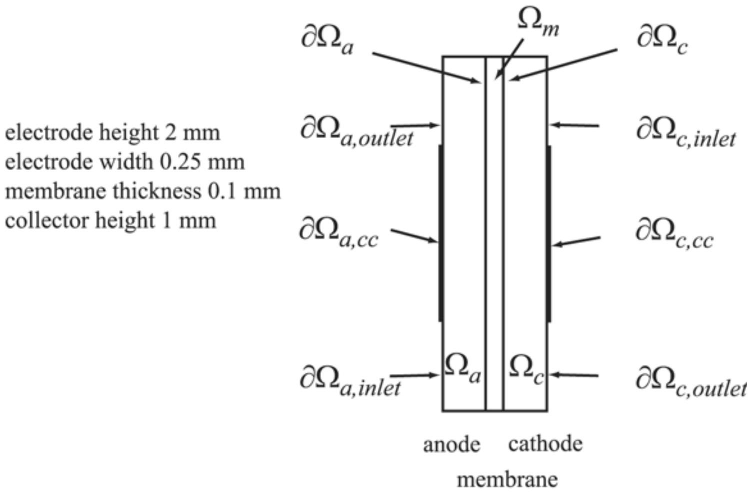


Figure 9-22: Model geometry with subdomain and boundary labels.

Humidified hydrogen and air are supplied to the inlet channels of the anode and cathode, respectively. Hydrogen reacts and is consumed at the anodic active layer to form protons that carry the ionic current to the cathode. Each proton is assumed to drag three molecules of water from the anode to the cathode. At the cathode, oxygen reacts together with the protons to form water at the active layer.

Both feed gases (humified hydrogen and humidified air) are treated as ideal and are transported through diffusion and convection. The electrodes are treated as homogeneous porous media with uniform morphological properties such as porosity and permeability. The gas within each of the electrodes exists as a continuous phase so Darcy's law applies.

An agglomerate model describes the electrode reactions in the active catalyst layers. The agglomerates consist of catalyst and carbon particles embedded in polymer electrolyte. The equations for the agglomerate model originate from the analytical solution of a diffusion-reaction problem in a spherical porous particle (References 5 and 6). At the anodic active catalyst layer, hydrogen is the diffusing and reacting species in the agglomerates, while oxygen is the diffusion and reacting species in the agglomerates at the cathode. An agglomerate model of the cathodic active catalyst layer of a PEM fuel cell has been presented by Broka et al. (Ref. 7).

CHARGE BALANCES

A Conductive Media DC application mode describes the potential distributions in the three subdomains using the following equations:

$$
\begin{aligned}
\nabla \cdot (-\kappa_{\mathrm{s,\,eff}} \nabla \phi_{\mathrm{s}}) &= 0 \quad \text{in } \Omega_{\mathrm{a}} \\
\nabla \cdot (-\kappa_{\mathrm{m,\,eff}} \nabla \phi_{\mathrm{m}}) &= 0 \quad \text{in } \Omega_{\mathrm{m}} \\
\nabla \cdot (-\kappa_{\mathrm{s,\,eff}} \nabla \phi_{\mathrm{s}}) &= 0 \quad \text{in } \Omega_{\mathrm{c}}
\end{aligned}
\qquad (9\text{-}47)
$$

Here $\kappa_{\mathrm{s,eff}}$ is the solid-phase effective electronic conductivity (S/m) and $\kappa_{\mathrm{m,eff}}$ is the membrane ionic conductivity (S/m). The potential (V) in the electrode phases is denoted by ϕ_{s} and that in the membrane by ϕ_{m}.

This example models the active layer of the two electrodes as boundaries. This means that you treat the charge-transfer current density expression, generally described using the Butler-Volmer electrochemical kinetic expression, as a boundary condition.

For the electrolyte potential equation, this results in a condition where the inward normal ionic current densities at the anode and cathode boundaries, i_{a} and i_{c}, are specified according to the equation

$$
i_e = L_{\mathrm{act}}(1 - \varepsilon_{\mathrm{mac}}) j_{\mathrm{agg},\,e} \qquad (9\text{-}48)
$$

where the index *e* stands for “a” (anode) or “c” (cathode). Further, L_{act} is the active layer’s thickness (m), $\varepsilon_{\mathrm{mac}}$ its porosity (the macroscopic porosity), and $j_{\mathrm{agg,a}}$ and $j_{\mathrm{agg,c}}$ are the current densities given by the agglomerate model.

AGGLOMERATE MODEL FOR ANODE AND CATHODE

The agglomerate model describes the current density in an active layer consisting of agglomerates of ionic conductor material and electrically conducting particles covered partially with catalyst. The local current density can be expressed analytically by solving a combination of the diffusion equation and the Butler-Volmer electrode kinetic equation for an agglomerate with constant electric and ionic potentials. The resulting equations for the current density in the anode and cathode are (Ref. 7)

$$
j_{\mathrm{agg},\,e} = -6 n_e F \left(\frac{D_{\mathrm{agg}}}{R_{\mathrm{agg}}^2} \right) (1 - \lambda_e \coth \lambda_e) \beta_e \qquad (9\text{-}49)
$$

where, again, the index *e* stands for “a” (anode) or “c” (cathode), and

$$\lambda_a = \sqrt{\frac{i_{0a}SR_{agg}^2}{2Fc_{H_2,\,ref}D_{agg}}} \qquad \lambda_c = \sqrt{\frac{i_{0c}SR_{agg}^2}{4Fc_{O_2,\,ref}D_{agg}}\exp\left(-\frac{F}{2RT}\eta_c\right)} \tag{9-50}$$

$$\beta_a = \left[c_{H_2,\,ref} - c_{H_2,\,ref}\exp\left(\frac{-2F}{RT}\eta_a\right)\right] \qquad \beta_c = c_{O_2,\,agg} \tag{9-51}$$

In these equations, D_{agg} is the agglomerate gas diffusivity (m^2/s), R_{agg} is the agglomerate radius (m), n_e is a "charge transfer" number (1 for the anode and –2 for the cathode), S is the specific area of the catalyst inside the agglomerate (1/m), and F is Faraday's constant (C/mol). Furthermore, $c_{i,ref}$ are the reference concentrations of the species (mol/m^3), $c_{i,agg}$ are the corresponding concentrations in the agglomerate surface (mol/m^3), i_{0a} and i_{0c} are the exchange current densities (A/m^2), R is the gas constant, T is the temperature (K), and the overvoltages at the anode and the cathode are given by

$$\eta_a = \phi_s - \phi_m - E_{eq,\,a} \qquad \eta_c = \phi_s - \phi_m - E_{eq,\,c} \tag{9-52}$$

where E_{eq} (V) denotes the equilibrium voltage.

You set the anodic and cathodic reference states equal to the molar fractions at the inlet channels of the anode and cathode, respectively, at 1 atm. The dissolved hydrogen and oxygen concentrations at the surface of the agglomerates are related to the molar fractions of the respective species in the gas phase through Henry's law

$$\begin{aligned} c_{agg,\,H2} &= \frac{p_H x_H}{K_H} \\ c_{agg,\,O2} &= \frac{p_O x_O}{K_O} \end{aligned} \tag{9-53}$$

where K is Henry's constant ($Pa\cdot m^3/mol$).

CHARGE BALANCES, CONTINUED

For the electric potential, the electrode boundary conditions are identical, setting the boundary normal current density but using the opposite sign. In addition, the potential difference between the cathode and anode current collectors corresponds to the total cell voltage. Choose the potential at the anode current collector as the reference level by setting it to zero. Then the total cell voltage serves as the boundary condition at the cathode current collector:

$$\begin{aligned}\phi_s &= 0 \quad \text{at } \partial\Omega_{\text{a, cc}} \\ \phi_s &= V_{\text{cell}} \text{ at } \partial\Omega_{\text{c, cc}}\end{aligned} \qquad (9\text{-}54)$$

For the other boundaries you have electric insulation boundary conditions.

POROUS MEDIA FLUID FLOW

To model the gas flows in the gas backings, this example uses the Darcy's Law application mode. The gas velocity is given by the continuity equation according to

$$\nabla \cdot (\rho \mathbf{u}) = 0 \text{ in } \Omega_{\text{a}} \text{ and } \Omega_{\text{c}} \ . \qquad (9\text{-}55)$$

where ρ is the mixture density of the gas phase (kg/m^3) and **u** denotes the gas velocity (m/s). Darcy's law for porous media states that the gradient of pressure, the viscosity of the fluid, and the structure of the porous media determine the velocity:

$$\mathbf{u} = -\frac{k_p}{\eta}\nabla p \qquad (9\text{-}56)$$

Here k_p denotes the electrode's permeability (m^2), η represents the gas viscosity (Pa·s), and p is the pressure (Pa). The ideal gas law gives the gas phase's mixture density, ρ:

$$\rho = \frac{p}{RT}\sum_i M_i x_i \qquad (9\text{-}57)$$

In this equation, R denotes the gas constant (J/(mol·K)), T is the temperature (K), M is the molar mass (kg/mol), and x is the mole fraction.

At the inlets and outlets you specify the pressure:

$$\begin{aligned} p &= p_{\text{a, in}} \text{ at } \partial\Omega_{\text{a, inlet}} \\ p &= p_{\text{ref}} \ \text{ at } \partial\Omega_{\text{a, outlet}} \\ p &= p_{\text{c, in}} \text{ at } \partial\Omega_{\text{c, inlet}} \\ p &= p_{\text{ref}} \ \text{ at } \partial\Omega_{\text{c, outlet}} \end{aligned} \qquad (9\text{-}58)$$

At the electrode boundary for the anode and cathode, the gas velocity is calculated from the total mass flow given by the electrochemical reaction rate according to

$$-\mathbf{n} \cdot \mathbf{u}|_{\text{anode}} = \frac{j_{\text{anode}}}{\rho F}\left(\frac{M_{\text{H2}}}{2} + \lambda_{\text{H2O}} M_{\text{H2O}}\right) \qquad (9\text{-}59)$$

$$-\mathbf{n}\cdot\mathbf{u}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{\rho F}\left[\frac{M_{\mathrm{O2}}}{4} + \left(\frac{1}{2} + \lambda_{\mathrm{H2O}}\right)M_{\mathrm{H2O}}\right]. \tag{9-60}$$

Combined with these boundary conditions, Darcy's law determines the gas flow velocity and preserves the total mass conservation in the anode and cathode gas backing.

MAXWELL-STEFAN MASS TRANSPORT

The model takes into account two species in the anode—H_2 and H_2O—and three at the cathode—O_2, H_2O, and N_2. The model uses one instance of the Maxwell-Stefan Diffusion and Convection application mode for each electrode. Maxwell-Stefan multicomponent diffusion is governed by the equations

$$\begin{gathered}\frac{\partial}{\partial t}\rho w_i + \nabla\cdot\left[-\rho w_i\sum_{j=1}^{N}\mathsf{D}_{ij}\left\{\frac{M}{M_j}\left(\nabla w_j + w_j\frac{\nabla M}{M}\right) + (x_j - w_j)\frac{\nabla p}{p}\right\} + \right.\\ \left. w_i\rho\mathbf{u} + D_i^T\frac{\nabla T}{T}\right] = R_i\end{gathered} \tag{9-61}$$

which the software solves for the mass fractions, w_i. This particular PEM fuel cell model assumes that the temperature-driven diffusion is insignificant and sets the source term, R, to zero. For the cathode gas, with three species (oxygen = 1, water = 2, nitrogen = 3), the mass transport is described by the following three equations together with Darcy's law, describing the flow rate:

$$\nabla\cdot\left\{-\rho w_1\sum_j\left[D_{1j}(\nabla x_j + (x_j - w_j)(\nabla p/p))\right]\right\} = -(\rho\mathbf{u}\cdot\nabla w_1) \tag{9-62}$$

$$\nabla\cdot\left\{-\rho w_2\sum_j\left[D_{2j}(\nabla x_j + (x_j - w_j)(\nabla p/p))\right]\right\} = -(\rho\mathbf{u}\cdot\nabla w_2) \tag{9-63}$$

$$w_3 = 1 - w_1 - w_2 \tag{9-64}$$

Here p is the pressure (Pa), T is the temperature (K), and $\mathbf{u}$ is the velocity (m/s). The density of the mixture is given by Equation 9-57. The Maxwell-Stefan diffusivity matrix, D_{ij} (m^2/s), is calculated from the binary diffusivities you specify in the application mode.

The feed-gas mass fractions are specified at the inlets. At the outlets, convective flux boundary conditions are applied, meaning that the flux is convection dominated. At the electrode-membrane boundary, the mass fluxes of hydrogen in the cathode, and of oxygen and water in the cathode, are determined by the electrochemical reaction rate:

$$-\mathbf{n}\cdot\mathbf{N}_{\mathrm{H2}}\big|_{\mathrm{anode}} = \frac{j_{\mathrm{anode}}}{2F}M_{\mathrm{H2}} \tag{9-65}$$

$$-\mathbf{n}\cdot\mathbf{N}_{\mathrm{O2}}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{4F}M_{\mathrm{O2}} \tag{9-66}$$

$$-\mathbf{n}\cdot\mathbf{N}_{\mathrm{H2O}}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{F}\left(\frac{1}{2}+\lambda_{\mathrm{H2O}}\right)M_{\mathrm{H2O}} \tag{9-67}$$

Results

Figure 9-23 shows the current distribution in the PEM fuel cell. There are significant current spikes present at the corners of the current collectors.

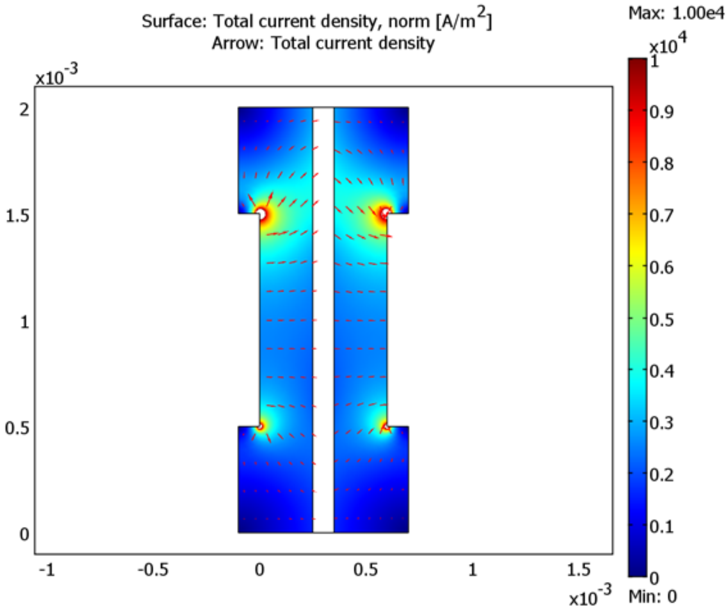


Figure 9-23: Current density (surface plot) and current vector field (arrow plot) in the fuel cell operating at 0.7 V. The anode is on the left and the cathode is on the right

To further analyze the cell's behavior, plot the current density at the active layer as a function of cell height (y) as in Figure 9-24.

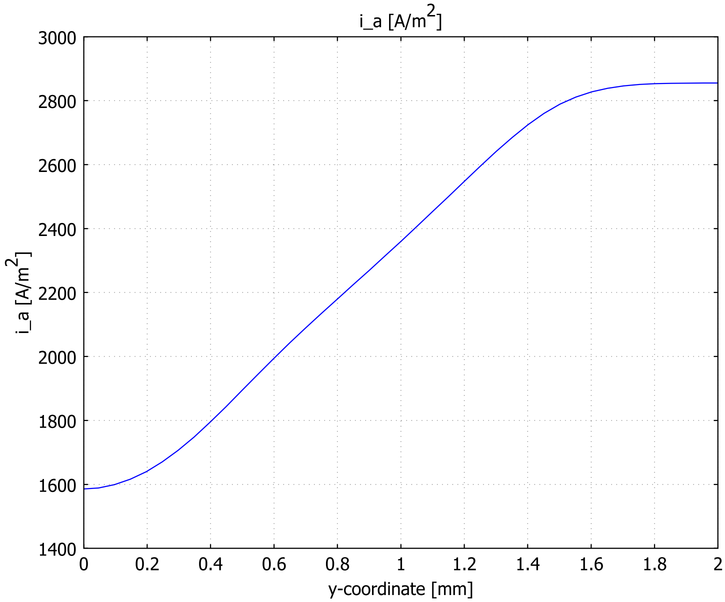


Figure 9-24: Current-density distribution at the active layer at the anode.

The current density is uneven with the highest density in the cell's upper region. This means that the oxygen-reduction reaction rate in the cathode determines the current-density distribution. The maximum current density arises close to the air inlet.

The convective fluxes generally dominate mass transport in the cell. To study the convective effects, plot the velocity field as in Figure 9-25.

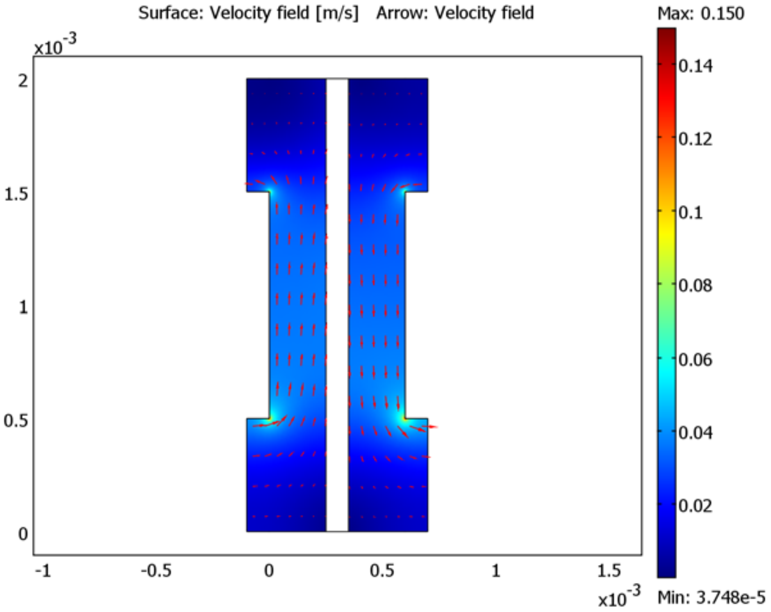


Figure 9-25: Gas velocity field in the anode and cathode compartments.

The flow-velocity magnitude attains its highest values at the current collector corners.

Figure 9-26 shows the reactant (oxygen and hydrogen) weight fractions in the cathode and anode gases. Surprisingly, the hydrogen fraction increases as the anode gas flows from the inlet (at the bottom) to the outlet (at the top). This is the result of the electroosmotic drag of water through the membrane, which results in a higher flux than the consumption of hydrogen. This means that the resulting convective flux of anode gas towards the membrane causes the weight fraction of hydrogen to go up. In the cathode gas, there is an expected decrease in oxygen content along the flow direction.

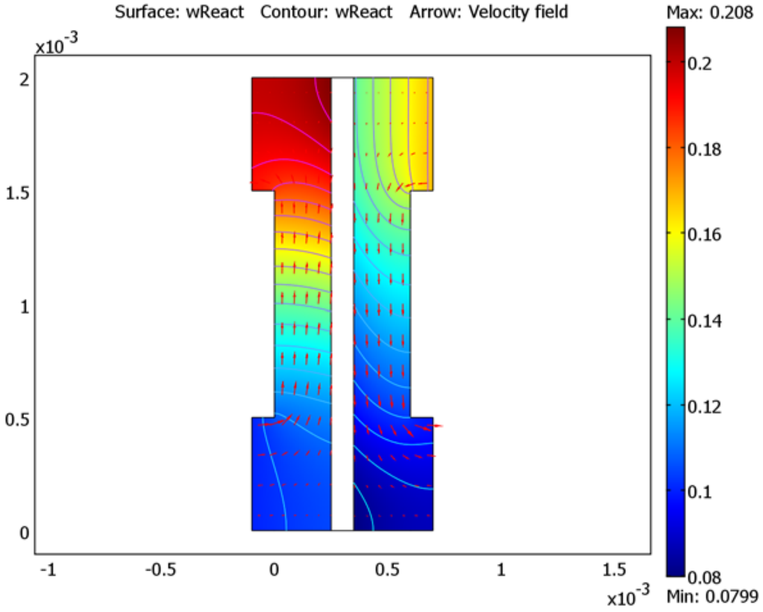


Figure 9-26: Reactant mass fractions, normalized by their inlet values, on the anode side (left) and cathode side (right). The reactant in the anode is hydrogen and that in the cathode is oxygen.

Although oxygen consumption is small, the concentration overvoltage in the agglomerates gives a substantial contribution to the concentration overvoltage. A small change in the oxygen flow gives a substantial change in cell polarization.

Figure 9-27 depicts the water mass fraction in the anode and cathode gases as well as the diffusive flux of water in the anode. It is apparent that water is transported through both diffusion and convection to the membrane on the anode side. The results show a minimum occurring in the upper corner of the membrane on the anode side. This is known to limit fuel cell performance. If the anode gas becomes too dry, the membrane dries out, resulting in decreasing ionic conductivity and the cell subsequently fails.

On the other hand, on the cathode side water levels increase with the direction of flow, and a local maximum in water current occurs in the lower corner to the membrane. This might also be critical because water droplets can clog the pores and effectively hinder gas transport to the active layer.

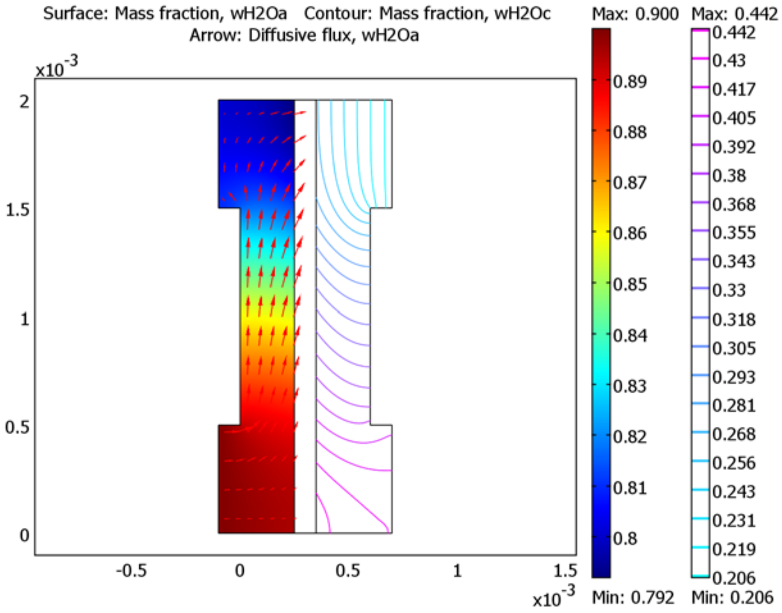


Figure 9-27: Water mass fraction in the anode (left, surface plot) and the cathode (right, contour plot). The arrows visualize the diffusive flux vector field on the anode side.

References

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Model Library path:
`Chemical_Engineering_Module/Electrochemical_Engineering/pemfc`

Modeling Using the Graphical User Interface

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, select **2D** in the **Space dimension** list.
3. Click the **Multiphysics** button.
4. From the **Application Modes** tree, select **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**.
5. Type `phi_s` in the **Dependent variables** edit field and `electrodes` in the **Application mode name** edit field. Click **Add**.
6. Select the **Conductive Media DC** application mode once again.
7. Type `phi_m` in the **Dependent variables** edit field and `membrane` in the **Application mode name** edit field. Click **Add**.
8. Select the application mode **Chemical Engineering Module>Momentum Transport>Porous Media Flow>Darcy's Law**.
9. Type `p` in the **Dependent variables** edit field and `Darcy` in the **Application mode name** edit field. Click **Add**.
10. Select the application mode **Chemical Engineering Module>Mass Transport>Maxwell-Stefan Diffusion and Convection**.
11. In the **Dependent variables** edit field, type `wH2 wH2Oa`. In the **Application mode name** edit field type `MSa`, then click **Add**.
12. Finally, add a second **Maxwell-Stefan Diffusion and Convection** application mode. In the **Dependent variables** edit field type `wO2 wH2Oc wN2`, and in the **Application mode name** edit field type `MSc`. Click **Add**, then click **OK**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar. Create the rectangle R1 by entering the properties in the Rectangle 1 column below; when done, click **OK**.

OBJECT DIMENSIONS	RECTANGLE 1	RECTANGLE 2	RECTANGLE 3	RECTANGLE4
Width	`2.5e-4`	`1e-4`	`2.5e-4`	`1e-4`
Height	`2e-3`	`2e-3`	`2e-3`	`5e-4`
Position base	Corner	Corner	Corner	Corner
Position x	`0`	`2.5e-4`	`3.5e-4`	`-1e-4`

2 Repeat the previous step three times using the properties listed in the remaining three columns to create the rectangles R2, R3, and R4.

3 Click the **Zoom Extents** button on the Main toolbar.

4 Select the rectangle R4, then click the **Array** button on the Draw toolbar.

5 In the **x-displacement** and **y-displacement** edit fields, type `7e-4` and `1.5e-3`, respectively. Type `2` in both the **x-array size** and **y-array size** edit fields. Click **OK**.

6 Select the rectangle R1 and the two small rectangles to the left (Press Ctrl to make multiple selections).

7 Click the **Create Composite Object** button on the Draw toolbar. Clear the **Keep interior boundaries** check box, then click **OK**.

8 Select the rectangle R3 and the two small rectangles to the right. Repeat the previous step for these objects.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`kappa_s`	`1000[S/m]`	`Conductivity, solid phase`
`kappa_m`	`9[S/m]`	`Conductivity, membrane`
`V_cell`	`0.7[V]`	`Cell voltage`
`R`	`8.314[J/(mol*K)]`	`Gas constant`
`T`	`353[K]`	`Temperature`
`F`	`96485[C/mol]`	`Faraday's constant`
`kappa_p`	`1e-13[m^2]`	`Permeability`
`eta`	`2.1e-5[Pa*s]`	`Fluid viscosity`
`p_ref`	`1.013e5[Pa]`	`Reference pressure`

NAME	EXPRESSION	DESCRIPTION
p_a_in	1.1*p_ref	Inlet pressure, anode
p_c_in	1.1*p_ref	Inlet pressure, cathode
drag	3	Water drag coefficient
E_eq_a	0[V]	Equilibrium potential, anode
E_eq_c	1[V]	Equilibrium potential, cathode
i0_a	1e5[A/m^2]	Exchange current density, anode
i0_c	1[A/m^2]	Exchange current density, cathode
S	1e7[1/m]	Specific surface area
R_agg	0.1[um]	Aggregate radius
l_act	10[um]	Active-layer length
eps_mic	0.2	Microscopic porosity inside agglomerate
eps_mac	0.4	Macroscopic porosity between agglomerates
D_agg	1.2e-10[m^2/s]*((1-eps_mac)*(eps_mic))^1.5	Gas diffusivity in agglomerate
D_effH2_H2O	0.915e-4[m^2/s]*(T/307.1[K])^1.5*(eps_mac)^1.5	Effective binary diffusivity, H2_H2O
D_effO2_H2O	0.282e-4[m^2/s]/(T/308.1[K])^1.5*(eps_mac)^1.5	Effective binary diffusivity, O2_H2O
D_effO2_N2	0.22e-4[m^2/s]*(T/293.2[K])^1.5*(eps_mac)^1.5	Effective binary diffusivity, O2_N2
D_effH2O_N2	0.256e-4*(T/307.5[K])^1.5*(eps_mac)^1.5	Effective binary diffusivity, H2O_N2
wH2_in	0.1	Inlet weight fraction, H2
wO2_in	0.21*0.8	Inlet weight fraction, O2
wH2Oc_in	0.2	Cathode inlet weight fraction, H2O
MH2	2[g/mol]	Molar mass, H2
MO2	32[g/mol]	Molar mass, O2
MH2O	18[g/mol]	Molar mass, H2O
MN2	28[g/mol]	Molar mass, N2

NAME	EXPRESSION	DESCRIPTION
xH2_in	(wH2_in/MH2)/(wH2_in/MH2+(1-wH2_in)/MH2O)	Inlet mole fraction, H2
xO2_in	(wO2_in/MO2)/(wO2_in/MO2+wH2Oc_in/MH2O+(1-wO2_in-wH2Oc_in)/MN2)	Inlet mole fraction, O2
KH2	3.9e4[Pa*m^3/mol]	Henry's law constant, H2 in agglomerate
KO2	3.2e4[Pa*m^3/mol]	Henry's law constant, O2 in agglomerate
cH2_ref	xH2_in*p_ref/KH2	Reference concentration, H2
cO2_ref	xO2_in*p_ref/KO2	Reference concentration, O2

3 From the **Options** menu, select **Expressions>Scalar Expressions**.

4 Enter the following expressions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
eta_a	phi_s-phi_m-E_eq_a	Anodic overvoltage
eta_c	phi_s-phi_m-E_eq_c	Cathodic overvoltage
cH2_agg	p*xH2/KH2	Henrys law agglomerate concentration, H2
cO2_agg	p*xO2/KO2	Henry's law agglomerate concentration, O2
K	-6*l_act*(1-eps_mac)*F*D_agg/R_agg^2	Agglomerate current density subexpression
beta_a	cH2_agg-cH2_ref*exp(-2*F*eta_a/(R*T))	Anodic current density subexpression
lda_a	sqrt(i0_a*S*R_agg^2/(2*F*cH2_ref*D_agg))	Anodic current density subexpression
lda_c	sqrt(i0_c*S*R_agg^2*exp(-F*eta_c/(2*R*T))/(4*F*cO2_ref*D_agg))	Cathodic current density subexpression
i_a	K*(1-lda_a*coth(lda_a))*beta_a	Anodic current density
i_c	-2*K*(1-lda_c*coth(lda_c))*cO2_agg	Cathodic current density

5 From the **Options** menu, select **Expressions>Subdomain Expressions**.

6 Define the following subdomain expressions; when done, click **OK**.

NAME	SUBDOMAIN 1	SUBDOMAIN 2	SUBDOMAIN 3
`rho_mix`	`(x_wH2_MSa*MH2+ x_wH2Oa_MSa*MH2O)* p/(R*T)`		`(x_wO2_MSc*MO2+ x_wH2Oc_MSc*MH2O+ x_wN2_MSc*MN2)*p/(R*T)`
`E`	`phi_s`	`phi_m`	`phi_s`
`xH2`	`x_wH2_MSa`		
`xO2`			`x_wO2_MSc`
`wReact`	`wH2`		`wO2`
`wH2O`	`wH2Oa`		`wH2Oc`

7 From the **Options** menu, select **Expressions>Boundary Expressions**.

8 Select Boundary 10. Define a variable with the **Name** `u_a` by the **Expression** `i_a*(MH2/2+drag*MH2O)/(F*rho_mix)`.

9 Select Boundary 13. On the table's second row, define a variable with the **Name** `u_c` by the **Expression** `i_c*(MO2/4-(1/2+drag)*MH2O)/(F*rho_mix)`.

10 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Electrodes

1 From the **Multiphysics** menu, select **1 Conductive Media DC (electrodes)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 1 and 3. In the σ edit field, type `kappa_s`.

4 Select Subdomain 2. Deactivate the application mode by clearing the **Active in this domain** check box. Click **OK**.

Boundary Conditions—Electrodes

1 From the **Physics** menu, select **Boundary Settings**.

2 Apply the following conditions; when done, click **OK**.

SETTINGS	BOUNDARIES 1–7, 9, 14–16, 18–22	BOUNDARY 8	BOUNDARY 10	BOUNDARY 13	BOUNDARY 17
Type	Electric insulation	Electric potential	Inward current flow	Inward current flow	Electric potential
Value		0	`-i_a`	`-i_c`	`V_cell`

Subdomain Settings—Membrane

1 From the **Multiphysics** menu, select **2 Conductive Media DC (membrane)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 2. In the σ edit field, type `kappa_m`.

4 Select Subdomains 1 and 3. Deactivate the application mode by clearing the **Active in this domain** check box. Click **OK**.

Boundary Conditions—Membrane

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 10	BOUNDARIES 11, 12	BOUNDARY 13
Type	Inward current flow	Electric insulation	Inward current flow
Value	`i_a`		`i_c`

Subdomain Settings—Darcy

1 From the **Multiphysics** menu, select **3 Darcy's Law (Darcy)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 1 and 3, then apply settings according to the following table:

PROPERTY	VALUE
ρ	`rho_mix`
κ	`kappa_p`
η	`eta`

4 On the **Init** page, type `p_ref` in the **$p(t_0)$** edit field.

5 Select Subdomain 2, then clear the **Active in this domain** check box.

6 Click **OK**.

Boundary Conditions—Darcy

1 From the **Physics** menu, select **Boundary Settings**.

2 Apply conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 4, 21	BOUNDARY 22	BOUNDARY 10	BOUNDARY 13
Type	Pressure condition	Pressure condition	Pressure condition	Inflow/ Outflow	Inflow/ Outflow
p_0	`p_a_in`	`p_ref`	`p_c_in`		
u_0				`-u_a`	`u_c`

Subdomain Settings—MSa

1 From the **Multiphysics** menu, select **4 Maxwell-Stefan Diffusion and Convection (MSa)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 2 and 3, then clear the **Active in this domain** check box.

4 Select Subdomain 1, then apply the following settings:

PAGE	PROPERTY	VALUE
General	ρ	`rho_mix`
General	p	`p`
General	T	`T`
General	u	`u_Darcy`
General	v	`v_Darcy`
wH2	M	`MH2`
wH20a	M	`MH2O`
Init	$wH2(t_0)$	`wH2_in`

5 On the **General** page, click the **Edit** button for the **Maxwell-Stefan diffusivity matrix**. In the dialog box that appears, type `D_effH2_H2O` in the edit field. Click **OK**.

6 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Settings—MSa

1 From the **Physics** menu, select **Boundary Settings**.

2 Specify conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 4	BOUNDARY 10
Type	Mass fraction	Convective flux	Flux
$wH2_0$	`wH2_in`		
n_0			`-i_a*MH2/(2*F)`

Subdomain Settings—MSc

1 From the **Multiphysics** menu, select **5 Maxwell-Stefan Diffusion and Convection (MSc)**.

2 From the **Physics** menu, select **Subdomain Settings**.

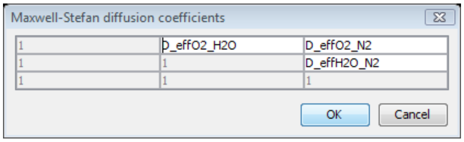
3 Select Subdomains 1 and 2, then clear the **Active in this domain** check box.

4 Select Subdomain 3, then apply the following settings:

PAGE	PROPERTY	VALUE
General	ρ	`rho_mix`
General	p	`p`
General	T	`T`

PAGE	PROPERTY	VALUE
General	u	`u_Darcy`
General	v	`v_Darcy`
wO2	M	`MO2`
wH20c	M	`MH2O`
wN2	M	`MN2`
Init	wO2(t_0)	`wO2_in`
Init	wH2Oc(t_0)	`wH2Oc_in`

5 On the **General** page click the **Edit** button for the **Maxwell-Stefan diffusivity matrix**. In the dialog that appears, type `D_effO2_H2O` and `D_effO2_N2` in the edit fields on the first row and `D_effH2O_N2` in that on the second row. Click **OK**.



1	D_effO2_H2O	D_effO2_N2
1	1	D_effH2O_N2
1	1	1

6 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Settings—MSc

1 From the **Physics** menu, select **Boundary Settings**.

2 Specify conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 13	BOUNDARY 21	BOUNDARY 22
Type (wO2 and wH2Oc))	Flux	Convective flux	Mass fraction
n_0 (wO2)	`i_c*MO2/(4*F)`		
n_0 (wH2Oc)	`-i_c*MH2O*(1/2+drag)/F`		
wO2$_0$			`wO2_in`
wH2Oc$_0$			`wH2Oc_in`

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Boundary** tab. Select Boundaries 10 and 13. Set the **Maximum element size** to `5e-5`.

3 Click the **Point** tab. Select Points 6, 7, 14, and 15. Set the **Maximum element size** to `1e-5`.

4 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1. Click the **Solver Manager** button on the Main toolbar.
2. On the **Solve For** page, select the two **Conductive Media DC** application modes and the **Darcy's Law** application mode. Click **Apply**.
3. On the **Script** page, select the **Solve using a script** check box.
4. Click the **Add Current Solver Settings** button.
5. On the **Initial Value** page, click the **Current solution** option button in the **Initial value** area.
6. On the **Solve For** page, select all the application modes by clicking on the icon **Geom1 (2D)**.
7. Click **Apply**.
8. On the **Script** page, click the **Add Current Solver Settings** button.
9. Click **Solve**.
10. When the solver has finished, click **OK** to close the **Solver Manager**.

POSTPROCESSING AND VISUALIZATION

The following steps reproduce the plot in Figure 9-23 on page 587:

1. Click the **Plot Parameters** button on the Draw toolbar.
2. On the **Surface** page, make sure the **Surface plot** check box is selected.
3. From the **Predefined quantities** list on the **Surface Data** page, select **Conductive Media DC (electrodes)>Total current density, norm**.
4. Click the **Range** button. Clear the **Auto** check box, then type `0` and `1e4` in the **Min** and **Max** edit fields, respectively. Click **OK**.
5. On the **Arrow** page, select the **Arrow plot** check box.
6. From the **Predefined quantities** list on the **Subdomain Data** page, select **Conductive Media DC (electrodes)>Total current density**.
7. From the **Arrow type** list, select **3D arrow**. Click **OK** to generate the plot.

To generate Figure 9-24, proceed as follows:

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.
2. On the **Line/Extrusion** page, select Boundary 10, then type `i_a` in the **Expression** edit field.

3 In the **x-axis data** area, click the lower option button, then click **Expression**.

4 From the **Predefined quantities** list on the **X-Axis Data** dialog box, select **Geometry and Mesh>y-coordinate**. From the **Unit** list, select **mm**, then click **OK**.

5 Click **OK** to close the **Domain Plot Parameters** dialog box and generate the plot.

To generate Figure 9-25 follow these instructions:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **Surface** page, select **Darcy's Law (Darcy)>Velocity field** from the **Predefined quantities** list on the **Surface Data** page.

3 Click the **Range** button. Select the **Auto** check box, then click **OK**.

4 Click the **Arrow** tab.

5 From the **Predefined quantities** list on the **Subdomain Data** page, select **Darcy's Law (Darcy)>Velocity field**.

6 Click **Apply** to generate the plot.

Generate Figure 9-26 with these steps:

7 Back in the **Plot Parameters** dialog box, click the **Surface** tab.

8 In the **Expression** edit field on the **Surface Data** page, type `wReact`.

9 Click the **Contour** tab. Select the **Contour plot** check box.

10 In the **Expression** edit field, type `wReact`.

11 In the **Contour color** area, clear the **Color scale** check box.

12 Click **Apply**.

Finally, to generate Figure 9-27 do the following:

13 Still on the **Contour** page, select the **Color scale** check box. In the **Expression** edit field, type `wH2Oc`.

14 Click the **Surface** tab. In the **Expression** edit field on the **Surface Data** page, type `wH2Oa`.

15 Click the **Arrow** tab. From the **Predefined quantities list** on the **Subdomain Data** page, select **Maxwell-Stefan Diffusion and Convection (MSa)>Diffusive flux, wH2Oa**. Click **OK**.

Serpentine Proton Exchange Membrane Fuel Cell Cathode

Introduction

During the last several years, the use of fuel cells as power sources has been demonstrated in cell phones, computers, cars, and apartment buildings. The requirements for each of these applications are diverse, and the design of fuel cell units are consequently also different. Despite this, the phenomena that describe the characteristics of the electrodes and electrolyte in a fuel cell are identical for all types. In most types, the costs of the components of the fuel cell unit, electrodes, electrolyte, and current collectors are high, which implies that the degree of utilization of catalyst and unit cell surface area must be maximized. Modeling is an efficient way of saving time and money in the design stage.

This study illustrates the use of modeling in the design of a proton exchange membrane fuel cell (PEMFC) cathode. The model is based on simple charge and mass balances in the gas diffusion electrodes and the electrolyte in the fuel cell. It can help optimize the electrode structure in order to minimize concentration and activation polarization. The phenomena described in this paper appears in all types of fuel cells.

The specific purpose of the model is to estimate the influence of the serpentine channel and electrode design on the current-density distribution and the distribution of reacting oxygen gas in the cathode.

Model Definition

The model domain consists of a unit cell of the cathode where the gas channel is configured in a serpentine shape (see Figure 9-28). The active layer is the domain's bottom boundary. Thus the model neglects current-distribution effects along the thickness of the catalyst layer.

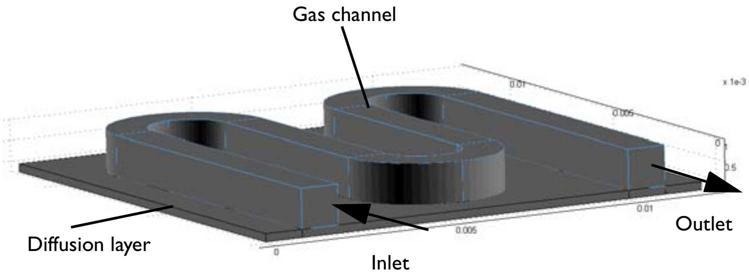


Figure 9-28: Geometrical depiction of the serpentine PEM fuel cell cathode. Gas flows through the curved serpentine channels, which sit flush against the cathode layer. Surrounding the channels is the current collector. The bottom boundary of the cathode layer is the catalytic active layer.

In the gas channel section, this example models fluid flow in combination with diffusion and convective transport. The plate-shaped subdomain at the bottom represents the porous diffusion layer of the PEMFC cathode. The bottom boundary is the active catalyst layer where the reaction takes place. The electrode reaction in the active layer couples the concentration of oxygen to the electric current density. The electrode reaction is treated as a boundary condition at the cathode's bottom surface.

The gas flow in the gas channel is modeled with the momentum and continuity equations (the Navier-Stokes equations):

$$\begin{gathered}\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 \\ \nabla\cdot\mathbf{u} = 0.\end{gathered} \tag{9-68}$$

The pressure difference, Δp, drives the flow in the channel. All walls in the channel except the inflow and outflow have no-slip boundary conditions. The inlet and outlet boundary conditions are

$$\begin{array}{cc} p = p_0 + \Delta p & \text{inlet} \\ p = p_0 & \text{outlet} \\ \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} = 0 & \text{inlet/outlet} \\ \mathbf{u} = \mathbf{0} & \text{wall} \end{array} \tag{9-69}$$

The mass flux in the gas phase is based on the Maxwell-Stefan diffusion and convection equations. It is described by this expression for species i:

$$\nabla\cdot\left[-\rho\omega_i\sum_{j=1}^{N}\mathrm{D}_{ij}\frac{M}{M_j}\left(\nabla\omega_j+\omega_j\frac{\nabla M}{M}\right)+\rho\omega_i\mathbf{u}\right]=0 \tag{9-70}$$

Here ρ denotes the density of the mixture (kg/m^3), M equals the total molar mass of the mixture (kg), M_j represents the molar mass of species j (kg), ω_j gives the mass fraction of species j, and $\mathbf{u}$ is the velocity (m/s). You can also express M and ρ in terms of the mass fractions, ω_j. The multicomponent Fick diffusivities, D_{ij}, which COMSOL Multiphysics calculates automatically, depend strongly on the composition and are given by the following expressions (Ref. 2 and Ref. 3):

$$\mathrm{D}_{11}=-\frac{\dfrac{(\omega_2+\omega_3)^2}{x_1D_{23}}+\dfrac{\omega_2^2}{x_2D_{13}}+\dfrac{\omega_3^2}{x_3D_{12}}}{\dfrac{x_1}{D_{12}D_{13}}+\dfrac{x_2}{D_{12}D_{23}}+\dfrac{x_3}{D_{13}D_{23}}} \tag{9-71}$$

$$\mathrm{D}_{12}=\frac{\dfrac{\omega_1(\omega_2+\omega_3)}{x_1D_{23}}+\dfrac{\omega_2(\omega_1+\omega_3)}{x_2D_{13}}-\dfrac{\omega_3^2}{x_3D_{12}}}{\dfrac{x_1}{D_{12}D_{13}}+\dfrac{x_2}{D_{12}D_{23}}+\dfrac{x_3}{D_{13}D_{23}}} \tag{9-72}$$

where x_j denotes the molar fraction of species j and D_{ij} are the Maxwell-Stefan diffusivities (m^2/s). The Maxwell-Stefan diffusivities, which the user enters in COMSOL Multiphysics, can be described with an empirical equation based on kinetic gas theory (Ref. 4):

$$D_{ij}=k\frac{T^{1.75}}{p(\nu_i^{1/3}+\nu_j^{1/3})^2}\left[\frac{1}{M_i}+\frac{1}{M_j}\right]^{1/2} \tag{9-73}$$

Here k is a constant equal to $3.16\cdot10^{-8}$ Pa·m^2/s, T represents the temperature expressed in kelvin, p equals pressure (Pa), ν_i is the molar diffusion volume of species i expressed in m^3/mol, and M_i is the molar mass of species i expressed in kg/mol.

The molar diffusion volumes appear in Table 9-3 (see Ref. 1).

TABLE 9-3: MOLAR DIFFUSION VOLUMES

SPECIES	DIFFUSION VOLUME
O_2	$16.6 \cdot 10^{-6}$
H_2O	$12.7 \cdot 10^{-6}$
N_2	$17.9 \cdot 10^{-6}$

In the porous cathode, the effective Maxwell-Stefan diffusivities depend on the porosity, ε, according to:

$$D_{\mathrm{eff},\,ij} = D_{ij}\varepsilon^{1.5} . \tag{9-74}$$

At the inlet, the composition is specified according to Table 9-4 (corresponding to air, steam saturated at 80 °C (Ref. 1)):

TABLE 9-4: INLET COMPOSITION

SPECIES	MASS FRACTION
O_2	0.1447
H_2O	0.3789
N_2	0.4764

At the outflow, assume that convective flux dominates the mass transport. This boundary condition is defined by the expression

$$\mathbf{n}_i \cdot \mathbf{n} = (\rho\omega_i\mathbf{u}) \cdot \mathbf{n} \tag{9-75}$$

where $\mathbf{n}_j$ represents the mass flux of species j.

The electrochemical reaction at the active layer determines the flux at the reactive boundary, where oxygen is consumed and water is produced (and dragged) according to these expressions:

$$\begin{aligned} \mathbf{n}_{\mathrm{O2}} \cdot \mathbf{n} &= M_{\mathrm{O2}_2}\frac{i_c}{4F} \\ \mathbf{n}_{\mathrm{H2O}_2} \cdot \mathbf{n} &= -M_{\mathrm{H2O}}\frac{i_c}{F}\left(\frac{1}{2} + t_{\mathrm{H2O}}\right) \end{aligned} \tag{9-76}$$

where $\mathbf{n}_j$ represents the mass flux of j, F denotes Faraday's constant (C/mol), t_{H2O} is the water transport number or drag number (that is, the number of water molecules dragged across the PEMFC membrane for each electron transferred), and i_c is the current density (A/m^2) given by the expression

$$i_c = (-S_a \delta i_0) \frac{\omega_{O2}}{\omega_{O2,0}} \exp\left(\frac{F\eta}{2RT}\right) . \tag{9-77}$$

Here S_a denotes the specific surface area (m^2/m^3), δ is the thickness of the active layer (m), R represents the gas constant (J/(mol·K)), T equals the temperature (K), i_0 gives the exchange current density (A/m^2), and η is the overpotential (V). The weight fraction of oxygen, ω_{O2}, normalized with a reference fraction, is also included.

The nitrogen flux across the reactive boundary is zero. As a consequence, there is a convective flux present at steady state, working counter to the nitrogen diffusive flux, $\mathbf{n}_{N2,d}$. This means that a gas velocity is present even in the porous domain. It is given by

$$\mathbf{u} = \frac{-\mathbf{n}_{N2,\,d}}{\rho\omega_{N2}} . \tag{9-78}$$

This condition is applied in the model's porous domain.

Results

Table 9-29 shows the composition of the gas in the porous electrode and in the channel.

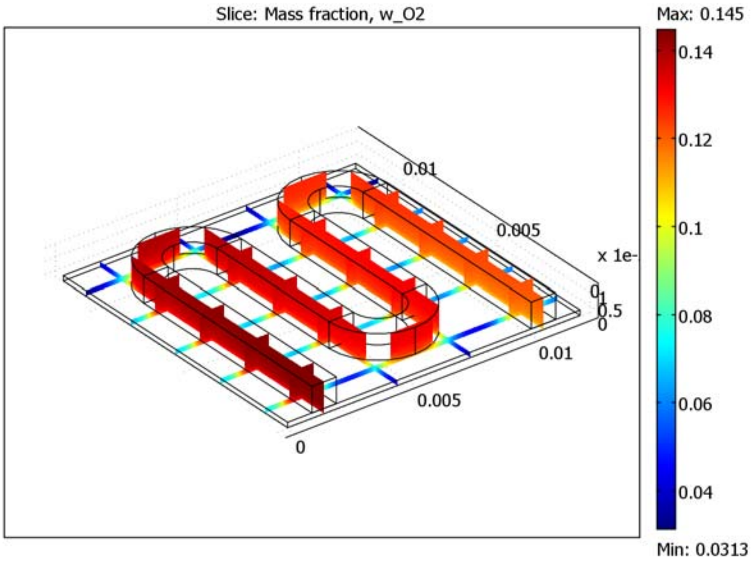


Figure 9-29: Mass fraction in the channel and porous cathode.

In this case, the high current density results in a substantial oxygen depletion in the regions far away from the gas channel. The oxygen weight fraction reaches values as low as 0.03 in the corner to the left in the figure. There is also a substantial decrease in oxygen weight fraction along the gas channel from inlet to outlet, from 0.145 to approximately 0.1. This solution is based on applying a pressure drop of 25 Pa between the inlet and outlet. Figure 9-30 depicts the resulting gas-velocity distribution in the gas channel.

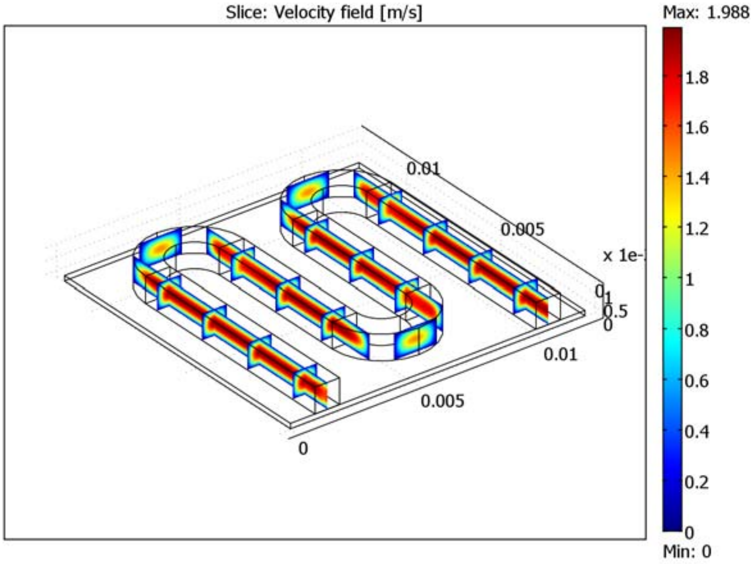


Figure 9-30: Velocity distribution in the gas channel for a 25 Pa pressure drop between the inlet and outlet.

The applied pressure difference results in a maximum gas velocity of approximately 2 m/s. A typical laminar flow profile is present in the straight sections. In the curved sections, on the other hand, the velocity distribution is asymmetric, resulting in an asymmetric concentration distribution there.

In designing the cathode it is important to exploit the expensive catalyst layer to its maximum. The current-density distribution gives a quantitative measure of this utilization. Figure 9-31 displays a top view of that distribution throughout the entire active layer. The current density is significantly higher below the gas channels. A maximum current density of 2400 kA/m^2 is reached under the center of the channel in the inlet region. The lowest current density is only 420 kA/m^2. This uneven use of the active layer indicates that the thickness of the diffusion layer might need to be increased to optimize the electrode's performance.

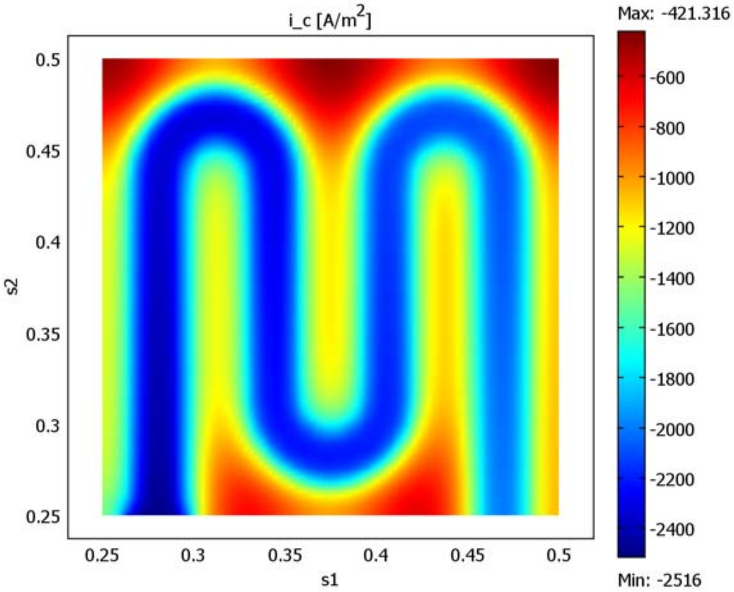


Figure 9-31: Top view of the current-density distribution on the surface of the catalytic active layer.

This model neglects the voltage drop in the electrode. The electronic conductivity of the porous electrode is typically quite high, in the range of 10,000 S/m. The conductivity is related to the voltage drop through the current density according to

$$\Delta E = \frac{-i_c}{\kappa} L . \tag{9-79}$$

An electrode thickness of 0.2 mm means that the maximum voltage drop across the electrode is in the range of 0.05 mV, which is indeed negligible.

An interesting effect in the PEMFC cathode is its water management. Water is present initially in the gas phase at close to saturation concentration. There is a water influx at the reactive boundary due to both reaction and drag. In practice, the water content must not become too high because water droplets would form, clog the electrode, and cause performance to decrease. This is often called "flooding." Figure 9-32 studies water management by plotting the water fraction in the gas.

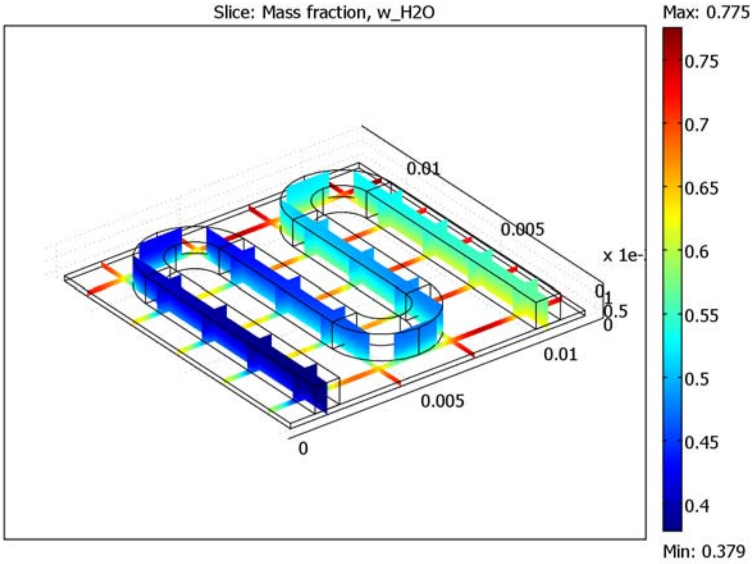


Figure 9-32: Weight fraction of water in the cathode gas.

Clearly the water fraction increases significantly in the electrode. It reaches a maximum value of 0.77 in the corner at the top of the figure. It is probable that water droplets would start forming in this region. To avoid this problem, the design should decrease the inlet water fraction and increase the thickness of the diffusion layer.

References

1. R. Perry and D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

2. J.A. Wesselingh and R. Krishna, *Mass Transfer in Multicomponent Mixtures*, Delft University Press, 2000.

3. R. Bird, W. Stewart, and E. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2002.

4. J. A. Wesselingh and R. Krishna, *Mass Transfer in Multicomponent Mixtures*, Delft University Press, 2000.

Model Library path:

`Chemical_Engineering_Module/Electrochemical_Engineering/serpentine`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 From the **Space dimension** list, select **2D**.

3 Click **OK**.

GEOMETRY AND MESHING

1 Press Shift and click the **Rectangle/Square** button on the Draw toolbar. Create the rectangle R1 using data from the following table. Click **OK**, then repeat the procedure for the rectangles R2–R5.

SETTINGS	R1	R2	R3	R4	R5
Width	`1e-3`	`1e-3`	`1e-3`	`1e-3`	`4e-3`
Height	`9e-3`	`9e-3`	`6e-3`	`6e-3`	`2e-3`
Base	Corner	Corner	Corner	Corner	Corner
x	`1e-3`	`10e-3`	`4e-3`	`7e-3`	`1e-3`
y	`0`	`0`	`3e-3`	`3e-3`	`7e-3`

2 Click the **Zoom Extents** button on the Main toolbar.

3 Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar. Create the circle C1 using data from following table. Click **OK**, then repeat the procedure for C2.

SETTINGS	C1	C2
Radius	`2e-3`	`1e-3`
x	`3e-3`	`3e-3`
y	`9e-3`	`9e-3`

4 Click **Zoom Extents**.

5 Click the **Create Composite Object** button on the Draw toolbar.

6 In the **Set formula** edit field, type `C1-C2-R5`, then click **OK**.

7 Select the generated object, then press Ctrl+C to copy it.

8 Press Ctrl+V to paste the copy. In the **Paste** dialog box specify an **x-displacement** of `6e-3`. Click **OK**.

9 Repeat the paste operation, this time with the **x-displacement** and **y-displacement** set to `3e-3` and `-6e-3`, respectively.

10 Select the last pasted object, click the **Mirror** button on the Draw toolbar, specify `0` and `3e-3` as **Point on line** for **x** and **y**, respectively. Type `0` and `1` in the edit fields for **Normal vector x** and **y**, respectively. Click **OK**.

11 Delete the original object you used to create the mirror image.

Now start creating the 3D objects by extruding the 2D versions:

1 From the **Draw** menu, select **Extrude**.

2 Select all objects, type `1e-3` in the **Distance** edit field and click **OK**.

3 Click the **Coerce to Solid** button on the Draw toolbar.

4 Go back to **Geom1**.

5 Draw an additional **Rectangle** with a width of `12e-3`, a height of `12e-3`, and starting with a lower left corner at the origin (0, 0).

6 Go to the **Draw** menu and select **Extrude**. Select the large rectangle **R5**, type `-0.2e-3` in the **Distance** edit field and click **OK**.

7 Press shift and click the two geometry objects to select both of them.

8 Click the **Create Pairs** (without imprints) button on the Draw toolbar. This allows you to mesh the two objects independently by creating an assembly with two parts that are connected by the identity pairs.

9 Go to the **Mesh** menu and select **Mapped Mesh Parameters**. Select Boundaries 10, 14, 24, 25, 34, 38, and 46.

10 Select **Extra fine** from the **Predefined mesh sizes** list and click **Mesh Selected.** Click **OK**.

11 Click the **Subdomain Mode** button on the Main toolbar.

12 Press shift and click the subdomains of the gas channel to select these domains.

13 Click the **Mesh Selected (Swept)** button on the Mesh toolbar.

14 Click the **Boundary Mode** button on the Main toolbar.

15 Go to the **Mesh** menu and select **Mapped Mesh Parameters**. Select Boundary 3.

16 Select **Finer** from the **Predefined mesh sizes** list and click **Mesh selected.** Click **OK**.

17 Go to the **Mesh** menu and select **Swept Mesh Parameters**. Select Subdomain 1 and select the **Manual specification of element layers** check box. Type 2 in the **Number of element layers** edit field. Click **Mesh selected** and then **OK**.

MODEL NAVIGATOR

Next, add the necessary application modes:

1 From the **Multiphysics** menu, open the **Model Navigator**.

2 Select **Geom2** in the **Multiphysics** area.

3 In the list of application modes select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes**. Click **Add**.

4 In the list of application modes select **Chemical Engineering Module>Mass Transport>Maxwell-Stefan Diffusion and Convection**. Type `w_O2 w_H2O w_N2` in the **Dependent variables** edit field. Click **Add**.

5 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
mu	2e-5[Pa*s]	Dynamic viscosity
p0	1.013e5[Pa]	Outlet pressure
dp	2.5e-4*p0	Pressure drop
R	8.314[J/(mol*K)]	Gas constant
T0	353[K]	Temperature
F	96485[C/mol]	Faraday's constant
rho_M0	p0/(R*T0)	Molar density
eta	0.2[V]	Overvoltage
M_O2	32[g/mol]	Molar mass, O2
M_H2O	18[g/mol]	Molar mass, H2O
M_N2	28[g/mol]	Molar mass, N2
v_O2	16.6e-6	Molar diffusion volume, O2
v_H2O	12.7e-6	Molar diffusion volume, H2O
v_N2	17.9e-6	Molar diffusion volume, N2
eps	0.5	Porosity, cathode

NAME	EXPRESSION	DESCRIPTION
w_O20	0.1447	Inlet mass fraction, O2
w_H2O0	0.3789	Inlet mass fraction, H2O
k	3.16e-8[Pa*m^2/s]	MS diffusivity prefactor
D_O2_H2O	k*(T0[1/K])^1.75*(1[kg/mol]/M_O2+1[kg/mol]/M_H2O)^0.5/(p0*(v_O2^(1/3)+v_H2O^(1/3))^2)	MS diffusivity, O2-H2O component
D_O2_N2	k*(T0[1/K])^1.75*(1[kg/mol]/M_O2+1[kg/mol]/M_N2)^0.5/(p0*(v_O2^(1/3)+v_N2^(1/3))^2)	MS diffusivity, O2-N2 component
D_H2O_N2	k*(T0[1/K])^1.75*(1[kg/mol]/M_H2O+1[kg/mol]/M_N2)^0.5/(p0*(v_H2O^(1/3)+v_N2^(1/3))^2)	MS diffusivity, H2O-N2 component
DO2_H2O_eff	D_O2_H2O*por^1.5	Effective MS diffusivity, O2-H2O component
DO2_N2_eff	D_O2_N2*por^1.5	Effective MS diffusivity, O2-N2 component
DH2O_N2_eff	D_H2O_N2*por^1.5	Effective MS diffusivity, H2O-N2 component
S_a	1e7[1/m]	Specific surface area
d	10[um]	Active-layer thickness
i0	1[A/m^2]	Exchange current density
t_H2O	3	Drag number, H2O

3 From the **Options** menu, select **Expressions>Scalar Expressions**.

4 Enter the following expressions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
M_g	M_O2*x_w_O2_chms+M_H2O*x_w_H2O_chms+M_N2*x_w_N2_chms	Total molar mass
i_c	-S_a*d*i0*exp(0.5*F*eta/(R*T0))*w_O2/w_O20*(w_O2>0)	Current density

PHYSICS SETTINGS

Subdomain Settings— Incompressible Navier-Stokes

1 From the **Multiphysics** menu, select **Geom2: Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then clear the **Active in this domain** check box.

4 Select Subdomains 2–8. Type `rho_chms` and `mu` in the ρ and η edit fields, respectively.

5 Click the **Artificial diffusion** button.

6 Clear the **Streamline diffusion** check box. Click **OK**.

7 Click **OK**.

Boundary Conditions—Incompressible Navier-Stokes

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 8	BOUNDARY 44
Type	Inlet	Outlet
Condition	Pressure, no viscous stress	Pressure, no viscous stress
Value p_0	`p0+dp`	`p0`

Subdomain Settings—Maxwell-Stefan Diffusion and Convection

1 From the **Multiphysics** menu, select **Geom2: Maxwell-Stefan Diffusion and Convection (chms)**.

2 From the **Physics** menu, select **Subdomain Settings**.

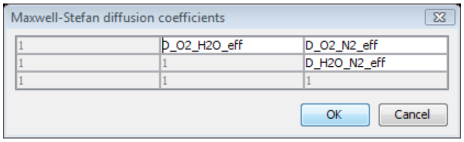
3 On the **General** page, select all subdomains.

4 Type `M_g*rho_M0` in the ρ edit field., Similarly, type `p0`, `T0`, `u`, `v`, and `w` in the edit fields for **Pressure**, **Temperature**, **x-velocity**, **y-velocity**, and **z-velocity**, respectively.

5 Select Subdomain 1 only. Replace the expression in the **x-velocity** edit field by `-dflux_w_N2_x_chms/(w_N2*rho_chms)`.

6 Similarly type `-dflux_w_N2_y_chms/(w_N2*rho_chms)` and `-dflux_w_N2_z_chms/(w_N2*rho_chms)` in the **y-velocity** and **z-velocity** edit fields, respectively.

7 Select Subdomain 1 and click **Edit**. Set the **Maxwell-Stefan diffusion coefficients** to `D_O2_H2O_eff`, `D_O2_N2_eff`, and `D_H2O_N2_eff`(see the following image). Click **OK**.



1	D_O2_H2O_eff	D_O2_N2_eff
1	1	D_H2O_N2_eff
1	1	1

8 Select Subdomains 2–8, then click **Edit**. Set the **Maxwell-Stefan diffusion coefficients** to `D_O2_H2O`, `D_O2_N2`, and `D_H2O_N2`. Click **OK**

9 Select all subdomains. Click the tabs for each species and set the **Molecular weight** to `M_O2`, `M_H2O`, and `M_N2` respectively.

10 Click the **Init** tab and set the initial conditions according to the following table:

PROPERTY	VALUE
w_O2(t_0)	`w_O20`
w_H2O(t_0)	`w_H2O0`

11 Click **OK**.

Boundary Conditions—Maxwell-Stefan Diffusion and Convection

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions for `w_O2` as follows:

SETTINGS	BOUNDARY 8	BOUNDARY 44
Type	Mass fraction	Convective flux
Value	`w_O20`	

3 On the **w_H2O** page, enter the same boundary conditions but specify the **Mass fraction** `w_H2O0`.

4 Select Boundary 3. From the **Boundary condition** list, select **Flux**. In the **Inward mass flux** edit field, type `-i_c*M_H2O*(1/2+t_H2O)/F`.

5 Click the **w_O2** tab. From the **Boundary condition** list, select **Flux**. In the **Inward mass flux** edit field, type `i_c*M_O2/(4*F)`.

6 Click **OK**.

COMPUTING THE SOLUTION

Because there is only a one-way coupling between the Navier-Stokes and Maxwell-Stefan equations, solve first the momentum transport and then the mass transport equations. In this case you set up and use a script to solve the problem.

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Linear system solver** list, select **Direct (UMFPACK)**.

3 Click **OK**.

4 Click the **Solver Manager** button on the Main toolbar.

5 On the **Initial Value** page, select **Initial value expression** in the **Initial value** area.

6. On the **Solve For** page, select **Incompressible Navier-Stokes (chns)** from the **Solve for variables** list. Click **Apply**.
7. On the **Script** page select the **Solve using a script** check box and click the **Add Current Solver Settings** button to generate the first part of the script.
8. Go to the **Initial Value** page and select **Current Solution** in the **Initial value** area.
9. On the **Solve For** page, select the application mode **Maxwell-Stefan Diffusion and Convection (chms)**. Click **Apply**.
10. On the **Script** page, click the **Add Current Solver Settings** button to generate the second part of the solver script. Click **OK**.
11. Click the **Solve** button on the Main toolbar.

To calculate the solution, your computer needs approximately 850 MB of free memory. The solution converges in approximately 500 seconds on a 1.5 GHz Intel Pentium M processor.

POSTPROCESSING AND VISUALIZATION

1. Click the **Plot Parameters** button on the Main toolbar.
2. To generate Figure 9-29, go to the **Slice** page. From the **Predefined quantities** list, select **Maxwell-Stefan Diffusion and Convection (chms)>Mass fraction, w_O2**.
3. In the **Slice positioning** area, type `5` in the **Number of levels** edit field for **y levels**.
4. For **x levels**, click the **Vector with coordinates** option button to specify coordinates manually. In the **Vector with coordinates** edit field, type `1.5e-3 4.5e-3 7.5e-3 10.5e-3`. Click **Apply**.

   To produce Figure 9-30, proceed as follows:
5. On the **Slice** page, select **Incompressible Navier-Stokes (chns)>Velocity field** from the **Predefined quantities** list. Click **OK**.

   Reproduce the plot in Figure 9-31 with the following steps:
6. From the **Postprocessing** menu, select **Domain Plot Parameters**.
7. On the **Surface** page, select Boundary 3. Type `i_c` in the **Expression** edit field, then click **OK**.

   Finally, generate the plot in Figure 9-32 as follows:
8. Click the **Plot Parameters** button on the Main toolbar.
9. On the **Slice** page, select **Maxwell-Stefan Diffusion and Convection (chms)>Mass fraction, w_H2O** from the **Predefined quantities** list.
10. Click **OK**.

10

Electrophoresis and Chromatography

This chapter contains examples of mass transport coupled to momentum transport, where the systems are generally found in microsystems and are often affected by electrical fields. The diffusion of ionic species through charged media or carried by electrolytes can be quite difficult to model. Yet, an electric field is quite easy to control, which means that the flow and distribution of charged ions, particularly with analysis instruments, is best steered by this media. COMSOL Multiphysics is well suited to analyze these types of processes for two reasons:

- *Its ability to model multiphysics applications easily and quickly*—often you need to model momentum and mass transport to a description of the electric potential field. The system could depend on an arbitrary description of the double charge layer at a boundary or could depend on another description of the electric field.
- *Its ability to handle equation-based modeling*—the coupling between the physics that describes such systems can be unusual. Furthermore, chemical kinetics can be involved along with sudden changes in time-based phenomena or phases. The ability to quickly type in your own equations is therefore useful.

Electrophoresis—Transport in a Capillary Column

Introduction

In analytical chemistry, CZE (capillary zone electrophoresis) is the most common electrophoretic separation technique. A typical CZE instrument consists of a capillary, a detector, and a high-voltage power supply (see Figure 10-1).

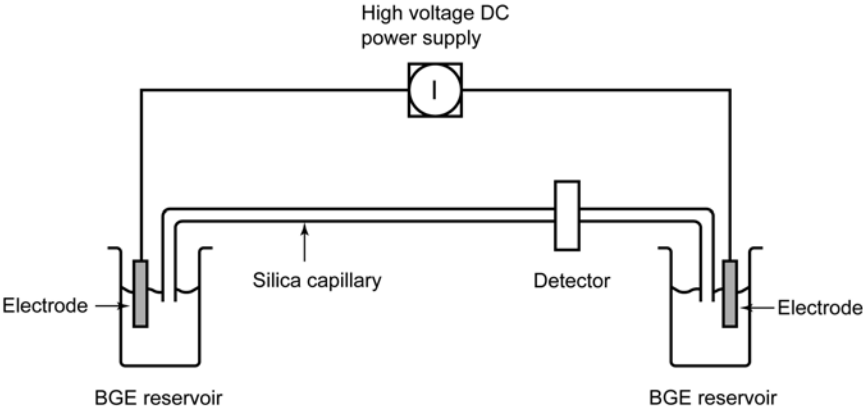


Figure 10-1: Configuration of a CZE instrument.

The capillary is made of fused silica clad with a thin polymer layer to make the capillary flexible. The outer diameter is roughly 375 μm, and the inner diameter is between 25 μm and 100 μm. The length of the capillary varies and can be as much as 1 m long while bridging two buffer reservoirs. A voltage applied between the reservoirs generates a field strength in the capillary of 70–100 kV/m. When a sample is introduced at one end of the capillary, the applied voltage induces migration of the different ions. Separation occurs due to differences in the ions' electrophoretic mobilities.

This example illustrates the basic principles of electrophoretic separation with the help of two models. In Model 1, you consider a simplified system that does not include any protolytic equilibria, that is, the electrolyte and analyte ions are completely ionized. Model 2 is experimentally more realistic because it considers a buffered electrolyte. In this case both the electrolyte and analyte ions can be partially ionized so the simulation includes protolytic equilibria.

Model Definitions

MODEL 1

The first model demonstrates some principles of the theory of electrophoresis. The mass transport equation for species i in an electrophoretic system reads

$$\frac{\partial c_i}{\partial t} = -\frac{\partial \Phi_i}{\partial x} + D_i \frac{\partial^2 c_i}{\partial x^2} \tag{10-1}$$

where c_i denotes the concentration (mol/m^3), Φ_i equals the migrational flux (mol/(m^2·s)), and D_i refers to the diffusion coefficient (m^2/s).

For an ionic species in CZE, two effects cause the migrational flux: a flow of the background electrolyte (BGE), usually an electroosmotic flow, and the local electric field strength in the column. The mass-balance analysis gives

$$\Phi_i = c_i\left(u + F\frac{z_i}{|z_i|}u_{\mathrm{m}i}E\right) \tag{10-2}$$

where u denotes the linear velocity (or electroosmotic flow) of the BGE (m/s), F refers to Faraday's constant (96,485 C/mol), z_i is the charge number of species i, $u_{\mathrm{m}i}$ gives the electrophoretic mobility of species i (mol·m^2/(J·s)), and E is the local electric field strength within the column (V/m).

The local electric field strength in the column depends on the current density through the column and on the concentration profiles for the different charged species. Assuming that electroneutrality is maintained at all times, implies that

$$\rho_{\mathrm{e}} \equiv F\sum_i z_i c_i = 0 \tag{10-3}$$

Multiplying Equation 10-1 for each species i by z_i, and summing the so obtained equations over all species, leads upon using Equation 10-3 to the equation

$$\frac{\partial}{\partial x}\left[\kappa E - \frac{\partial}{\partial x}\left(\sum_i D_i z_i F \frac{\partial c_i}{\partial x}\right)\right] = 0 \tag{10-4}$$

which can be integrated to give

$$\kappa E = j + \sum_i D_i z_i F \frac{\partial c_i}{\partial x} \tag{10-5}$$

Here j denotes the current density through the column (A/m^2) and κ equals the local electrolyte conductivity (S/m). The latter quantity depends on the local concentration of the different ionic species through the equation

$$\kappa = F^2 \sum_i |z_i| u_{\mathrm{m}i} c_i \tag{10-6}$$

This treatment assumes that the current through the column is constant during the experiment. The model also makes use of the following relationship between mobility and diffusion constant for an ionic species:

$$D_i = \frac{RTu_{\mathrm{m}i}}{|z_i|} \tag{10-7}$$

where R is the gas constant (8.314 J/(mol·K)) and T denotes the temperature (K).

It is well known that ionic mobility decreases with increasing ionic strength in the solution. However, this treatment assumes that the mobility is constant and independent of the ionic strength of the BGE.

Input Data

This study covers the migration of two analyte ions (benzoic acid and chlorobenzoic acid) migrating in a BGE consisting of sodium acetate at pH = 7. Such a BGE is not suitable for practical use because of the extremely low buffer capacity of acetate at this pH. This means that you can neglect protolytic equilibria in this model.

The model domain is a uniform 2 mm long column. The two analyte ions are injected with a Gaussian initial concentration profile around the column center at $x = 0$:

$$c_i(x) = c_{i0} \exp(-ax^2)\,. \tag{10-8}$$

This example uses the values $a = 1 \cdot 10^9$ (m^{-2}) and $c_{i0} = 10$ mol/m^3 for the two analyte ions. The concentration of sodium acetate in the BGE is 50 mol/m^3. Sodium is also the counter ion to the two analyte ions in the analyte zone. The BGE's relative permittivity, ε_r, equals 80. The current density through the column is 19.23 A/m^2, and the mobilities for the ionic species are as listed in the following table:

ION SPECIES	INDEX	MOBILITY
Na^+	1	$5.19 \cdot 10^{-8}$ m^2/(V·s)
AcO^-	2	$4.23 \cdot 10^{-8}$ m^2/(V·s)
Bz^-	3	$3.36 \cdot 10^{-8}$ m^2/(V·s)
$ClBz^-$	4	$3.42 \cdot 10^{-8}$ m^2/(V·s)

To obtain the corresponding electrophoretic mobilities, u_{mi} (mol·s/kg), divide these quantities by Faraday's constant, $F = 96{,}485$ C/mol.

MODEL 2

The previous case studies the migration of ionic analytes in a BGE consisting of completely ionized species. A more realistic CZE-system consists of a buffered BGE with analytes that are only partially ionized due to the acid-base equilibrium. Consider a sodium acetate buffer at pH = 4.2 and the migration of the same mixture as before, that is, benzoic acid and o-chlorobenzoic acid. In this case you must consider the following equilibria:

$$\begin{gathered} \mathrm{AcOH} \leftrightarrow \mathrm{AcO^-} + \mathrm{H^+} \quad \mathrm{pK_a(AcOH)} = 4.76 \\ \mathrm{K_{AcOH}} = \frac{[\mathrm{AcO^-}][\mathrm{H^+}]}{[\mathrm{AcOH}]} = 10^{-1.76}\ \mathrm{mol/m^3} \end{gathered} \tag{10-9}$$

$$\begin{gathered} \mathrm{HBz} \leftrightarrow \mathrm{Bz^-} + \mathrm{H^+} \quad \mathrm{pK_a(HBz)} = 4.21 \\ \mathrm{K_{HBz}} = \frac{[\mathrm{Bz^-}][\mathrm{H^+}]}{[\mathrm{HBz}]} = 10^{-1.21}\ \mathrm{mol/m^3} \end{gathered} \tag{10-10}$$

$$\begin{gathered} \mathrm{HBzCl} \leftrightarrow \mathrm{BzCl^-} + \mathrm{H^+} \quad \mathrm{pK_a(HBzCl)} = 2.94 \\ \mathrm{K_{HBzCl}} = \frac{[\mathrm{BzCl^-}][\mathrm{H^+}]}{[\mathrm{HBz}]} = 10^{0.06}\ \mathrm{mol/m^3} \end{gathered} \tag{10-11}$$

$$\begin{gathered} \mathrm{H_2O} \leftrightarrow \mathrm{OH^-} + \mathrm{H^+} \quad \mathrm{pK_w} = 14 \\ \mathrm{K_w} = [\mathrm{OH^-}][\mathrm{H^+}] = 10^{-8}\ \mathrm{mol/m^3} \end{gathered} \tag{10-12}$$

At pH = 4.2, half of the total concentration of benzoic acid is in the acidic form and the other half is in the basic form; this contrasts to o-Chlorobenzoic acid, which 95%

is in the basic form. Therefore, at pH = 4.2 the migration velocity for o-Chlorobenzoic acid is almost twice that of Benzoic acid, and they are therefore easily separated.

To readily allow for a comparison of the results with those of the previous model, this case keeps the current density and the concentrations of all anions at the same values as before, that is, the total concentration of all species is adjusted with the acid dissociation constant.

Results and Discussion

MODEL I

The first model demonstrates some electrophoretic principles by studying a simplified system, that is, the simultaneous movement in the electric field of five ions, maintaining local electroneutrality and overall conservation of mass for each one. Figure 10-2a depicts the concentration profiles for the sodium ion and the two analyte ions at $t = 0$. The initial concentration of AcO^- is constant at all points in the system.

Figure 10-2b shows the concentration profiles for the sodium, acetate, and the two analyte ions after 0.4 s of electrophoretic migration. The small difference in mobility between the two benzoic acids is not large enough to bring any significant separation between them. It is interesting to note that the concentration of both sodium and acetate is lower in the zones containing the analyte ions than in the BGE.

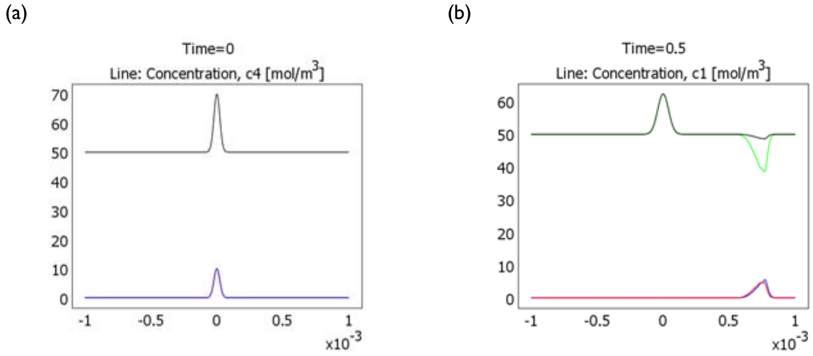


Figure 10-2: Concentration profiles: (a) Na^+, Bz^-*, and* $BzCl^-$ *at* $t = 0$*; (b)* Na^+, AcO^-, Bz^-*, and* $BzCl^-$ *at* $t = 0.5$ *s.*

The difference in ionic composition at different locations in the column gives a difference in the local conductivity. Because the current is constant throughout the column, the variation in ionic conductivity leads to a variation in the local electric field strength, E. This is illustrated in Figure 10-3 for $t = 0$ and $t = 0.4$ s.

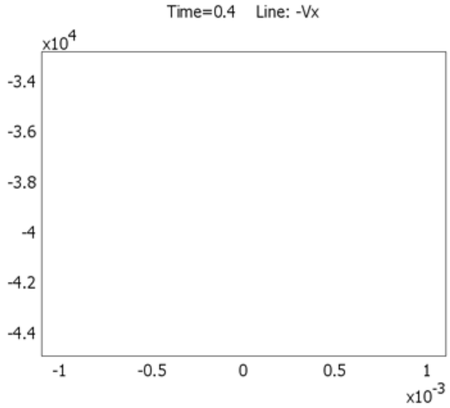


Figure 10-3: Electric field strength at $t = 0$ *and* $t = 0.4$ *s.*

According to classical electrophoretic theory, the Kolrausch regulating function

$$K = \sum_i \frac{|z_i| c_i}{u_{\mathrm{m}i}} \tag{10-13}$$

should be constant across all moving boundaries. Figure 10-4 plots this function at $t = 0.4$ s for the same conditions as in Figure 10-3. It is clearly visible that the function is constant across all moving fronts and that its value varies only across the stationary zone situated at $x = 0$.

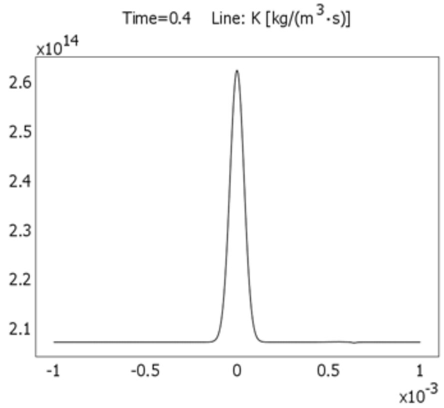


Figure 10-4: The Kohlrausch regulating function at $t = 0.4$ *s.*

MODEL 2

The second model studies a more realistic electrophoretic experiment. Here pH is lowered so that the difference in pK_a values between Benzoic acid and o-Chlorobenzoic acid is applied to achieve a separation between the two components in the column. The value for the current density and concentration of the ionic form of the analytes is the same as in the previous example. The total acetate ion concentration is also adjusted so that the acetate anion concentration in the BGE is the same as before.

In contrast to the previous example, in this second model you also include the H^+ concentration in the calculations. This implies that pH is allowed to vary in the column and that all protolytic equilibria must be satisfied simultaneously and in combination with the ionic mass balances and the electroneutrality condition.

Figure 10-5 shows the total concentration of the two analytes together with a $pH = -\log(cH^+) = 4.2$ at $t = 0$. This decreases the migration velocity of Benzoic acid so that the two anions can now be separated after only 0.4 s of electrophoretic migration (see Figure 10-6.

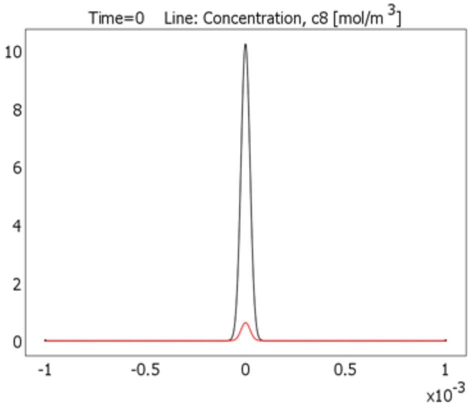


Figure 10-5: The concentration profiles for benzoic acid (black) and o-chlorobenzoic acid (red) at t = 0.

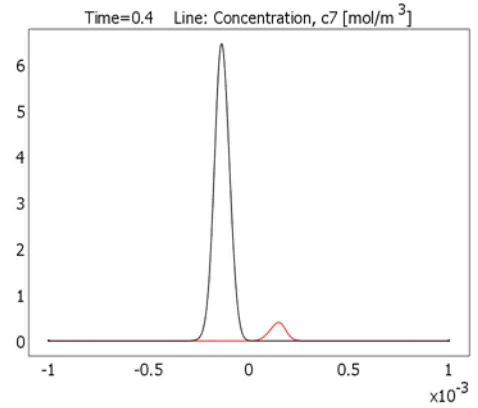


Figure 10-6: The concentration profiles for benzoic acid (black) and o-chlorobenzoic acid (red) at t = 0.4 s.

Figure 10-7 displays the pH at t = 0.4 s. As the figure shows, the value is lower in the analyte zones and higher in the stationary zone compared to the pH value in the BGE.

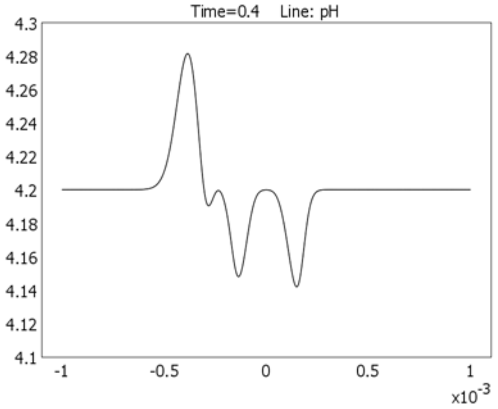


Figure 10-7: pH in the system at t = 0.4 s.

References

1. R.A. Mosher, D.A. Saville, and W. Thormann, *The Dynamics of Electrophoresis, Electrophoresis Library* (B.J. Radola, ed.), Weinheim, VCH, 1992.

2. E.V. Dose and G.A. Guiochon, “High-Resolution Modeling of Capillary Zone Electrophoresis and Isotachophoresis,” *Analytical Chemistry*, vol. 63, p. 1083, 1991.

Model Library path: `Chemical_Engineering_Module/Electrophoresis_and_Chromatography/capillary_electrophoresis_1`

Modeling Using the Graphical User Interface—Model 1

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **1D** from the **Space dimension** list.

3 In the list of application modes select **Chemical Engineering Module>Mass Transport>Electrokinetic Flow>Transient analysis**.

4 In the **Dependent variables** edit field, type `c1 c2 c3 c4`.

5 Click first the **Multiphysics** button and then the **Add** button.

6 Select the application mode **COMSOL Multiphysics >PDE Modes>PDE, General Form**.

7 In the **Dependent variables** edit field, type `V`.

8 Click **Add**, then click **OK**.

GEOMETRY MODELING

1 Shift-click the **Line** button on the Draw toolbar.

2 Enter the **Coordinates** `-1e-3 1e-3`, then click **OK**.

3 Click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
a	1.0e9[1/m^2]	Gaussian distribution inverse-variance parameter
c0	10[mol/m^3]	Initial peak concentration, analyte ions
c_BGE0	50[mol/m^3]	Initial BGE concentration
u_m1	5.19e-8[m^2/(V*s)]/F	Electrophoretic mobility, Na+
u_m2	4.23e-8[m^2/(V*s)]/F	Electrophoretic mobility, AcO-

NAME	EXPRESSION	DESCRIPTION
u_m3	3.36e-8[m^2/(V*s)]/F	Electrophoretic mobility, Bz-
u_m4	3.42e-8[m^2/(V*s)]/F	Electrophoretic mobility, ClBz-
eps_BGE	80*8.854e-12[F/m]	Electric permittivity of BGE
F	96485[C/mol]	Faraday's constant
RT	2476.38[J/mol]	Gas constant times temperature
D1	RT*u_m1	Diffusion coefficient, Na+
D2	RT*u_m2	Diffusion coefficient, AcO-
D3	RT*u_m3	Diffusion coefficient, Bz-
D4	RT*u_m4	Diffusion coefficient, ClBz-
j0	19.23[kA/m^2]	Current density
kappa0	F^2*(u_m1+u_m2)*c_BGE0	Conductivity at boundaries
E0	j0/kappa0	Electric field at boundaries

3 Select **Options>Expressions>Scalar Expressions**.

4 Enter the following expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
c_G	c0*exp(-a*x^2)	Gaussian concentration distribution
c10	2*c_G+c_BGE0	Initial concentration, Na+
c30	c_G	Initial concentration, Bz-
c40	c_G	Initial concentration, ClBz-
K	c1/u_m1+c2/u_m2+ c3/u_m3+c4/u_m4	Kolrausch regulating function

PHYSICS

Subdomain Settings—Electrokinetic Flow

1 From the **Physics** menu, select **Subdomain Settings**.

2 On each page listed in the table heading, enter the corresponding coefficients.

QUANTITY	**c1**	**c2**	**c3**	**c4**
D	D1	D2	D3	D4
u_m	u_m1	u_m2	u_m3	u_m4
z	1	-1	-1	-1
V	V	V	V	V

3 On the **Init** page, set the following initial values; when done, click **OK**.

VARIABLE	INITIAL VALUE
$c1(t_0)$	`c10`
$c2(t_0)$	`c_BGE0`
$c3(t_0)$	`c30`
$c4(t_0)$	`c40`

Boundary Conditions—Electrokinetic Flow

1 From the **Multiphysics** menu, select **1 Electrokinetic Flow (chekf)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 For each species, `i` = `1`, `2`, `3`, and `4`, select **Concentration** as the **Boundary condition**. Specify the concentrations according to the following table:

QUANTITY	**c1**	**c2**	**c3**	**c4**
ci_0	`c10`	`c_BGE`	`c30`	`c40`

4 Click **OK**.

Subdomain Settings—PDE, General Form

1 From the **Multiphysics** menu, select **2 PDE, General Form (g)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Enter the following values; when done, click **OK**.

COEFFICIENTS	VALUE
Γ	`-Vx`
F	`eps_BGE*(c1-c2-c3-c4)/F`

Boundary Conditions—PDE, General Form

1 From the **Physics** menu, select **Boundary Settings**.

2 Select Boundary 1.

3 Click the **Neumann boundary condition** option button, then set **g** to –`E0`.

4 Select Boundary 2.

5 Click the **Dirichlet boundary condition** option button, then set **R** to –`V`.

6 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 On the **Global** page, set the **Maximum element size** to `2e-6`.

3 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 Set **Times** to `0:0.05:0.5`.

3 Click the **Time Stepping** tab.

4 In the **Advanced** area, select **On** in the **Consistent initialization of DAE systems** list. Click **OK**.

5 Click the **Solve** button on the Main toolbar.

Model Library path: `Chemical_Engineering_Module/Electrophoresis_and_Chromatography/capillary_electrophoresis_2`

Modeling Using the Graphical User Interface—Model 2

1 In the **Model Navigator**, select **1D** from the **Space dimension** list.

2 In the list of application modes select **Chemical Engineering Module>Mass Transport>Electrokinetic Flow>Transient analysis**.

3 In the **Dependent variables** edit field, type `c1 c2 c3 c4 c5`.

4 Click first the **Multiphysics** button and then the **Add** button.

5 From the list of application modes, select **Chemical Engineering Module>Mass Transport>Convection and Diffusion>Transient analysis**.

6 In the **Dependent variables** edit field, type `c6 c7 c8`. Click **Add**.

7 From the list of application modes, select **COMSOL Multiphysics>PDE Modes>PDE, General Form**.

8 In the **Dependent variables** edit field, type `V`. Click **Add**.

9 Click **OK**.

GEOMETRY MODELING

Generate the geometry in the same way as in Model 1.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 To the constants from Model 1, add the following ones; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`u_m5`	`1e-7[m^2/(V*s)]/F`	`Electrophoretic mobility, H+`
`D5`	`RT*u_m5`	`Diffusion coefficient, H+`
`c50`	`0.06310[mol/m^3]`	`Initial concentration, H+`
`c60`	`181.54[mol/m^3]`	`Initial concentration, AcOH`
`K_HBz`	`(10^(-1.21))[mol/m^3]`	
`K_HBzCl`	`(10^0.006)[mol/m^3]`	
`k1_Ac`	`1e8[1/s]`	`Reaction rate constant`
`k2_Ac`	`5.754e9[m^3/(mol*s)]`	`Reaction rate constant`
`k1_HBz`	`1e8[1/s]`	`Reaction rate constant`
`k2_HBz`	`1.622e9[m^3/(mol*s)]`	`Reaction rate constant`
`k1_HBzCl`	`1e8[1/s]`	`Reaction rate constant`
`k2_HBzCl`	`9.863e7[m^3/(mol*s)]`	`Reaction rate constant`
`u0`	`1[mm/s]`	`Flow velocity`

3 From the **Options** menu, select **Expressions>Scalar Expressions**.

4 Change the expression for `c10` from Model 1 to `2*c_G+c_BGE0-c50`.

5 Add the following expressions to those you entered in Model 1:

NAME	EXPRESSION	DESCRIPTION
`c70`	`c30*c50/K_HBz`	`Initial concentration, HBz`
`c80`	`c40*c50/K_HBzCl`	`Initial concentration, HBzCl`
`r_Ac`	`k1_Ac*c6-k2_Ac*c5*c2`	`Reaction rate`
`r_Bz`	`k1_HBz*c7-k2_HBz*c5*c3`	`Reaction rate`
`r_BzCl`	`k1_HBzCl*c8-k2_HBzCl*c5*c4`	`Reaction rate`
`pH`	`-log10(c5/1[mol/l])`	`pH value`

6 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings—PDE, General Form

1 From the **Physics** menu, select **Subdomain Settings**.

2 Set Γ to `-Vx` and **F** to `F*(c1-c2-c3-c4+c5)/eps_BGE`.

3 Click **OK**.

Boundary Conditions—PDE, General Form

Use the same boundary conditions as in Model 1.

Subdomain Settings—Electrokinetic Flow

1. From the **Physics** menu, select **Subdomain Settings**.
2. Enter the following coefficients:

QUANTITY	c1	c2	c3	c4	c5
D	`D1`	`D2`	`D3`	`D4`	`D5`
R		`r_Ac`	`r_Bz`	`r_BzCl`	`r_Ac+r_Bz+r_BzCl`
u_m	`u_m1`	`u_m2`	`u_m3`	`u_m4`	`u_m5`
z	`1`	`-1`	`-1`	`-1`	`1`
u	`-u0`	`-u0`	`-u0`	`-u0`	`-u0`
V	`V`	`V`	`V`	`V`	`V`

3. Click the **Init** tab.
4. The initial conditions are the same as in Model 1 for the concentrations **c1**, **c2**, **c3**, and **c4**.
5. For **c5** set the initial condition to `c50`.
6. Click **OK**.

Boundary Conditions—Electrokinetic Flow

1. From the **Physics** menu, select **Boundary Settings**.
2. Specify the same boundary conditions as in Model 1 for species 1–4.
3. For species 5, set the boundary condition to **Concentration**. In the **$c5_0$** edit field, type `c50`.
4. Click **OK**.

Subdomain Settings—Convection and Diffusion

1. From the **Physics** menu, select **Subdomain Settings**.
2. Enter the following values:

QUANTITY	c6	c7	c8
D	`D2`	`D3`	`D4`
R	`-r_Ac`	`-r_Bz`	`-r_BzCl`
u	`-u0`	`-u0`	`-u0`

3. Click the **Init** tab.

4 Enter the following initial conditions:

VARIABLE	INITIAL VALUE
$c6(t_0)$	c60
$c7(t_0)$	c70
$c8(t_0)$	c80

5 Click **OK**.

Boundary Condition—Convection and Diffusion

1 From the **Physics** menu, select **Boundary Settings**.

2 Select both boundaries and enter the following conditions; when done, click **OK**.

PAGE	c6	c7	c8
Type	Concentration	Concentration	Concentration
Value	c60	c70	c80

MESH GENERATION

Generate the mesh in the same way as in Model 1.

COMPUTING THE SOLUTION

Use the same solver settings as in Model 1.

Liquid Chromatography

Introduction

Chromatography is an important group of methods to separate closely related components of complex mixtures. The following examples simulate the separation in High Performance Liquid Chromatography (HPLC). In this technique an injector introduces a sample as a zone in a liquid mobile phase. The mobile phase containing the sample zone is pumped through a column containing a solid stationary phase; Figure 10-8 shows a diagram of such an instrument.

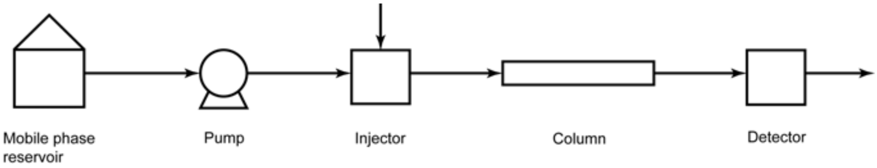


Figure 10-8: Diagram of an HPLC system.

The mobile and stationary phases are chosen so that the sample components are distributed to varying degrees between the two phases. Those components that strongly adsorb to the stationary phase move only slowly with the flow of the mobile phase, and those that are weakly adsorbed move more rapidly. As the sample zones migrate through the column, the components are separated into discrete zones that are recognized in a detector, situated after the outlet of the column.

Model Definitions

The first two models study the separation of two species under conditions of non-linear chromatography, where the analyte concentration is high, and in a 1D geometry. The first model considers only the column itself. The second model considers a complete system, from injector to detector. The third model examines the transport of a single band of solute through a column under conditions of linear chromatography, where the analyte concentration is low, but in a complex 3D geometry[1]. In addition, it factors in temperature rise effects due to viscous friction.

---

[1] Courtesy of Bernard Bunner, Waters Corporation.

DEFINITION—MODEL I

The mass transport equation is valid for the analyte component during its migration through the chromatographic column. If you neglect the dispersion of the chromatographic zone during the migration, the mass transport equation takes the form

$$S\frac{\rho(1-\varepsilon)}{\varepsilon}\cdot\frac{\partial n_i}{\partial t}+\frac{\partial c_i}{\partial t} = -\frac{\mathrm{v}}{\varepsilon A}\cdot\frac{\partial c_i}{\partial x} \qquad (10\text{-}14)$$

where S denotes the surface area of the particles in the column (m^2/kg), ρ denotes the density of the solid particles (kg/m^3), ε equals the column porosity, A gives the inner area of the column tube, n_i equals the analyte concentration in the stationary phase of component i ($\mathrm{mol}/\mathrm{m}^2$), v is the mobile phase flow (m^3/s), and c_i equals the analyte concentration in the mobile phase of component i ($\mathrm{mol}/\mathrm{m}^3$).

The ideal model for chromatography assumes that the equilibrium for the analyte between the mobile and stationary phases is immediate, that is,

$$\frac{\partial n}{\partial t} = \left(\frac{dn}{dc}\right)\cdot\frac{\partial c_i}{\partial t}\ . \qquad (10\text{-}15)$$

The mass transport equation for the ideal chromatography model therefore becomes

$$\left(1+S\frac{\rho(1-\varepsilon)}{\varepsilon}\cdot\frac{dn}{dc}\right)\cdot\frac{\partial c_i}{\partial t} = -\frac{v}{\varepsilon A}\frac{\partial c_i}{\partial x}\ . \qquad (10\text{-}16)$$

The dispersion or band broadening of the analyte zone that is obtained during the migration through the column is a result of a great number of random processes that the analyte experiences (for example, inhomogeneous flow and diffusion in pores and the mobile phase). It is therefore possible to formally express the band broadening as a diffusion process with an effective diffusion constant, D_{eff}. Thus, D_{eff} is a measure of the chromatographic system's efficiency for a particular analyte. This constant is closely related to the concept of the height equivalent of a theoretical plate, H, that is customarily used in chromatographic practice. It can be shown that

$$D_{\mathrm{eff}} = \frac{Hv_{zi}}{2} \qquad (10\text{-}17)$$

where v_{zi} is the migration velocity of the analyte zone through the column. A mass balance that includes the zone-dispersion term gives the following equation:

$$\left(1+\Phi\cdot\frac{dn}{dc}\right)\cdot\frac{\partial c_i}{\partial t} = -v_1\frac{\partial c_i}{\partial x}+D_{\mathrm{eff}}\frac{\partial^2 c_i}{\partial x^2} \qquad (10\text{-}18)$$

Here $\Phi = S\rho(1-\varepsilon)/\varepsilon$ denotes the phase ratio of the column ($\mathrm{m}^2/\mathrm{m}^3$), $v_1 = v/(\varepsilon A)$ gives the linear velocity of the mobile phase in the column (m/s), and D_{eff} is the effective diffusion constant (m^2/s).

This first example covers the migration within the column of two components. The adsorption isotherm for both components is assumed to follow a Langmuir adsorption isotherm, that is,

$$n_i = \frac{n_{0i}K_ic_i}{1+K_ic_i} \qquad (10\text{-}19)$$

and

$$\frac{dn_i}{dc_i} = \frac{n_{0i}K_i}{(1+K_ic_i)^2} \qquad (10\text{-}20)$$

where K_i is the adsorption constant for component i ($\mathrm{m}^3/\mathrm{mol}$), and n_{0i} is the monolayer capacity of the stationary phase for component i ($\mathrm{mol}/\mathrm{m}^2$).

INPUT DATA

This example looks at the migration of a chromatographic zone migrating only within the column. The physical data for the column correspond to a 12 cm×4 mm inner diameter column filled with 5 µm porous particles ($\varepsilon_{\mathrm{column}} = 0.6$) with a specific surface area of 100 m^2/g, which gives a column phase ratio, Φ, of $1.533\cdot10^8\ \mathrm{m}^{-1}$. Additional input data appear in Table 10-1.

TABLE 10-1: INPUT DATA

NAME	VALUE
v_1	2.22 mm/s
D_{eff1}	$1\cdot10^{-8}$ m^2/s
D_{eff2}	$3\cdot10^{-8}$ m^2/s
K_1	0.04 $\mathrm{m}^3/\mathrm{mol}$
n_{01}	$1\cdot10^{-6}$ $\mathrm{mol}/\mathrm{m}^2$
K_2	0.05 $\mathrm{m}^3/\mathrm{mol}$
n_{02}	$5\cdot10^{-7}$ $\mathrm{mol}/\mathrm{m}^2$

The initial concentrations for the two components are described by the normal distribution

$$c_{i0}(x) = c_{0i} \cdot e^{-a(x-0.01)^2} \qquad (10\text{-}21)$$

where a equals $1 \cdot 10^5$ m^{-2}, and the starting point at $t = 0$ is at $x = 0.01$ m. You first solve the model for the initial injector concentrations $c_{01} = c_{02} = 0.1$ mol/m^3, which corresponds to the linear regime for the adsorption isotherm. In a second stage, you increase the injector concentrations to $c_{01} = 1$ mol/m^3 and $c_{02} = 10$ mol/m^3.

DEFINITION—MODEL 2

The second example studies a complete chromatographic system. The analyte is introduced through an injector at $t = 0$ and then transported in a tube to the column inlet. The initial concentration at the injector is $c_{01} = 1$ mol/m^3 and $c_{02} = 10$ mol/m^3. In the injector, the initial concentration profile is a pulse that is smoothed at the end points. When the analyte has migrated through the column, it is eluted into a tube and then transported to the detector. Figure 10-9 shows the setup.

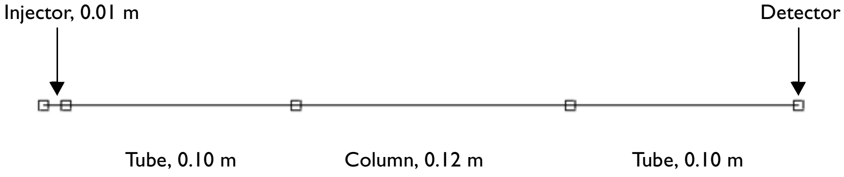


Figure 10-9: Geometry of the simulated model.

The injector volume is 20 µl (corresponding to an inner diameter of 1.6 mm), and the volumetric flow is 1 ml/min, which gives a linear velocity through the injector of v_{li} = 0.0083 m/s. The tube that connects the injector and the column has an inner diameter of 0.25 mm and is 10 cm long. These dimensions result in a linear velocity through the tube of 0.333 m/s. The tube's dimensions between the column and the detector are the same as the previous tube. The data characteristic for the column and the analytes are the same as in the previous example.

DEFINITION—MODEL 3

This model was provided by Bernard Bunner of Waters Corporation.

A bed of particles of diameter d_p = 1.7 um is packed inside a 5 cm long, 2.1 mm diameter stainless steel column. The bed is held in place by 1 mm thick, 2.1 mm diameter frits at both ends of the column. Steel tubes are attached at both ends to provide fluid connections to the injector and detector. You will model the bed as well as the frits as porous subdomains. The problem's symmetry allows for a 2D axisymmetric model geometry.

The analysis includes flows in the column interior and in the pipes. The model computes the temperature rise due to viscous friction, accounting for the temperature dependences in both the fluid viscosity and diffusion coefficient.

Once you have computed the velocities and temperature field, you use the solution to calculate the transport by convection-diffusion of a narrow band of analyte that enters the inlet tube, travels through the column interior, and exits via the outlet tube.

Momentum transport

Unlike the examples of model 1 and 2, you assume that the analyte concentration is very small, and that the analyte does not have an influence on the viscosity and density, so that the flow problem is steady-state. Hence, the mass balance includes the continuity equation:

$$\nabla \cdot \mathbf{u} = 0 \tag{10-22}$$

The Navier-Stokes equations govern the flow in the pipes:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla \cdot [p\mathbf{I} + (-\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))] = 0 \tag{10-23}$$

Here ρ is the density (kg/m^3), η denotes the viscosity (kg/(m· s)), and p refers to the pressure (Pa).

In the porous subdomains (that is, the packed bed and frits) the Brinkman equations apply:

$$\frac{\eta}{\kappa}\mathbf{u} + \nabla \cdot \left[p\mathbf{I} - \frac{\eta}{\varepsilon}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\right] = 0 \tag{10-24}$$

Here ε is the porosity and κ is the hydraulic permeability (m^2) of the porous medium, for the latter you use the following formula:

$$\kappa = \frac{(d_p)^2\varepsilon^3}{180(1-\varepsilon)^2} \tag{10-25}$$

The momentum transport boundary conditions are axial symmetry at $r = 0$:

$$\begin{aligned} p &= p_{\mathrm{in}} && \text{inlet} \\ p &= 0 && \text{outlet} \\ \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} &= 0 && \text{inlet/outlet} \end{aligned} \qquad (10\text{-}26)$$

and no-slip conditions at all the other interior walls of the column.

Heat transport

The trend towards higher performance has led to the use of smaller particles for beds. However, smaller particles create larger back pressures, which can lead to significant heat generation through viscous friction inside the bed. In turn, this can lead to significant variations in the temperature across the column—and hence in the viscosity and the diffusion coefficient as well.

The temperature field is computed for the column interior, the tubes, and the column walls. The heat transport equation is

$$\rho c_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q \qquad (10\text{-}27)$$

where k is the thermal conductivity, and the heat source inside the bed is modeled as

$$Q = -v\frac{\partial p}{\partial z} \qquad (10\text{-}28)$$

Within the column walls, Equation 10-27 is reduced to a heat conduction equation.

The boundary conditions are the following: insulation on the tube walls and column outer walls, axial symmetry at $r = 0$, convective flux at the outlet, and

$$T = T_{\mathrm{in}} \quad \text{inlet} \qquad (10\text{-}29)$$

The temperature variation of the viscosity is modeled by

$$\eta = 10^{-3}\exp(-0.02\ \mathrm{K}^{-1}(T - 293\ \mathrm{K}))\ \ \mathrm{Pa{\cdot}s} \qquad (10\text{-}30)$$

The molecular diffusion coefficient depends on the viscosity according to the Wilke-Chang relation

$$D_{\mathrm{mol}}(T) = D_{\mathrm{mol}}(T_0)\frac{T}{\eta(T)} \qquad (10\text{-}31)$$

which together with Equation 10-30 gives

$$D_{\mathrm{mol}} = 10^{-9}\frac{T}{293\ \mathrm{K}}\exp(0.02\ \mathrm{K}^{-1}(T-293\ \mathrm{K}))\ \ \mathrm{m}^2/\mathrm{s} \tag{10-32}$$

In this example, you model the propagation of the Gaussian analyte-concentration peak

$$c_{\mathrm{in}}(t) = c_0\exp[-a_0(t-t_0)^2] \tag{10-33}$$

where $c_0 = 1\ \mathrm{mol/m}^3$, $t_0 = 1$ s, and $a_0 = 5\ \mathrm{s}^{-2}$. At the inlet, the pressure is $p_{\mathrm{in}} = 5.45\cdot10^7$ Pa, and the temperature is $T_{\mathrm{in}} = 303$ K.

Analyte transport

For the free flow domains, the total molar flux of analyte is

$$\mathbf{N} = -D_{\mathrm{mol}}\nabla c + c\mathbf{u} \tag{10-34}$$

where c is the molar concentration of analyte (mol/m^3), $\mathbf{u}$ is the velocity (m/s), and D_{mol} is the diffusion coefficient (m^2/s). The mass balance gives the following convection and diffusion transport equation for the analyte:

$$\frac{\partial c}{\partial t} + \nabla\cdot\mathbf{N} = 0 \tag{10-35}$$

For the porous subdomains, use the superficial volume-averaged molar flux (that is, the number of moles transferred per unit area and time):

$$\mathbf{N} = -\varepsilon D_{\mathrm{eff}}\nabla c + c\mathbf{u} \tag{10-36}$$

Here $\mathbf{u}$ is the superficial volume-averaged velocity of the mobile phase, ε is the porosity, and D_{eff} is the effective diffusion coefficient.

Note that c in Equation 10-36 presents the intrinsic volume-averaged molar concentration of analyte (mol/m^3), which is the number of moles per unit volume of the mobile phase. The resulting transport equation for the analyte in the porous subdomains is

$$\varepsilon\frac{\partial c}{\partial t} + \nabla\cdot\mathbf{N} = 0 \tag{10-37}$$

For the porous subdomains, model the diffusion using the Van Deemter equation

$$H(|\mathbf{u}|) = 1.5d_p + \frac{D_{\mathrm{mol}}}{|\mathbf{u}|} + \frac{(d_p)^2|\mathbf{u}|}{6D_{\mathrm{mol}}} \tag{10-38}$$

and the effective diffusion coefficient

$$D_{\mathrm{eff}} = 0.5|\mathbf{u}|H(|\mathbf{u}|) \tag{10-39}$$

where d_p is the particle diameter, and

$$|\mathbf{u}| = \frac{1}{\varepsilon}\sqrt{u^2 + v^2} \tag{10-40}$$

is the absolute linear velocity.

Both concentration and flux remain continuous across the boundaries of the adjacent porous and free-flow subdomains, as defined above. This allows you to use a single convection and diffusion mode for modeling the analyte transport.

Use the following boundary conditions:

- axial symmetry at $r = 0$
- concentration at the inlet:

$$c = c_{\mathrm{in}}(t) \tag{10-41}$$

- convective flux at the outlet:

$$\mathbf{n} \cdot (-D_{\mathrm{mol}} \nabla c) = 0 \tag{10-42}$$

At all other interior column and tube walls, insulation conditions apply.

Results and Discussion

MODEL I

Figure 10-10 shows the zones of the two components at various times (0 s, 80 s, and 160 s) as they migrate within the column. In this example, the analyte concentration at $t = 0$ is low for both components ($c_{0i} = 0.1\ \mathrm{mol/m^3}$); the solution is in the linear domain of the adsorption isotherm. This implies that the zones are symmetrical and normally distributed.

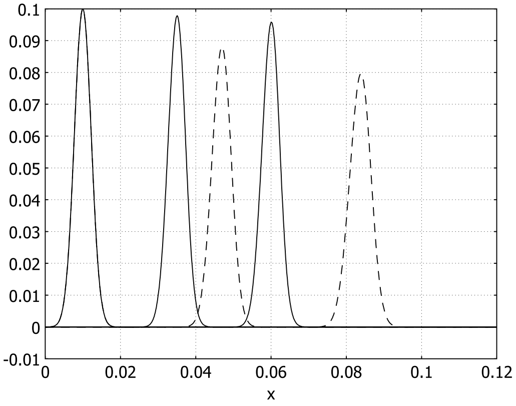


Figure 10-10: The concentrations of components 1 (solid) and 2 (dashed) in the mobile phase during the migration through the column at times 0, 80, and 160 s for initial injector concentrations $c_{01} = c_{02} = 0.1$ *mol/m*^{3}*.*

When the initial concentrations increase, $c_{01} = 1$ mol/m^3 and $c_{02} = 10$ mol/m^3, the solution enters into the nonlinear domain of the adsorption isotherm, changing the behavior radically (see Figure 10-11). A comparison of the zone for component 2 between the two simulations clearly shows that both the zone width and form is strongly influenced by migrating into the adsorption isotherm's nonlinear domain.

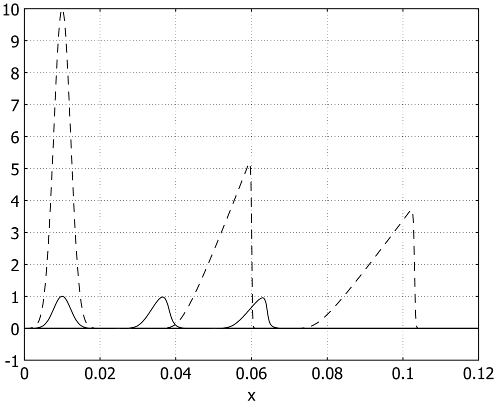


Figure 10-11: The concentrations of components 1 (solid) and 2 (dashed) in the mobile phase during migration through the column at times 0 s, 80 s, and 160 s for initial injector concentrations $c_{01} = 1$ *mol/m*^{3} *and* $c_{02} = 10$ *mol/m*^{3}*.*

MODEL 2

The second example studies the migration process from the injector, through the column, and to the detector. The initial concentration of the components in the injector is $c_{01} = 1\ \mathrm{mol/m^3}$ and $c_{02} = 10\ \mathrm{mol/m^3}$, and the characteristic data for the column and the two components are the same as in previous example. Figure 10-12 displays the zone for the two components at $t = 4$ s, 80 s, and 160 s.

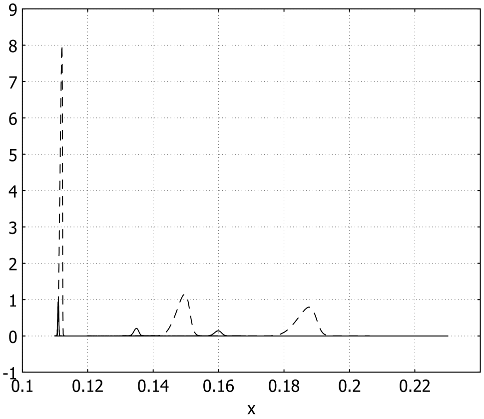


Figure 10-12: The concentration of components 1 (solid lines) and 2 (dashed lines) in the mobile phase during migration through the column at times 4, 80, and 160 s. In the injector, the concentrations of the components at t = 0 are $c_{01} = 1\ \mathrm{mol/m^3}$ and $c_{02} = 10\ \mathrm{mol/m^3}$.

At $t = 4$ s, the two components have just entered the column, and they have accumulated into very narrow zones close to the column inlet at $x = 0.11$ m. It is interesting to look at the concentration profile of the zones during the accumulation process at the column inlet. Figure 10-13 shows the concentration for component 2 in the mobile phase and stationary phase as well as the total column concentration at $t = 2.0$ s. At this time the component has not completely entered the column and the concentration in the tube prior to the column inlet ($x < 0.11$ m) is still non-zero. The figure illustrates the strong accumulation at the column inlet, and, additionally, the zone has a non-Gaussian form. When the components have migrated through the column they are transported to a detector, and Figure 10-14 shows the chromatogram as it is obtained by the chromatographer.

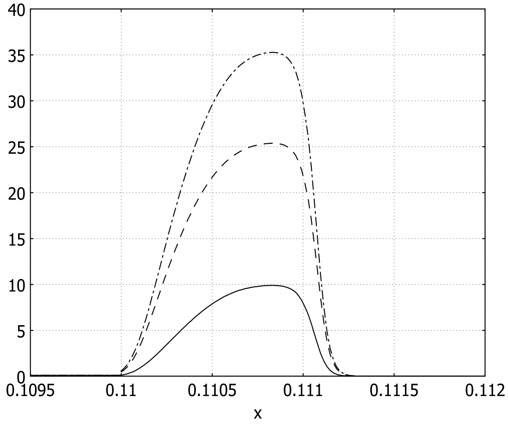


Figure 10-13: Close-up of the concentration profile of component 2 during the entrance into the column. The solid line corresponds to the mobile phase concentration, the dashed line to the stationary phase concentration, and the dash-dotted line to the sum of mobile and stationary phase concentrations.

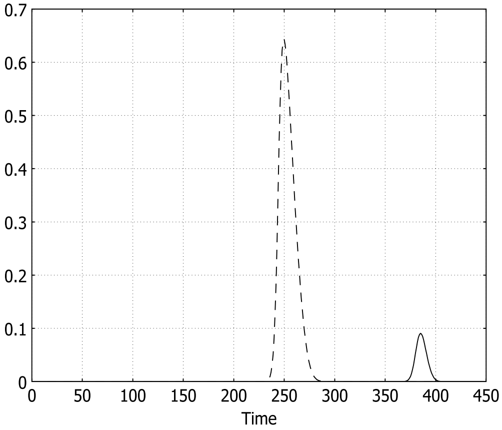


Figure 10-14: The chromatogram registered by the detector. The solid and dashed lines show the concentrations c_1 and c_2, respectively, as functions of time.

MODEL 3

The flow discharge of 0.58 ml/min is calculated. Figure 10-15 shows the temperature distribution within the column. The temperature rise is caused by friction in the bed, and the maximum temperature increase is about 18 degrees.

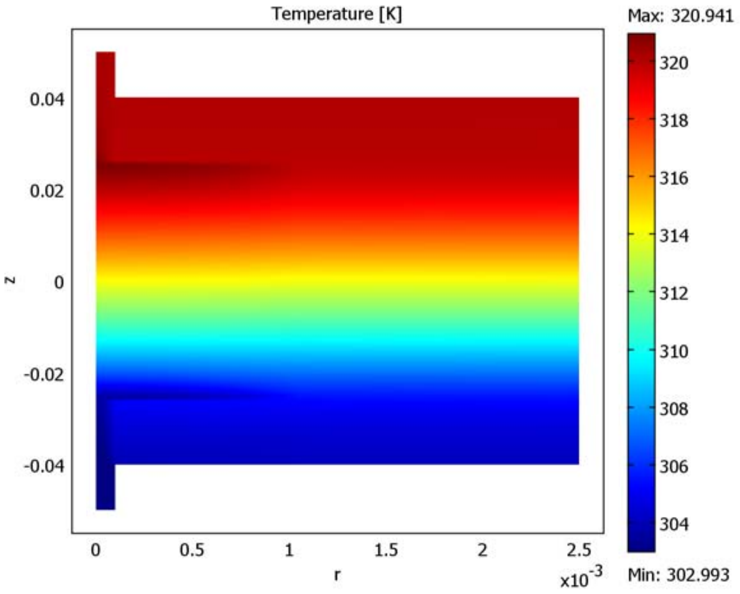


Figure 10-15: Temperature distribution.

Figure 10-16 illustrates the band broadening of the peak in terms of the total analyte flux, Φ_{tot}, obtained by integrating over the cross-section areas of the inlet and outlet tubes (R denotes the tube radius):

$$\Phi_{\text{tot}}(z, t) = 2\pi\int_0^R \left(-D\frac{\partial c}{\partial z} + cv\right) r\,dr \quad (\text{mol/s}) \tag{10-43}$$

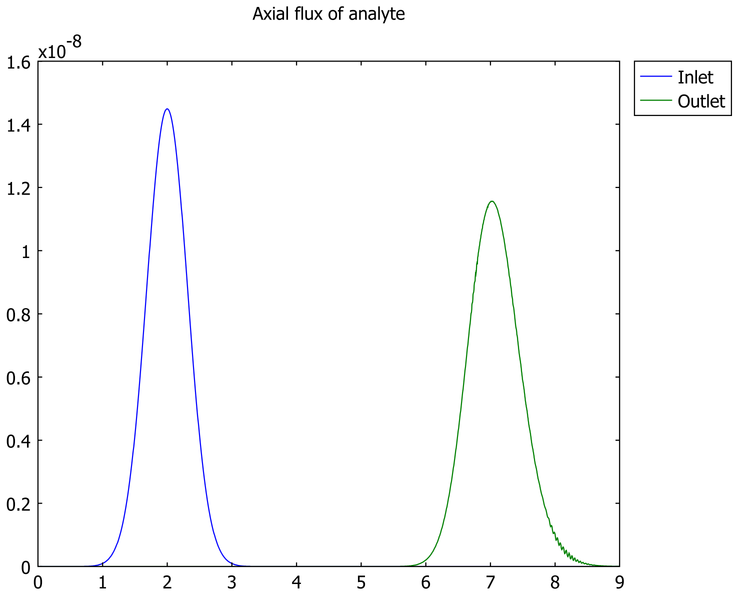


Figure 10-16: Analyte flux through inlet (blue) and outlet (green) as functions of time.

References

1. D. DeVault, *J. Am. Chemical Soc.*, vol. 65, p. 532, 1943.

2. S. Golshan-Shirazi and G. Guiochon, *Analytical Chemistry*, vol. 60, p. 2364, 1988.

3. B. Lin and G. Guiochon. *Modeling for Preparative Chromatography*, Elsevier Publishing, Amsterdam, 2003.

Model Library path: `Chemical_Engineering_Module/ Electrophoresis_and_Chromatography/liquid_chromatography_1`

Modeling Using the Graphical User Interface—Model 1

1 Start COMSOL Multiphysics.

2 In the **Model Navigator** select **1D** from the **Space dimension** list.

3 From the **Application Modes** list, select **Chemical Engineering Module>Mass Transport>Convection and Diffusion>Transient analysis**. In the **Dependent variables** edit field, type `c1 c2`.

4 Click **OK**.

OPTIONS AND SETTINGS

Enter the following constants in the **Options/Constants** dialog box:

NAME	EXPRESSION	DESCRIPTION
`Phi`	`1.533e8[1/m]`	`Phase ratio`
`v_l`	`2.22[mm/s]`	`Linear velocity, mobile phase`
`D_eff1`	`1e-8[m^2/s]`	`Effective diffusion constant, component 1`
`D_eff2`	`1e-8[m^2/s]`	`Effective diffusion constant, component 2`
`c01`	`0.1[mol/m^3]`	`Initial injector concentration, component 1`
`c02`	`0.1[mol/m^3]`	`Initial injector concentration, component 2`
`K1`	`0.04[m^3/mol]`	`Adsorption constant, component 1`
`K2`	`0.05[m^3/mol]`	`Adsorption constant, component 2`
`n01`	`1e-6[mol/m^2]`	`Monolayer capacity, component 1`
`n02`	`5e-7[mol/m^2]`	`Monolayer capacity, component 2`
`a`	`1e5[1/m^2]`	`Normal-distribution parameter`
`x0`	`0.01[m]`	`Starting point`

GEOMETRY MODELING

1 Select **Draw>Specify Objects>Line**.

2 In the **Coordinates** edit field, type `0 0.12`.

3 Click **OK**.

4 Click the **Zoom Extents** button on the Main toolbar.

PHYSICS SETTINGS

In order to define the problem, you must define two expression variables on the subdomain level.

1 Select **Options>Expressions>Scalar Expressions**.

2 Enter expressions for dn_i/dc_i according to this table; when done, click **OK**.

NAME	EXPRESSION
`dn1_dc1`	`n01*K1/(1+K1*c1)^2`
`dn2_dc2`	`n02*K2/(1+K2*c2)^2`

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**. Select Subdomain 1.

2 Enter subdomain settings for species 1 as follows:

PROPERTY	VALUE
δ_{ts}	`1+Phi*dn1_dc1`
D	`D_eff1`
R	`0`
u	`v_l`

3 Enter subdomain settings for species 2 as follows:

PROPERTY	VALUE
δ_{ts}	`1+Phi*dn2_dc2`
D	`D_eff2`
R	`0`
u	`v_l`

4 Click the **Artificial Diffusion** button.

5 Select the **Streamline diffusion** check box.

6 Select **Anisotropic diffusion** from the list and type `0.05` in the **Tuning parameter** edit field. Note that artificial diffusion should be used only for species 2.

7 On the **Init** page, enter these initial values:

VARIABLE	INITIAL VALUE
$c1(t_0)$	`c01*exp(-a*(x-x0)^2)`
$c2(t_0)$	`c02*exp(-a*(x-x0)^2)`

8 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter boundary conditions for species 1 as follows:

SETTINGS	BOUNDARY 1	BOUNDARY 2
Type	Concentration	Convective flux
$c1_0$	0	-

3 Enter boundary conditions for species 2 as follows:

SETTINGS	BOUNDARY 1	BOUNDARY 2
Type	Concentration	Convective flux
$c2_0$	0	-

4 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 Click the **Custom mesh size** button and type `3e-4` in the **Maximum element size** edit field.

3 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Time stepping** area, type `0:10:180` in the **Times** edit field.

3 Set the **Relative tolerance** to `1e-4` and the **Absolute tolerance** to `1e-7`.

4 Click **OK**.

5 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To reproduce the plots in Figure 10-10, perform the following steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 From the **Solutions to use** list, select **0**, **80**, and **160**.

3 On the **Line/Extrusion** page, select Subdomain 1.

4 In the **Expression** edit field in the **y-axis data** area, type `c1`.

5 From the **x-axis data** list, select **x**.

6 Click the **Line Settings** button. Set the **Line color** to black, then click **OK**.

7 Click **Apply** to generate the graphs of c_1.

8 In the **Expression** edit field, type `c2`.

9 Click the **Line Settings** button. Set the **Line style** to **Dashed line**, then click **OK**.

10 On the **General** page, select the **Keep current plot** check box.

11 Click the **Title/Axis** button. In the **Title/Axis Settings** dialog box, click the option buttons next to the **Title** and **Second axis label** edit fields (leave the edit fields empty). Click **OK**.

12 Click **OK** to finalize the plot and close the **Domain Plot Parameters** dialog box.

Next, increase the initial injector concentrations and solve the model again.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Change the values of `c01` and `c02` to `1[mol/m^3]` and `10[mol/m^3]`, respectively.

3 Click **OK**.

SOLVING THE MODEL

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Reproduce the plots in Figure 10-11 with the following steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 On the **General** page, select **0**, **80**, and **160** from the **Solutions to use** list.

3 Clear the **Keep current plot** check box, then click **Apply** to generate the c_2 graphs.

4 Select the **Keep current plot** check box.

5 On the **Line/Extrusion** page, type `c1` in the **Expression** edit field.

6 Click the **Line Settings** button. Set the **Line style** to **Solid line**, then click **OK**.

7 Click **OK**.

Model Library path: `Chemical_Engineering_Module/Electrophoresis_and_Chromatography/liquid_chromatography_2`

Modeling Using the Graphical User Interface—Model 2

Use the same application mode settings as in Model 1.

OPTIONS AND SETTINGS

In addition to the constants defined in Model 1, add the following ones:

NAME	EXPRESSION	DESCRIPTION
`A_i`	`2.01e-6`	`Time-scaling coefficient, injector`
`A_t`	`4.91e-8`	`Time-scaling coefficient, tube`
`A_c`	`7.54e-6`	`Time-scaling coefficient, column`
`D1`	`1.0e-9[m^2]`	`Diffusion coefficient, component 1`
`D2`	`5.0e-10[m^2]`	`Diffusion coefficient, component 2`
`V`	`1.67e-8[m/s]`	`Flow velocity`

GEOMETRY MODELING

1. Click the **Draw Mode** button on the Main toolbar.
2. Select the existing line by clicking on it.
3. Click the **Move** button on the Draw toolbar.
4. In the **Displacement** edit field, type `0.11`. Click **OK**.
5. Specify three more lines with the following properties:

LINE	COORDINATES
L2	`0 0.01`
L3	`0.01 0.11`
L4	`0.23 0.33`

PHYSICS SETTINGS

Subdomain Settings

To simplify the subdomain settings, first define three variables on the subdomain level.

1. From the **Options** menu, select **Expressions>Subdomain Expressions**.
2. Define the variables `A`, `n1`, and `n2` in the different subdomains as follows:

VARIABLE	SUBDOMAIN 1	SUBDOMAINS 2, 4	SUBDOMAIN 3
`A`	`A_i`	`A_t`	`A_c`
`n1`	`0`	`0`	`n01*K1*c1/(1+K1*c1)`
`n2`	`0`	`0`	`n02*K2*c2/(1+K2*c2)`

3. Click **OK**.
4. From the **Physics** menu, select **Subdomain Settings**.

5 Enter subdomain settings for species 1 according to the following table:

SETTINGS	SUBDOMAINS 1, 2, 4	SUBDOMAIN 3
δ_{ts}	`A`	`A*(1+Phi*dn1_dc1)`
D	`A*D1`	`A*D_eff1`
u	`V`	`V`

Artificial stabilization for species 1 is needed in Subdomains 1 and 2.

6 From the **Subdomain selection** list, select Subdomains 1 and 2.

7 Click the **Artificial Diffusion** button.

8 Select the **Streamline diffusion** check box, then select **Anisotropic diffusion**, and type `0.05` in the **Tuning parameter** edit field. Click **OK**.

9 Enter subdomain settings for species 2 according to the following table:

SETTINGS	SUBDOMAINS 1, 2, 4	SUBDOMAIN 3
δ_{ts}	`A`	`A*(1+Phi*dn2_dc2)`
D	`D2*A`	`D_eff2*A`
u	`V`	`V`

Artificial stabilization for species 2 is needed in all subdomains.

10 Select all four subdomains and click the **Artificial Diffusion** button.

11 Select the **Streamline diffusion** check box. Select **Anisotropic diffusion** and type `0.2` in the **Tuning parameter** edit field. Click **OK**.

12 The initial values in Model 2 are zero for both species in Subdomains 2, 3, and 4. In Subdomain 1, set **c1(t_0)** to `c01` and **c2(t_0)** to `c02`.

13 Click **OK**.

Boundary Conditions

Use the same boundary conditions as in Model 1, that is, zero concentrations at the inlet (Boundary 1) and convective flux conditions at the outlet (Boundary 5) for both species.

Mesh Generation

1 From the **Mesh** menu, choose **Free Mesh Parameters**.

2 On the **Global** page click the **Custom mesh size** button and enter `5e-3` in the **Maximum element size** edit field.

3 Go to the **Subdomain** page.

4 Select Subdomain 3 and type `1e-4` in the **Maximum element size** edit field.

5 Go to the **Boundary** page.

6 Select Boundaries 1, 2, 3, and 4. Type `1e-5` in the **Maximum element size** edit field.

7 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Keep the solver settings as in Model 1 but change the **Times** to `0:0.05:1.95 2:450` in the **Time stepping** frame. Compute the solution by clicking the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

You create Figure 10-12 on page 644 in the same way as you did Figure 10-10 on page 643, but his time do so for output times of 4 s, 80 s, and 160 s and in Subdomain 3.

To create Figure 10-13 on page 645, follow these steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 From the **Solutions to use** list, select **2**.

3 Click the **Line/Extrusion** tab.

4 From the **Subdomain selection** list, select Subdomains 2 and 3.

5 In the **y-axis data** area, type `c2` in the **Expression** edit field.

6 From the **x-axis data** list, select **x**.

7 Click the **Line Settings** button. From the **Line style** list, select **Solid line**. Click **OK**.

8 Click **Apply** to generate the graph of c_2.

9 On the **General** page, select the **Keep current plot** check box.

10 Return to the **Line/Extrusion** page. In the **y-axis data** area, type `Phi*n2` in the **Expression** edit field.

11 Click the **Line settings** button. Change **Line style** to **Dashed line**, then click **OK**.

12 Click **Apply** to generate the graph of Φn_2.

13 Finally, type `c2+Phi*n2` in the **Expression** edit field for the **y-axis data**.

14 Click the **Line settings** button. Change **Line style** to **Dash-dot line**, then click **OK**.

15 Click **OK** to plot $c_2 + \Phi n_2$ and close the dialog box.

16 In the figure window, use the **Zoom Window** tool to zoom in near the point connecting Subdomains 2 and 3.

To reproduce the plots in Figure 10-14 on page 645, follow these steps:

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.
2. Select all the output times in the **Solutions to use** list.
3. Click the **Point** tab.
4. From the **Boundary selection** list, select Boundary 5.
5. In the **y-axis data** area, type `c1` in the **Expression** edit field.
6. Click the **Line Settings** button.
7. Click the **Color** button. In the **Line color** dialog box, select black. Click **OK**.
8. From the **Line style** list, select **Solid line**. Click **OK**.
9. Back in the **Domain Plot Parameters** dialog box, click **Apply**.
10. On the **General** page, select the **Keep current plot** check box.
11. Return to the **Point** page and type `c2` in the **Expression** edit field.
12. Click the **Line Settings** button.
13. From the **Line style** list, select **Dashed line**. Click **OK**.
14. Click **OK** to finalize the plot and close the **Domain Plot Parameters** dialog box.

Model Library path: `Chemical_Engineering_Module/Electrophoresis_and_Chromatography/liquid_chromatography_3`

Modeling Using the Graphical User Interface—Model 3

1. Start COMSOL Multiphysics.
2. In the **Model Navigator** select **Axial symmetry (2D)** from the **Space dimension** list, then click the **Multiphysics** button.
3. From the **Application Modes** list, select **Chemical Engineering Module>Mass Transport>Convection and Diffusion>Transient analysis**. Click **Add**.
4. From the **Application Modes** list, select **Chemical Engineering Module>Momentum Transport>Laminar Flow>Incompressible Navier-Stokes>Steady-state analysis**.
5. From the **Element** list, select P_2P_{-1}, then click **Add**.
6. From the **Application Modes** list, select **Chemical Engineering Module>Energy Transport>Convection and Conduction>Steady-state analysis**. Click **Add**.
7. Click **OK**.

GEOMETRY MODELING

1 Press the Shift key and click the **Rectangle/Square** button on the Draw toolbar.

2 In the **Size** area of the **Rectangle** dialog box, set the **Width** to `1.05e-3` and the **Height** to `5e-2`. In the **Position** area, set **r** to `0` and **z** to `-2.5e-2`. Click **OK** to create the rectangle R1.

3 Repeat this procedure to create five more rectangles with the following properties:

SETTINGS	R2	R3	R4	R5	R6
Width	1.05e-3	1.05e-3	1e-4	1e-4	2.5e-3
Height	1e-3	1e-3	2.4e-2	2.4e-2	8e-2
r	0	0	0	0	0
z	2.5e-2	-2.6e-2	2.6e-2	-5e-2	-4e-2

4 Double-click the **EQUAL** button in the status bar at the bottom of the user interface.

5 Click the **Zoom Extents** button on the Main toolbar.

6 Click in the drawing area and then press Ctrl+A to select all six rectangles. Ctrl-click rectangle R6 to remove it from the selection.

7 Press Ctrl+C to copy the rectangles R1 through R5, then press Ctrl+V. In the **Paste** dialog box, click **OK** to paste the copies, R7 through R11, without displacement.

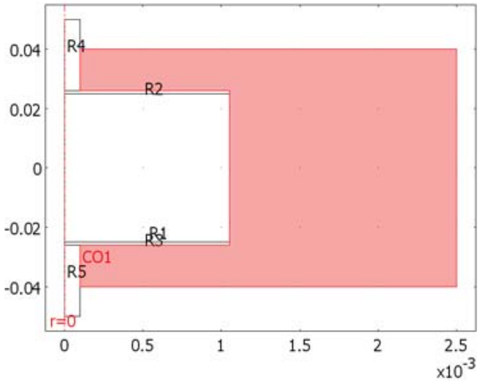
8 From the **Draw** menu, select **Create Composite Object**.

9 In the **Object selection** list, select **R6**, **R7**, **R8**, **R9**, **R10**, and **R11**.

10 In the **Set formula** edit field, edit the expression to read `R6-(R7+R8+R9+R10+R11)`.

11 Click **OK** to create the composite object CO1.

The geometry-modeling stage is now complete, and the result in the drawing area on your screen should look as in the figure below.



OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Constants** dialog box.

2 Enter the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho`	`1000[kg/m^3]`	`Fluid density`
`dp_bed`	`1.7[um]`	`Particle size for packed bed`
`dp_frit`	`3.5[um]`	`Particle size for frits`
`void_bed`	`0.4`	`Bed porosity`
`void_frit`	`0.4`	`Frit porosity`
`p_in`	`54.5[MPa]`	`Inlet pressure`
`p_out`	`0[Pa]`	`Outlet pressure`
`T_in`	`303[K]`	`Inlet temperature`
`c0`	`1[mol/m^3]`	`Inlet concentration peak maximum, c0*exp(-a0*(t-t0)^2)`
`t0`	`2[s]`	`Peak center time`
`a0`	`5[1/s^2]`	`Peak shape parameter`
`Cp`	`2.9[kJ/(kg*K)]`	`Heat capacity of fluid`
`k_f`	`0.25[W/(m*K)]`	`Thermal conductivity of fluid`
`k_e`	`0.5[W/(m*K)]`	`Thermal conductivity of bed and frit`
`k_s`	`15[W/(m*K)]`	`Thermal conductivity of column walls`
`eta0`	`1e-3[Pa*s]`	`Viscosity of fluid at T=293K`
`D_mol0`	`1e-9[m^2/s]`	`Molecular diffusion coefficient at T=293K`
`z_in`	`-5[cm]`	`Inlet position`
`z_out`	`5[cm]`	`Outlet position`

3 From the **Options** menu, point to **Expressions** and select **Subdomain Expressions**.

4 Enter the following expressions; when done, click **OK**.

SUBDOMAINS	NAME	EXPRESSION
1–5	`D_mol`	`D_mol0*exp(0.02[1/K]*(T-293[K]))*T/(293[K])`
1–5	`eta`	`eta0*exp(-0.02[1/K]*(T-293[K]))`
2–4	`u_lin`	`U_chns/epsilonp_chns`
2–4	`H_eff`	`1.5*dp+D_mol/u_lin+dp^2*u_lin/(6*D_mol)`
2–4	`D_eff`	`0.5*H_eff*u_lin`

SUBDOMAINS	NAME	EXPRESSION
2–4	`epsilon`	`dp^2*epsilonp_chns^3/(180*(1-epsilonp_chns)^2)`
2, 4	`dp`	`dp_frit`
3	`dp`	`dp_bed`

PHYSICS SETTINGS

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, select **1 Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 6, then clear the **Active in this domain** check box.

4 Select Subdomains 1–5. Set the **r-velocity** to `u` and the **z-velocity** to `v`.

5 Select Subdomains 1 and 5. In the **D (isotropic)** edit field, type `D_mol`.

6 Select Subdomains 2–4. In the **D (isotropic)** edit field type `D_eff*epsilonp_chns`, and in the δ_{ts} edit field type `epsilonp_chns`.

7 Click **OK**.

Subdomain Settings—Incompressible Navier Stokes

1 From the **Multiphysics** menu, select **2 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 6, then clear the **Active in this domain** check box.

4 Select Subdomains 1–5. In the ρ edit field type `rho`, and in the η edit field type `eta`.

5 Click the **Artificial Diffusion** button. Clear the **Streamline diffusion** check box, then click **OK**.

6 Select Subdomains 2–4. Select the **Flow in porous media (Brinkman equations)** check box, then type `epsilon` in the κ edit field.

7 Select Subdomains 2 and 4. In the ε_p edit field, type `void_frit`.

8 Select Subdomain 3. In the ε_p edit field, type `void_bed`.

9 Click **OK**.

Subdomain Settings—Convection and Conduction

1 From the **Multiphysics** menu, select **3 Convection and Conduction (chcc)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 On the **Physics** page, select Subdomains 1–5.

4 In the ρ edit field, type `rho`; in the **C_p** edit field, type `Cp`; and in the **u** edit fields, type `u` and `v`, respectively.

5 Select Subdomains 1 and 5. In the **k (isotropic)** edit field, type `k_f`.

6 Select Subdomains 2–4. In the **k (isotropic)** edit field, type `k_e`.

7 Select Subdomain 6. In the **k (isotropic)** edit field, type `k_s`.

8 Select Subdomain 3. In the **Q** edit field, type `-v*pz`.

9 Click the **Init** tab.

10 Select all subdomains. In the **Initial value** edit field, type `T_in-(z-z_in)*(p_out-p_in)/(z_out-z_in)/(rho*Cp)`.

11 Click **OK**.

Boundary Conditions—Convection and Diffusion

1 From the **Multiphysics** menu, select **1 Convection and Diffusion (chcd)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Enter the following boundary settings:

SETTINGS	BOUNDARIES 1, 3, 5, 7, 9	BOUNDARY 2	BOUNDARY 11
Boundary condition	Axial symmetry	Concentration	Convective flux
c_0		`c0*exp(-a0*(t-t0)^2)`	

For all other boundaries, the default boundary condition (insulation/symmetry) applies.

4 Click **OK**.

Boundary Conditions—Incompressible Navier Stokes

1 From the **Multiphysics** menu, select **2 Incompressible Navier-Stokes (chns)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Enter the following boundary settings:

SETTINGS	BOUNDARIES 1, 3, 5, 7, 9	BOUNDARY 2	BOUNDARY 11
Boundary type	Symmetry boundary	Stress	Stress
Boundary condition	Axial symmetry	Normal stress, normal flow	Normal stress
f_0		`p_in`	`p_out`

For all other boundaries the default settings apply (wall/no slip).

4 Click **OK**.

Boundary Conditions—Convection and Conduction

1. From the **Multiphysics** menu, select **3 Convection and Conduction (chcc)**.
2. From the **Physics** menu, select **Boundary Settings**.
3. Enter the following boundary settings:

SETTINGS	BOUNDARIES 1, 3, 5, 7, 9	BOUNDARY 2	BOUNDARY 11
Boundary condition	Axial symmetry	Temperature	Convective flux
T_0		`T_in`	

   For all other boundaries, the default boundary condition (thermal insulation) applies.

4. Click **OK**.

MESH GENERATION

1. From the **Mesh** menu, choose **Free Mesh Parameters**.
2. On the **Subdomain** page, enter the following settings:

SETTING	SUBDOMAINS 1, 5	SUBDOMAINS 2, 4	SUBDOMAIN 3	SUBDOMAIN 6
Maximum element size	`2.5e-5`	`1e-4`	`2e-4`	`3e-3`

3. Click the **Boundary** page. Select Boundaries 4 and 10, then set the **Maximum element size** to `5e-6`.
4. Click the **Advanced** tab. In the **z-direction scale factor** edit field, type `0.5`.
5. Click the **Remesh** button.
6. Click **OK**.

COMPUTING THE SOLUTION

First, compute the steady-state velocity and temperature fields. Then, using these fields as an initial value, compute the transient solution for the analyte concentration. Record the entire procedure in a Solver Manager script.

1. Click the **Solver Parameters** button on the Main toolbar.
2. From the **Analysis** list, select **Stationary**.
3. Click **OK** to close the **Solver Parameters** dialog box.
4. Click the **Solver Manager** button on the Main toolbar.
5. On the **Initial Value** page, go to the **Initial value** area and click the **Initial value expression** option button.

6 On the **Solve For** page, select **Incompressible Navier-Stokes (chns)** only.

7 On the **Output** page, select **Incompressible Navier-Stokes (chns)** and **Convection and Conduction (chcc)**.

8 Click **Apply**.

9 On the **Script** page, click the **Add Current Solver Settings** button.

10 On the **Initial Value** page, click the **Current solution** option button in the **Initial value** area.

11 On the **Solve For** page, select **Incompressible Navier-Stokes (chns)** and **Convection and Conduction (chcc)**.

12 Click **Apply**.

13 On the **Script** page, click the **Add Current Solver Settings** button.

14 Click **OK**.

Before completing the solver-script generation, set up the visualization of the time-dependent solution.

1 From the **Postprocessing** menu, choose **Probe Plot Parameters**.

2 Click **New**.

3 For the **Plot type** choose **Integration**, and for the **Domain type** choose **Boundary**.

4 In the **Plot name** edit field, type `Inlet`, then click **OK** to close the **New Probe Plot** dialog box.

5 From the **Boundary selection** list, select **2**. In the **Expression** edit field, type `2*pi*(v*c-Dzz_c_chcd*cz)*r`.

6 Click the **Title/Axis** button.

7 Click the option button next to the **Title** edit field, then enter the title `Axial flux of analyte`.

8 Click **OK** to close the **Title/Axis Settings** dialog box.

9 Select the **Plot all plots in the same axis** check box.

10 Click **Apply**.

11 Repeat Steps 2–10 to generate a second plot with the **Plot name** set to `Outlet` and with Boundary 11 selected from the **Boundary selection** list.

Continue with the transient solution set-up.

1 Click the **Solver Parameters** button on the Main toolbar.

2 Change the **Analysis** back to **Transient**.

3 In the **Time stepping** area, type `0:1:9` in the **Times** edit field.

4 On the **Time Stepping** page, select the **Manual tuning of step size** check box. Set the **Initial time step** to `1e-4` and the **Maximum time step** to `1e-2`.

5 Click **OK** to close the **Solver Parameters** dialog box.

6 Click the **Solver Manager** button on the Main toolbar.

7 On the **Solve For** page, select **Convection and Diffusion (chcd)** only.

8 On **Output** page, select all three application modes.

9 Click **Apply**.

10 On the **Script** page, click the **Add Current Solver Settings** button.

11 Select the **Solve using a script** check box.

The solver script is now complete and ready to run.

12 Click **OK** to close the **Solver Manager**, then click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

The default plot is the concentration-peak evolution plot shown in Figure 10-16.

To plot the temperature field, follow these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Click the **Surface** page. On the **Surface Data** page, type `T` in the **Expression** edit field.

3 Click **OK**.

4 Double-click the **EQUAL** button on the status bar at the bottom of the user interface, then click the **Zoom Extents** button on the Main toolbar to toggle the axis-scale status.

To reproduce Figure 10-15, follow these steps:

1 From the **Postprocessing** menu, select **Domain Plot Parameters**.

2 From the **Solutions to use** list, select **0**.

3 Click the **Surface** tab.

4 Select all subdomains.

5 In the **Expression** edit field, type `T`.

6 Click **OK** to generate the plot and close the dialog box.

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