COMSOL MULTIPHYSICS®

MODEL LIBRARY

VERSION 3.5a

COMSOL

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COMSOL Multiphysics Model Library

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1

Introduction

We have designed COMSOL Multiphysics to be an extremely flexible package applicable to virtually any area of research, science, and engineering. A consequence of this flexibility is that it becomes necessary to set up COMSOL Multiphysics for a specific modeling task. To relieve you of this work in many disciplines and application areas, we have created a series of time-saving preconfigured models and collected them in this *Model Library*. It ships as a standard component of COMSOL Multiphysics 3.5a, and it is just one of several collections available to COMSOL Multiphysics users. Similar libraries with models devoted to specific disciplines are also available in the range of add-on modules:

- AC/DC Module
- Acoustics Module
- Chemical Engineering Module
- Earth Science Module
- Heat Transfer Module
- MEMS Module
- RF Module
- Structural Mechanics Module.

These ready-to-run models cover many classic problems and equations from science and engineering, and they have two goals in mind:

- To show the versatility of COMSOL Multiphysics and the wide range of applications it covers
- To form an educational basis for you to learn about COMSOL Multiphysics and gain an understanding of the underlying physics

Each model entry consists of two elements: the documentation and a corresponding ready-to-run COMSOL Multiphysics Model MPH-file you load directly from the Model Navigator window in COMSOL Multiphysics. These model files are copied to your hard disk with the default installation.

The documentation for each model entry in this library includes a technical background, the model definition, and results. Each entry also contains a section that shows, step by step, how to implement the model in COMSOL Multiphysics. Following the model description, a series of instructions guide you in the process of building, solving, and postprocessing the model in COMSOL Multiphysics.

Note: In some cases, the settings appear in a table rather than giving a step-by-step procedure for each data entry.

Those users new to COMSOL Multiphysics might want start reading the *COMSOL Multiphysics Quick Start and Quick Reference*, which contains a detailed step-by-step instruction for a basic multiphysics model. During modeling, some general questions might arise about COMSOL Multiphysics, its various features, and how to use them. For the answers we suggest that you first refer to the *COMSOL Multiphysics User's Guide* and the *COMSOL Multiphysics Modeling Guide*.

The Model Library entries follow the basic structure of COMSOL Multiphysics and the modeling process you follow in using this package. Most of the chapters correspond to *application modes* in COMSOL Multiphysics. For a description of these application modes, including typical example models included in the Model Library, see the *COMSOL Multiphysics Modeling Guide*.

When describing *equation-based models*, which use partial differential equations (PDEs) directly, the text provides information about the model and the physical or mathematical background. In *benchmark models* you can compare a solution to analytical or established results. *Parametric studies* vary physical or geometrical

parameters in a series of solutions for optimization or evaluation of design criteria. To quickly locate models in each of the above categories, refer to the "Model Library Guide" on page 5.

One outstanding feature of COMSOL Multiphysics is the ability to include several interacting physics in one system using its multiphysics modeling features. To help you better appreciate this power, the Model Library includes a number of corresponding examples in the chapter "Multiphysics Models" on page 355. Additional information about multiphysics modeling is available in the *COMSOL Multiphysics User's Guide* and the *COMSOL Multiphysics Modeling Guide*.

The chapter "Multidisciplinary Models" on page 315 contains models that include control loops or other system simulation components. The models in this chapter show you how to combine COMSOL with MATLAB and Simulink for system simulations that include finite element models.

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 code.
- 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.

Model Library Guide

The table below summarizes key information about the entries in this *Model Library*.

The first three columns contain the model name, page number, and solution times. 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 combined solution time for all solution steps.

The subsequent three columns indicate whether the model geometry includes 1D, 2D, 3D, or multiple geometries (extended multiphysics).

The next several columns indicate the analysis types that the model covers, such as stationary, time-dependent, eigenvalue, sensitivity, or optimization.

The Multiphysics column shows which models include multiphysics couplings.

The final column indicates models that use parametric studies to evaluate and optimize their results by varying the value of one or more parameters.

TABLE 1-1: COMSOL MULTIPHYSICS MODEL LIBRARY MODELS

MODEL	PAGE	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME-DEPENDENT	EIGENVALUE	SENSITIVITY/OPTIMIZATION	MULTIPHYSICS	PARAMETRIC STUDY
ACOUSTICS MODELS	11										
automotive muffler	12	9 min			√	√					√
eigenmodes of room	21	12 s			√			√			
reactive muffler	35*	2 s		√		√					
BENCHMARK MODELS	597										
isospectral drum 1	598	1 s		√				√			
isospectral drum 2	598	1 s		√				√			
point source	279*	1 s		√		√					
CHEMICAL ENGINEERING MODELS	31										

TABLE 1-1: COMSOL MULTIPHYSICS MODEL LIBRARY MODELS

MODEL	PAGE	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME-DEPENDENT	EIGENVALUE	SENSITIVITY//OPTIMIZATION	MULTIPHYSICS	PARAMETRIC STUDY
adsorption	32	7 s		√		√				√	
tubular reactor	44	22 s		√		√				√	
DIFFUSION MODELS											
effective diffusivity	58*	45 s		√			√				
thin layer diffusion	434*	1 s			√	√					
ELECTROMAGNETICS MODELS	55										
electric sensor	121*	2 s		√		√					
electrochemical polishing	468*	2 s		√			√				
pacemaker electrode	68	4 s			√	√					
permanent magnet	126*	2 s		√		√					
potential between cylinders	57	1 s			√	√					
quadrupole	83	1 s		√		√					
skin effect	76	1 s		√		√					
spherical capacitor	93	1 s		√		√					
thin film resistance	422*	3 s			√	√					
EQUATION-BASED MODELS	99										
black-scholes put	100	1 s	√				√				
flywheel profile¤	104	16 s	√			√			√		
heart electrical clg	118	6 min			√		√			√	
heart electrical fhn	118	20 min			√		√			√	
integro partial	129	3 s	√				√				
kdv equation	138	4 s	√				√				
shallow water	145	10 s	√				√				
shell diffusion	153	1 s			√	√					
spherical symmetry ore	159	1 s	√				√				
telegraph equation	169	1 s	√				√				

TABLE 1-1: COMSOL MULTIPHYSICS MODEL LIBRARY MODELS

MODEL	PAGE	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME-DEPENDENT	EIGENVALUE	SENSITIVITY//OPTIMIZATION	MULTIPHYSICS	PARAMETRIC STUDY
transport problem	176	1 s		√		√					
two term boltzmann	183	2 min	√			√					√
FLUID DYNAMICS MODELS	203										
backstep	154*	10 s		√		√					√
backstep argyris	204	18 s		√		√					
backstep quad	154*	47 s		√		√					√
cylinder flow	211	25 min		√			√				
falling sand	220	20 min		√			√				
fluid valve	230	13 min		√			√				
micromixer	240	4 min			√	√					
reversed flow¤	326*	25 min		√		√			√		
shock tube	252	3 s		√		√					
sloshing tank	259	49 s		√			√				
GEOPHYSICS MODELS	269										
groundwater flow	270	17 s		√			√			√	
rock fracture	283	3 s		√		√					
HEAT TRANSFER MODELS	291										
heat convection 2D	192*	1 s		√		√					
heat radiation 1D	188*	1 s	√			√					
heat transient axi	196*	1 s		√			√				
laser heating	292	49 s			√		√			√	
dev merge lpd19	303	16 s			√		√				√
MULTIDISCIPLINARY MODELS	315										
magnet brake	316	4 s		√		√	√				
magnet brake simulink	316	1 s		√		√					
PID control	331	2 min		√			√			√	

TABLE 1-1: COMSOL MULTIPHYSICS MODEL LIBRARY MODELS

MODEL	PAGE	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME-DEPENDENT	EIGENVALUE	SENSITIVITY//OPTIMIZATION	MULTIPHYSICS	PARAMETRIC STUDY
thermal controller simulink	342	1 s		√			√			√	
MULTIPHYSICS MODELS	355										
electronic conductor	36**	2 min			√	√				√	√
free convection	356	41 s		√		√	√			√	
magnetic drug targeting	376	55 s		√			√			√	
marangoni	391	27 s		√		√				√	
microrobot	403	2 min		√			√			√	
milk container	414	1 s		√		√	√			√	
peristaltic pump	423	47 s		√			√			√	
resistive heating	387*	8 s		√		√	√			√	
QUANTUM MECHANICS MODELS	437										
conical quantum dot	438	1 s		√				√			
hydrogen atom	445	3 s		√				√			
SEMICONDUCTOR DEVICE MODELS	455										
bipolar transistor	456	2 min		√		√	√			√	
mos transistor	473	3 min		√		√				√	√
semiconductor diode	492	2 min		√		√				√	√
spice parameter extraction¤	507	2 min		√		√			√		√
STRUCTURAL MECHANICS MODELS	521										
crankshaft	521	54 s			√			√			
edge load 2d	235*	1 s		√		√					
feeder clamp	529	6 s			√	√					
gravity load 2d	240*	1 s		√		√					
loaded knee¤	548	21 min		√		√			√		
mast diagonal mounting	559	29 s			√	√					
mast diagonal mounting sensitivity	299*	2 min			√	√			√		

TABLE 1-1: COMSOL MULTIPHYSICS MODEL LIBRARY MODELS

MODEL	PAGE	SOLUTION TIME	1D	2D	3D	STATIONARY	TIME-DEPENDENT	EIGENVALUE	SENSITIVITY//OPTIMIZATION	MULTIPHYSICS	PARAMETRIC STUDY
pulley	571	8 s		√		√					√
WAVE PROPAGATION MODELS	589										
diffraction patterns	590	1 s		√		√	√				

¤ Requires the Optimization Lab.

* In the *COMSOL Multiphysics Modeling Guide*.

** In the *COMSOL Multiphysics Quick Start and Quick Reference*.

2

Acoustics Models

This chapter contains acoustics models solving for the pressure field using time-harmonic and eigenvalue formulation in the Acoustics application mode.

Acoustics of a Muffler

Introduction

This model describes the pressure wave propagation in a muffler for an explosion engine. The approach is general for analysis of damping of propagation of harmonic pressure waves.

The purpose of the model is to show how to treat 3D acoustics in a fairly complex geometry, consisting of several separate sections and pipes divided by thin perfectly rigid walls. The analysis gives the transmission loss in the frequency range 100 Hz–1000 Hz.

Model Definition

The model geometry consists of three separate resonator chambers divided by thin walls. The inlet and the outlet correspond to the connection in the direction of the engine and of free air, respectively.

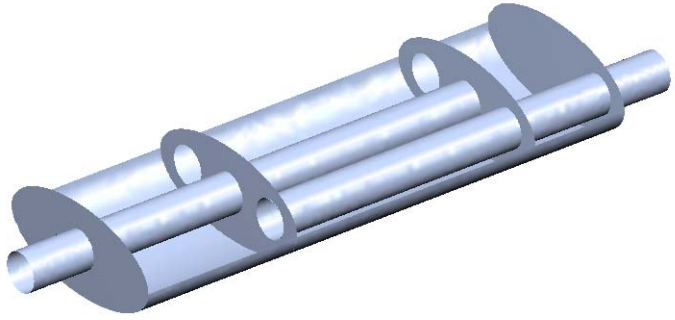


Figure 2-1: The geometry of a muffler. The exhaust fumes enter through the left pipe, pass the three resonator chambers, and exit through the right pipe.

DOMAIN EQUATIONS

The problem is solved in the frequency domain using the time-harmonic Acoustics application mode. The model equation is a slightly modified Helmholtz's equation for the acoustic pressure, p:

$$\nabla \cdot \left(-\frac{\nabla p}{\rho}\right) - \frac{\omega^2 p}{c_s^2 \rho} = 0$$

where ρ is the density, c_s is the speed of sound, and ω is the angular frequency. The density needs to be included in the equation in cases where variations in density in different materials exist. The model assumes that in the low-frequency range, reactive damping prevails. Resistive damping is therefore not included.

BOUNDARY CONDITIONS

The boundary conditions are of three different types. At all the solid boundaries, which include the outer walls of the muffler, the dividing walls between the resonator chambers, and the walls of the pipes, sound hard (wall) boundary conditions are used:

$$\left(-\frac{\nabla p}{\rho}\right) \cdot \mathbf{n} = 0 \tag{2-1}$$

At the inlet boundary is a combination of incoming and outgoing plane waves:

$$\left(-\frac{\nabla p}{\rho}\right) \cdot \mathbf{n} = \frac{i\omega}{\rho c_s} p - \frac{2\, i\omega}{\rho c_s} p_0$$

In this equation p_0 denotes the applied outer pressure and i the imaginary unit. At the outlet boundary, an outgoing plane wave is set:

$$\left(-\frac{\nabla p}{\rho}\right) \cdot \mathbf{n} = \frac{i\omega}{\rho c_s} p$$

Results and Discussion

The following equation defines the damping of the acoustic energy, d_w:

$$d_w = 10 \log\left(\frac{w_o}{w_i}\right)$$

Here, w_o and w_i denote the acoustic energy at the outlet and inlet, respectively. The acoustic energy is calculated using the following equations:

$$w_o = \int_{\partial\Omega} \frac{|p_c|^2}{2\rho c_s} dA$$

$$w_{\mathrm{i}} = \int_{\partial\Omega} \frac{p_0^{\,2}}{2\rho c_s} dA$$

Figure 2-2 shows the result of a parametric frequency study. This plot reveals that the damping is better at higher frequencies, with the exception of several deep dips throughout the frequency range. The dips correspond to the resonance frequencies for different parts of the muffler system.

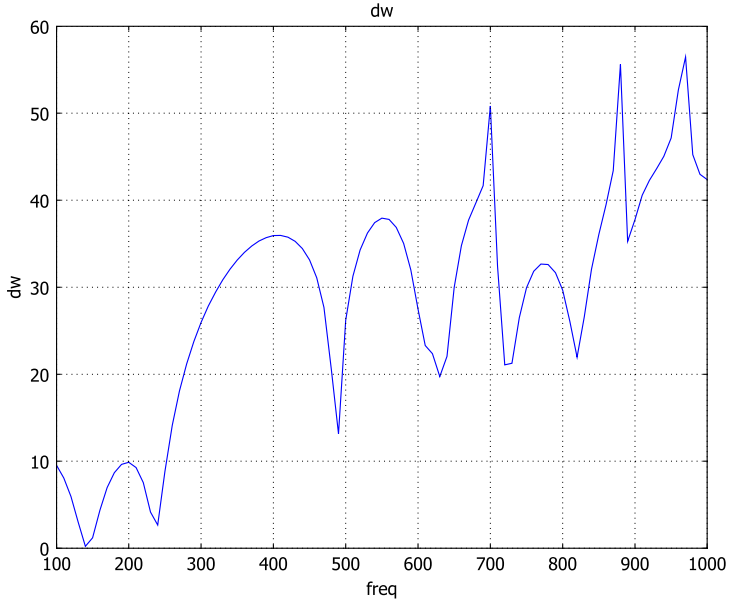


Figure 2-2: The damping (dB) in the muffler as a function of the frequency (Hz).

Modeling in COMSOL Multiphysics

The dividing walls between the resonator chambers and the walls of the pipes constitute interior boundaries. Because no waves propagate through these boundaries, the pressure between the inside and the outside of the pipe walls, as well as that between the chambers, must be decoupled. To accomplish this, use three dependent variables for the pressure (and three Acoustics application modes) in the model: one for the pipes, p_{p}, one for the first and the third resonator chambers, p_{c1}, and one for the second resonator chamber, p_{c2}. You implement this by deactivating the variables in the parts of the model where they do not exist. It is then possible to specify the dividing walls and the walls of the pipes as exterior boundaries for each pressure

variable. The pressure variables couple to each other where the pipes open up into the resonator chambers and at the openings between the chambers. You only have to specify this coupling in one direction; the implementation distributes the reaction forces evenly. To view the results for the entire pressure field simultaneously, you define a variable p for the common pressure.

Model Library path: `COMSOL_Multiphysics/Acoustics/automotive_muffler`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, click the **Multiphysics** button.

2 Add three Acoustics application modes. To do so, select **3D** in the **Space dimension** list and then select **Acoustics>Acoustics>Time-harmonic analysis** in the list of application modes (in the **COMSOL Multiphysics** folder if the license contains additional modules).

3 Before adding each application mode, name it and its dependent variable according to the following table:

APPLICATION MODE NAME	DEPENDENT VARIABLE
`pipe`	`p_p`
`chamber1`	`p_c1`
`chamber2`	`p_c2`

Type the names of the application mode and the dependent variable in the **Application mode name** and **Dependent variables** edit fields, respectively.

4 Click **Add** to add each of the application modes to the model.

5 When you have added the three application modes, click **OK** to exit the **Model Navigator** and continue modeling.

OPTIONS AND SETTINGS

1 Open the **Constants** dialog box from the **Options** menu, and enter the variable name `p0` and the expression `1`. Click **OK**.

2 From the **Physics** menu, choose **Scalar Variables** to open the **Application Scalar Variables** dialog box. Set the frequency to `freq` for all the three

application modes. It is sufficient to type `freq` in the **Expression** edit field for the variable `freq_pipe` only and press Enter. The synchronization of equivalent variables then sets the two other frequency variables to `freq`. When done, click **OK**.

GEOMETRY MODELING

1. Create a cylinder with radius 0.03, height 0.75, axis base point (–0.1, 0, 0), and axis direction vector (1, 0, 0).
2. Create another cylinder with radius 0.03, height 0.65, axis base point (0.25, –0.09, 0), and axis direction vector (1, 0, 0).
3. Go to the **Work-Plane Settings** dialog box in the **Draw** menu. On the **Quick** page, specify a **y-z** plane at $x = 0$. Click **OK**.
4. In this new work plane, specify an ellipse with semiaxes 0.15 and 0.07 centered at (0, 0).
5. In the **Extrude** dialog box in the **Draw** menu, select the ellipse and extrude it by a distance of 0.8.
6. In the **Work-Plane Settings** dialog box, set the **x** coordinate for the **y-z** plane to `0.25`. When done, click **OK**.
7. Specify a circle with radius 0.03 centered at (0.09, 0).
8. Go to the **Embed** dialog box in the **Draw** menu. Select both the circle and the ellipse, and embed them.
9. Go to the **Work-Plane Settings** dialog box again, and set the **x** coordinate for the **y-z** plane to `0.65`. Click **OK**.
10. Embed the circle and the ellipse from this plane.
11. Finally, click the **Zoom Extents** button on the Main toolbar to view the complete muffler geometry.

The geometry should now look like that in Figure 2-3.

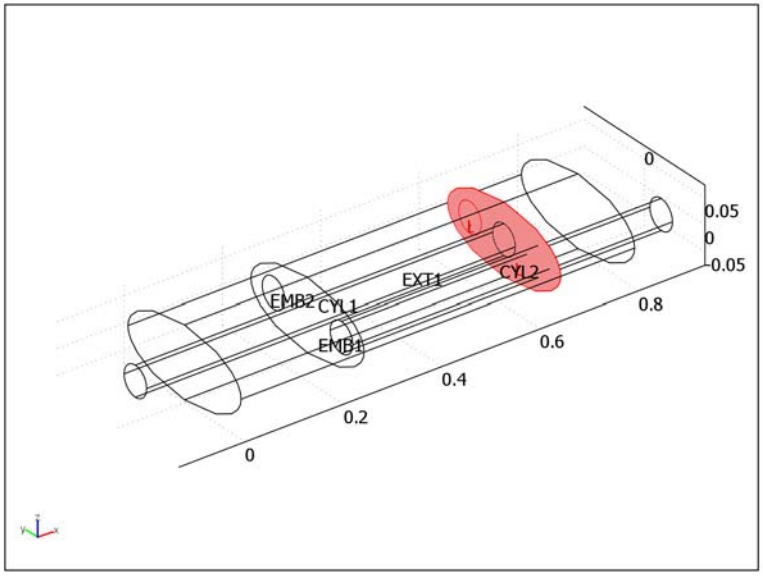


Figure 2-3: The muffler geometry.

PHYSICS SETTINGS

Subdomain Settings

In this model, use the default values for the subdomain settings. However, every subdomain should have only one active application mode. Open the **Subdomain Settings** dialog box from each application mode, select the **Active in this mode** check box in the following subdomains, and clear it in all other subdomains.

APPLICATION MODE	ACTIVE IN SUBDOMAINS
pipe	1, 3, 5, 6, 8, 9
chamber1	2, 7
chamber2	4

Boundary Conditions

1 In the **pipe** application mode, select **Radiation condition** from the **Boundary condition** list and then select **Plane wave** from the **Wave type** list on Boundaries 1 and 50; the pressure source **p_p0** should be p0 on Boundary 1 and 0 on Boundary 50. Use the default sound-hard boundary condition on all other boundaries.

2 In the **chamber1** application mode, use the **Pressure** boundary condition on Boundaries 19, 31, 40, and 43. Set the pressure source p_c1_0 to p_p on Boundaries 19 and 40 and p_c2 on Boundaries 31 and 43. Use the default sound-hard boundary condition on all other active boundaries.

3 In the **chamber2** application mode, use the default sound-hard boundary condition on all boundaries.

Coupling Variables

1 On the **Options** menu, point to **Integration Coupling Variables** and then click **Boundary Variables**.

2 In the **Boundary Integration Variables** dialog box, select Boundary 1 and create a boundary integration variable with **Name** Iin, **Expression** p0^2/(2*1.25*343), **Integration order** 4, and **Global destination**.

3 Select Boundary 50. On a new line, create a boundary integration variable with **Name** Iout, **Expression** p_p^2/(2*1.25*343), **Integration order** 4, and **Global destination**.

4 Click **OK** to close the **Boundary Integration Variables** dialog box.

Expression Variables

1 Open the **Scalar Expressions** dialog box from the **Options** menu. Create a scalar expression with **Name** dw and **Expression** 10*log10(Iin/Iout). This represents the damping in dB. When done, click **OK**.

2 Open the **Boundary Expressions** dialog box. Create a boundary expression with **Name** p and **Expression** depending on the boundary according to the following table; when done, click **OK**.

EXPRESSION	BOUNDARIES
p_p	2–5, 10, 11, 13, 14, 20–23, 25, 26, 28, 29, 36–39, 46–49
p_c1	6, 7, 12, 16, 33, 41, 44
p_c2	17, 27, 32

3 Open the **Subdomain Expressions** dialog box. Create a subdomain expression with **Name** p and **Expression** according to the following table; when done, click **OK**.

EXPRESSION	SUBDOMAINS
p_p	1, 3, 5, 6, 8, 9
p_c1	2, 7
p_c2	4

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar to generate the mesh.

COMPUTING THE SOLUTION

1. Click the **Solver Parameters** button on the Main toolbar.
2. In the **Solver Parameters** dialog box, select **Parametric** from the **Solver** list.
3. Type `freq` in the **Parameter names** edit field and `range(100,10,1000)` in the **Parameter values** edit field. This will compute the solution for 91 equally spaced frequencies from 100 Hz to 1000 Hz. Note that this process takes around 25 minutes; if you want to run a faster analysis, try the same frequency range but with a step of 100 Hz instead (to do so, type `range(100,100,1000)`).
4. Click **OK**.
5. Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

1. To see what goes on inside the muffler, hide the boundaries that obstruct the view. To do so, choose **Options>Suppress>Suppress Boundaries** and suppress Boundaries 1, 8, 9, 15, 18, 19, 24, 30, 31, 34, 35, 40, 42, 43, 45, and 50 by selecting them from the **Boundary selection** list in the **Suppress Boundaries** dialog box. Click **OK**.
2. Click the **Plot Parameters** button on the Main toolbar.
3. Visualize the pressure in the muffler with a boundary plot of the absolute value of the pressure and an isosurface plot of the pressure. To do so, click the **General** tab, clear the **Slice** check box and select the **Boundary** and **Isosurface** check boxes in the **Plot type** area.
4. Click the **Boundary** tab and type `abs(p)` in the **Expression** edit field.
5. Click the **Isosurface** tab. Type `p` in the **Expression** edit field on the **Isosurface Data** page. The suitable number of isosurface levels for the isosurface plot varies with the frequency. At frequencies with low damping many of the isosurfaces tend to congregate inside the pipe. For a frequency of 490 Hz (select this solution from the **General** page of the **Plot Parameters** dialog box), ten isolevels gives a nice plot.
6. Click **OK**.
7. Click the **Headlight** button on the Camera toolbar to make the visualization more viewer friendly. The plot should look like the one in Figure 2-4.

8 Click the **Go to XY View** toolbar button to see a projection of the plot on the *xy*-plane. You may need to click it twice, in case the muffler appears upside down.The pressure in the second chamber displays a resonance pattern.

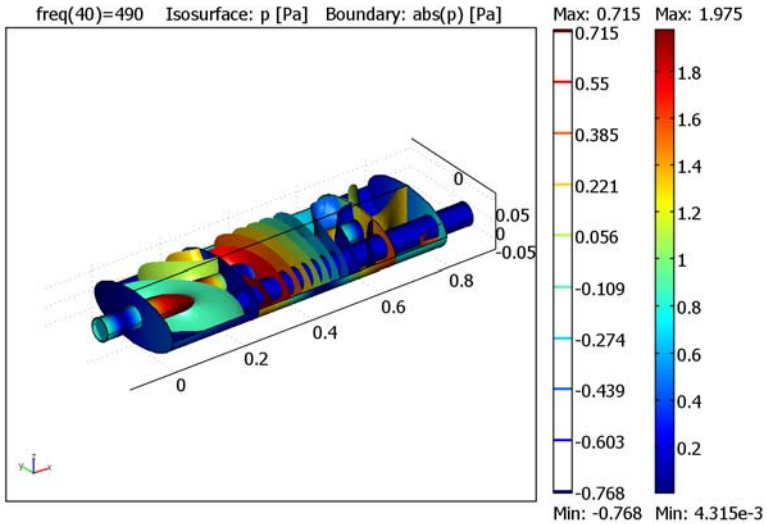


Figure 2-4: The solution at 490 Hz. The real value of the pressure is plotted as isosurfaces, and the absolute value of the pressure is displayed as a boundary plot on the inner walls of the muffler.

9 To see the damping as a function of the frequency, open the **Cross-Section Plot Parameters** dialog box.

10 On the **General** page, select all solutions in the **Solutions to use** area.

11 Click the **Point plot** button.

12 Click the **Point** tab and type `dw` in the **Expression** edit field to make a point plot of the damping in some arbitrary point located inside the geometry. The origin (the default point) will do.

13 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

The plot should look like in Figure 2-2. Notice the deep dip in the damping around 490 Hz caused by the resonance in the second chamber. If you plot the pressure in the muffler at other dips, resonances in the other chambers appear.

Eigenmodes of a Room

Resonance can at times be a problem in everyday life. The low bass notes from the music system or home theater in the living room can shake the windows and make the floor vibrate. This happens only for certain frequencies—the eigenfrequencies of the room.

It is only in the low-frequency range that the eigenfrequencies are well separated. In the mid- and high-frequency ranges, the eigenfrequencies are packed so closely, with less than a halftone between them, that the individual resonances are insignificant for music and other natural sounds. Nevertheless, the music experience is affected by the acoustics of the room.

When designing a concert hall, it is extremely important to take the resonances into account. For a clear and neutral sound, the eigenfrequencies should be evenly spaced. For the home theater or music system owner, who cannot change the shape of the living room, another question is more relevant: Where should the speakers be located for the best sound?

Model Definition

For example, take a room with the dimensions 5 by 4 by 2.6 meters equipped with a TV set, two speakers, and a couch. To illustrate the effects on the music, compute all eigenfrequencies below 100 Hz together with the corresponding eigenmodes. The eigenmode shows the sound intensity pattern for its associated eigenfrequency. From the characteristics of the eigenmodes, you can draw some conclusions as to where the speakers should be placed.

DOMAIN EQUATIONS

Sound propagating in free air is described by the wave equation:

$$-\Delta p + \frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} = 0$$

where p is the pressure, and c is the speed of sound. If the air is brought into motion by a harmonically oscillating source, for example, a loudspeaker, only one frequency f exists in the room. For that reason it makes sense to look for a time-harmonic solution on the form

$$p = \hat{p} e^{i\omega t}$$

The wave equation then simplifies to the Helmholtz equation for p, the amplitude of the acoustic disturbances:

$$\Delta \hat{p} + \frac{\omega^2}{c^2} \hat{p} = 0$$

BOUNDARY CONDITIONS

This model assumes that all boundaries—walls, floor, ceiling, and furniture —are perfectly rigid (sound hard boundaries).

ANALYTIC COMPARISON

It is possible to solve the simpler case of an empty room analytically. Each eigenfrequency corresponds to an integer triple (*i, l, m*):

$$f_{i,l,m} = \frac{c}{2} \sqrt{\left(\frac{i}{L_x}\right)^2 + \left(\frac{l}{L_y}\right)^2 + \left(\frac{m}{L_z}\right)^2}$$

The eigenmodes can be divided into three distinct classes:

- Eigenfrequencies with only one index different from zero give rise to axial modes, that is, plane standing waves between two opposite walls.
- If one index is zero, the mode is tangential.
- If all indices are different from zero, the mode is oblique.

Theoretical eigenvalues for a room without furniture are found in the following table.

MODE INDEX	$\omega^2/10^5$	MODE INDEX	$\omega^2/10^5$
0,0,0	0	0,1,1	2.444
1,0,0	0.465	2,1,0	2.584
0,1,0	0.726	0,2,0	2.902
1,1,0	1.191	1,1,1	2.908
0,0,1	1.718	1,2,0	3.367
2,0,0	1.858	2,0,1	3.575
1,0,1	2.182	3,0,0	4.180

Results and Discussion

The relevant quantity when it comes to placing the loudspeakers is the amplitude of the standing pressure wave. A sound source excites an eigenmode the most if it is placed in one of the pressure antinodes for the mode. Conversely, with the source in a pressure node, the eigenmode remains silent.

All modes have local maxima in the corners of an empty room so speakers in the corners excite all eigenfrequencies. This simulation predicts eigenmodes that strongly resemble those of the corresponding empty room. The higher the frequency, the more the placing of the furniture matters. For instance, some of the high-frequency eigenmodes are located behind the couch.

In the strictest sense, the results of this simulation only apply to a room with perfectly rigid walls and nonabsorbing furniture. The prediction that speakers placed in the corners of the room excite many eigenmodes and give a fuller and more neutral sound, however, holds for real-life rooms.

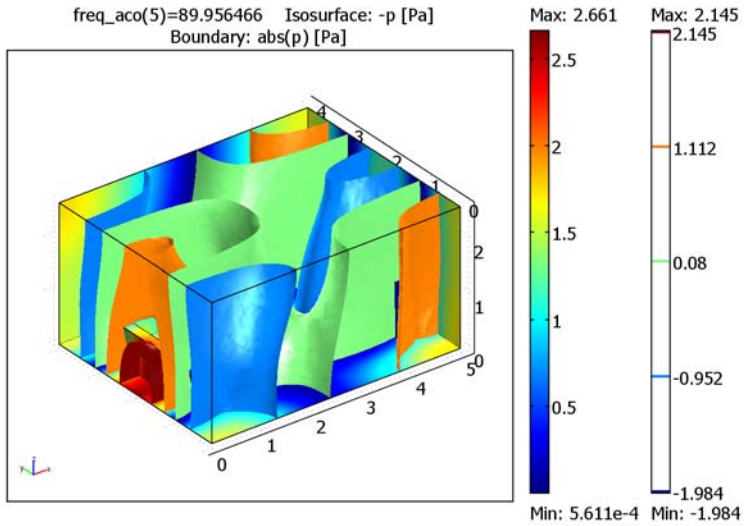


Figure 2-5: The sound pressure distribution for $\omega = 569$ *rad/s. The (negative of) the real part of the pressure is visualized as an isosurface plot, and the absolute value of the pressure as a boundary plot.*

Model Library path: `COMSOL_Multiphysics/Acoustics/eigenmodes_of_room`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Click **Multiphysics**.

2 Select **3D** in the **Space dimension** list.

3 In the list of application modes, select **Acoustics** (in the **COMSOL Multiphysics** folder if your license includes additional modules), and in the **Acoustics** folder, select **Eigenfrequency analysis**.

4 Click **Add**.

5 Add geometries according to the following table by clicking the **Add Geometry** button.

NAME	SPACE DIMENSION	INDEPENDENT VARIABLES
Floor	2D	x y z
Table	2D	x y z
TV	2D	x y z

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

GEOMETRY MODELING

1 Click the **Geom1** tab.

2 Click the **Block** button to create a block with the following dimensions that you enter in the **Length** area; when done, click **OK**.

PARAMETER	VALUE
X	5
Y	4
Z	2.6

3 Click to clear the **Highlight Face** button on the Draw toolbar for a wireframe view.

Now create the cross section of the geometry on the floor of the room. The floor is by default an xy-plane at $z = 0$.

1 Go to the **Floor** work plane and click the **Zoom Extents** button on the Main toolbar.

2 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

3 Click the **Grid** tab, clear the **Auto** check box, and change the grid according to the following table; when done, click **OK**.

GRID	
x spacing	`0.2`
Extra x	`1.7 2.1 4.5 4.7`
y spacing	`0.2`
Extra y	`1.7 2.3`

4 Draw a rectangle with top left corner at (0.4, 3) and bottom right corner at (1.2, 1).

5 Draw eight squares with side 0.1 and upper left corners at (1.6, 1.7), (1.6, 2.4), (2.1, 1.7), (2.1, 2.4), (4.4, 1.7), (4.4, 2.4), (4.7, 1.7), and (4.7, 2.4).

6 From the **Draw** menu, choose **Extrude**.

7 In the **Extrude** dialog box, select all objects and set the **Distance** parameter to `0.4`.

8 Click **OK**.

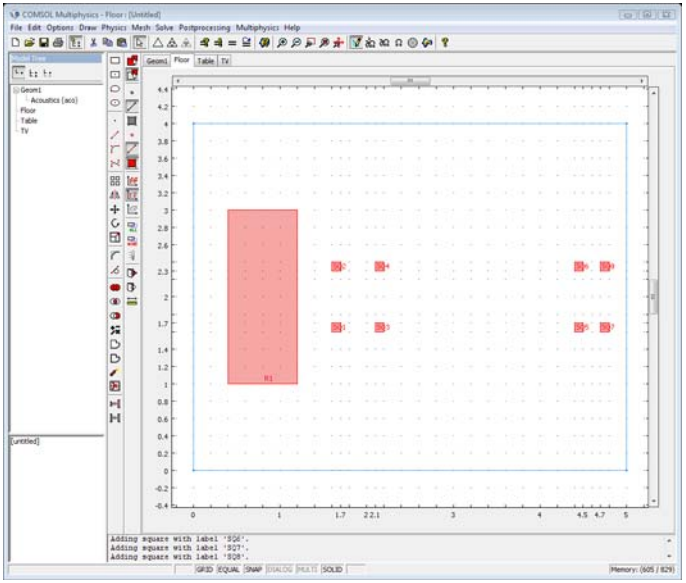


Figure 2-6: The geometry of the Floor work plane.

Now proceed to create the cross section of the geometry at the level of the table.

1. Go to the **Table** work plane.
2. Go to the **Work-Plane Settings** dialog box and change the **z** coordinate to `0.4`. When done, click **OK**.
3. Click the **Zoom Extents** button on the Main toolbar.
4. In the **Axes/Grid Settings** dialog box, click the **Grid** tab and clear the **Auto** check box. Then change the grid spacing according to the following table; when done, click **OK**.

GRID	
x spacing	`0.2`
y spacing	`0.2`

5. Draw a rectangle with top left corner at (1.6, 2.6) and bottom right corner at (2.2, 1.4).
6. Make sure the rectangle is selected and choose **Extrude** from the **Draw** menu. Set the distance to `0.1` and click **OK**.
7. Return to the **Table** work plane.
8. Draw a rectangle with top left corner at (0.4, 3) and bottom right corner at (1.2, 1), that is, following the blue projected contour.
9. Draw another rectangle with top left corner at (0.6, 2.8) and bottom right corner at (1.2, 1.2).
10. Select the two last rectangles and click the **Difference** button.

11 With the new composite object still selected, open the **Extrude** dialog box. Set **Distance** to `0.4` and **Displacement x** to `-0.1` and click **OK**.

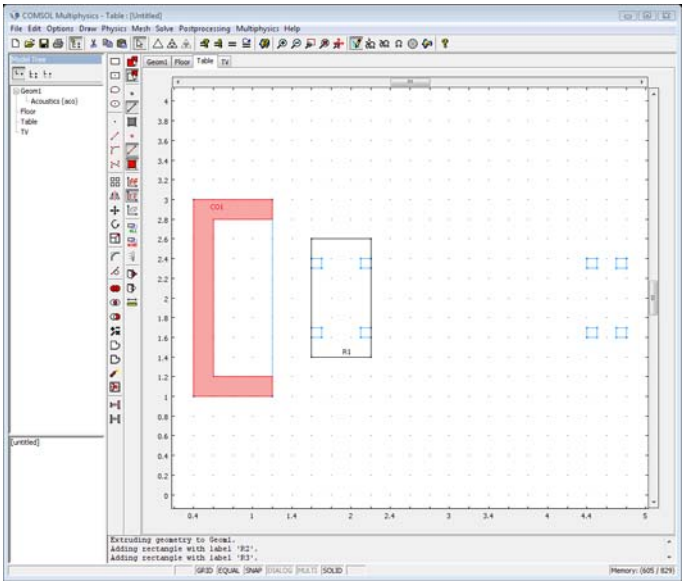


Figure 2-7: The geometry of the Table work plane.

Finally, create the geometry in the cross section of the TV.

1 Go the **TV** work plane.

2 Go to the **Work-Plane Settings** dialog box. Select the **y-z** plane and set the **x** coordinate to `4.4`.

3 Click **OK**.

4 Click the **Projection of All 3D Geometries** button and after that the **Zoom Extents** button.

5 Use **Axes/Grid Settings** to change the grid as in the following table; when done, click **OK**.

GRID	
x spacing	`0.2`
y spacing	`0.2`

6 Draw the TV set as a rectangle with top left corner at (1.6, 1.0) and bottom right corner at (2.4, 0.4).

7 Draw the left speaker as a rectangle with top left corner at (0.8, 1.0) and bottom right corner at (1.2, 0.0).

8 Draw the right speaker with the same size, but with top left corner at (2.8, 1.0).

9 Select all objects and open the **Extrude** dialog box. Set distance to `0.4`, then click **OK**.

10 In the 3D geometry, select all objects and click the **Difference** button.

Now the room is completed and should look like in Figure 2-8.

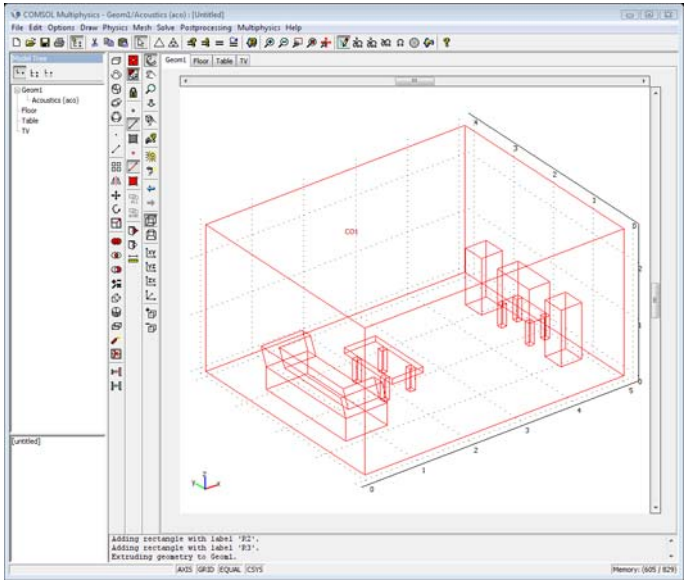


Figure 2-8: The 3D geometry.

PHYSICS SETTINGS

Boundary Conditions

Use the **Sound hard boundary (wall)** boundary condition for all boundaries.

Subdomain Settings

Use the default subdomain settings.

MESH GENERATION

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

COMPUTING THE SOLUTION

1. Make sure that **Eigenfrequency** is selected from the **Solver** list in the **Solver Parameters** dialog box.
2. To get 6 eigenfrequencies around 90 Hz enter `6` in the **Desired number of eigenfrequencies** edit field, this is default, and `90` in the **Search for eigenfrequencies around** edit field.
3. Click **OK** to close the **Solver Parameters** dialog box.
4. Click the **Solve** button to compute the solution.

POSTPROCESSING AND VISUALIZATION

The default plot style is a slice plot showing the sound pressure in five equally spaced slices. Try looking at some of the eigenmodes. The first eigenvalue in the list is very small. Its true value is zero, corresponding to the solution without any sound. The next few are axial and tangential modes. To get a better view of the more complicated eigenmodes, you can do a combined surface and boundary plot (see Figure 2-5).

1. In the **Suppress Boundaries** dialog box in the **Options** menu, suppress Boundaries 1, 2, and 4.
2. On the **General** page of the **Plot Parameters** dialog box, clear the **Slice** check box and select the **Isosurface**, **Boundary**, and **Geometry edges** check boxes in the **Plot type** area. In the **Eigenfrequency** list, select the eigenvalue of about `90.6`.
3. Click the **Boundary** tab and type `abs(p)` in the **Expression** edit field.
4. Click the **Isosurface** tab and type `-p` in the **Expression** edit field.
5. Click the **Scene Light** and **Perspective Projection** buttons in the Camera toolbar.
6. Click **OK**.

This particular mode is concentrated behind the couch. Try moving around the room and looking at other eigenmodes. It is possible that you can identify some of them with the exact solutions for the case of an empty room.

3

Chemical Engineering Models

This section contains a model of a tubular reactor and a model of surface diffusion and surface reactions coupled to transport of species to the reacting surface—a comprehensive set of chemical engineering models covering mass balances, energy balances, and momentum balances is available in the *Model Library* that comes with the Chemical Engineering Module.

Transport and Adsorption

This model demonstrates one of the unique features of COMSOL Multiphysics: the possibility to model phenomena defined in different numbers of dimensions in a fully coupled manner.

Whereas in most cases you define the reaction rate expression as a function of the concentrations of the reactants and products, in adsorption reactions it is also necessary to model the surface concentrations of the active sites or surface complex. This implies that the mass balance in the bulk of the reactor must be coupled to the mass balance for species present only at the surface of the device. This device could be a catalyst, a biochip, a semiconductor component, or any process with surface-specific species.

In this particular case, the model involves a small parallel-plate reactor with an active surface. It is a simple example of surface diffusion and surface reactions coupled to the transport of species between the reacting surface and the surrounding volume. Processes of this kind are found, for instance, in heterogeneous reactors and biacore chips.

The geometry of the domain appears in Figure 3-1.

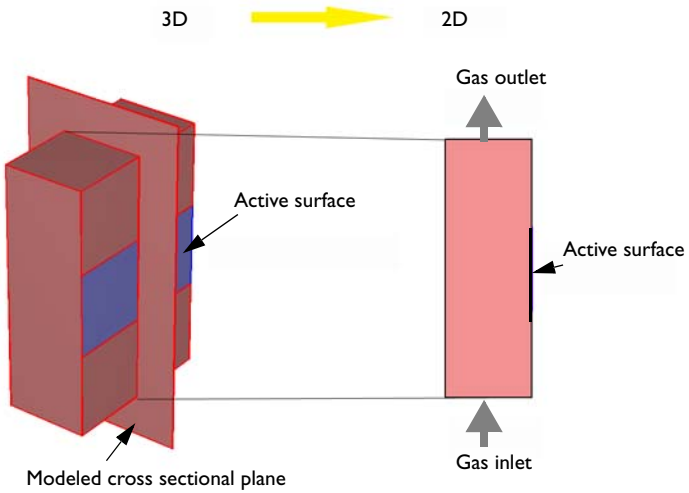


Figure 3-1: The modeled domain is a parallel plate reactor with an active surface where you want to model the concentration of surface species.

The first approximation you can make is to reduce the 3D geometry to a 2D approximation, which is reasonable if the variations in concentration are small along the depth of the domain.

DOMAIN EQUATIONS

The reaction at the active surface is given as

$$c + \theta \underset{k_{\text{des}}}{\overset{k_{\text{ads}}}{\Leftrightarrow}} c_s$$

where

- c is the bulk concentration (mol/m^3)
- θ is the surface concentration of active sites (mol/m^2)
- c_s is the surface concentration of adsorbed species (mol/m^2)

- k_{ads} is the rate constant for the forward reaction ($m^3/(mol \cdot s)$)
- k_{des} is the rate constant for the backward reaction ($1/s$)

Note: The surface concentration is in moles per unit surface.

The material balance for the surface, including surface diffusion and the reaction rate expression for the formation of the adsorbed species, c_s, is:

$$\frac{\partial c_s}{\partial t} + \nabla \cdot (-D_s \nabla c_s) = k_{ads} c\theta - k_{des} c_s$$

where D_s represents surface diffusivity. However, the concentration of active sites is equal to the difference between the total concentration of active sites and the number of sites occupied by the adsorbed species. This gives the following equation for the reaction rate:

$$\frac{\partial c_s}{\partial t} + \nabla \cdot (-D_s \nabla c_s) = k_{ads} c(\theta_0 - c_s) - k_{des} c_s \tag{3-1}$$

In the above equation, θ_0 represents the total number of active sites available on the surface of the catalyst. Equation 3-1 also defines the units of the rate constants: k_{ads} and k_{des}. The initial condition is that the concentration of adsorbed species is zero at the beginning of the process:

$$c_s = 0$$

The equation for the surface-reaction expression includes the concentration of the bulk species, c, at the position of the catalyst surface. Thus you must solve the equation for the surface reaction in combination with the mass balance in the bulk. The coupling between the mass balance in the bulk and the surface is obtained as a boundary condition in the bulk's mass balance. This condition sets the flux of c at the boundary equal to the rate of the surface reaction and is presented below. The transport in the bulk of the reactor is described by a convection-diffusion equation:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c + c\mathbf{u}) = 0 \tag{3-2}$$

The initial condition sets the concentration in the bulk at $t = 0$:

$$c = c_0$$

In the above equation, D denotes the diffusivity of the reacting species, c is its concentration, and $\mathbf{u}$ is the velocity. In this case, the velocity in the x direction equals 0 while the velocity in the y direction comes from the analytical expression for fully developed laminar flow between two parallel plates:

$$\mathbf{u} = (0, v_{\max}\left[1 - \left(\frac{(x - 0.5\delta)}{0.5\delta}\right)^2\right])$$

Here, δ is the distance between the plates, and $v_{\max}$ is the maximum local velocity. We assume that the origin for x is at the left edge of the model depicted in Figure 3-1.

BOUNDARY CONDITIONS

The boundary conditions for the material balance for the surface species are insulating conditions according to:

$$\mathbf{n} \cdot (-D_s \nabla c_s) = 0 \tag{3-3}$$

For the bulk, the boundary condition at the active surface couples the rate of the reaction at the surface with the flux of the reacting species and the concentration of the adsorbed species and bulk species:

$$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = -k_{\text{ads}} c(\theta_0 - c_s) + k_{\text{des}} c_s$$

The other boundary conditions for the bulk problem are:

- Inlet: $c = c_0$
- Outlet: $\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = \mathbf{n} \cdot c\mathbf{u}$
- Insulation: $\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = 0$

Modeling in COMSOL Multiphysics

This model deals with a phenomenon occurring in a 2D domain (convection-diffusion) coupled to another phenomenon occurring only at the 1D boundary of the 2D domain (diffusion-reaction). The COMSOL Multiphysics implementation is straightforward in every step except for the definition of the 1D problem, which requires some mathematical background. You need to use weak-form application modes for modeling PDEs on boundaries, edges, or points. To add the 1D boundary equation in the 2D model, use the Weak Form, Boundary application mode. This enables you to formulate the problem with the weak form instead of with the PDE form. An examination of the spatial diffusion on the boundary shows that only the flux tangential to the surface is defined. Therefore, in the weak-form specification you must

make use of the special *tangential derivative variable*. For more information about how to specify equations on the weak form, refer to the chapter "Deriving the Weak Form" on page 360 in the *COMSOL Multiphysics Modeling Guide*.

You define the two equations using the multiphysics feature of COMSOL Multiphysics. Select the two application modes, corresponding to the 2D and 1D material balances, in the Model Navigator.

Results

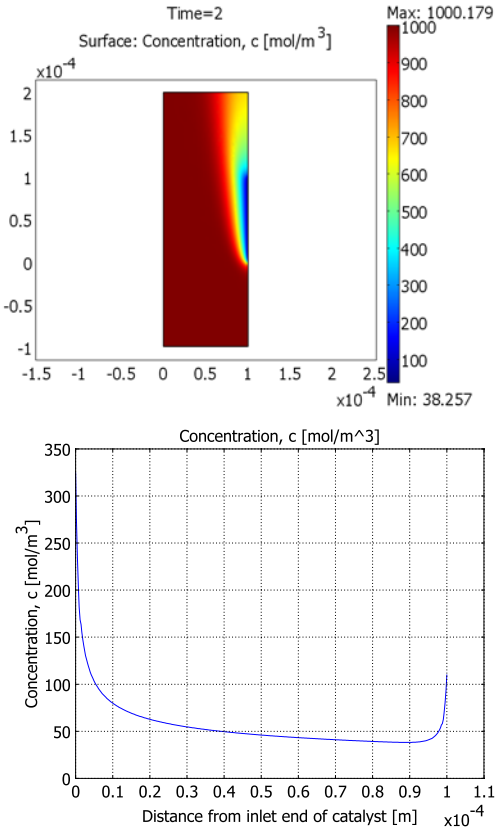


Figure 3-2: The concentration of the reacting species, c, after 2 seconds of operation in the 2D cross section (top) and along the active surface (bottom).

The upper plot in Figure 3-2 shows the concentration, c, of the reacting species in the 2D subdomain after 2 seconds of operation. The reaction is very fast and almost reaches steady state in that time frame. The lower plot, displaying the concentration along a vertical cross section of the active surface, shows that the concentration distribution exhibits edge effects at both ends of the catalyst. The higher concentration near $y = 0$ is easy to explain because this is the position closest to the inlet, and this end is therefore continuously supplied with fresh reactant. The increase in concentration at the end closer to the outlet is due to radial diffusion; the edge of the surface can receive diffusion in all directions within a 90° angle without having to "compete" for the reactant supply with other parts of the catalysts. This effect also appears at the edge close to the inlet.

The concentration of adsorbed species, c_s, shows a similar spatial distribution. However, while the concentration of the reactant decreases with time, the concentration of adsorbed species increases. You can also see that the slight spatial diffusion evens out the concentration gradients somewhat (see Figure 3-3).

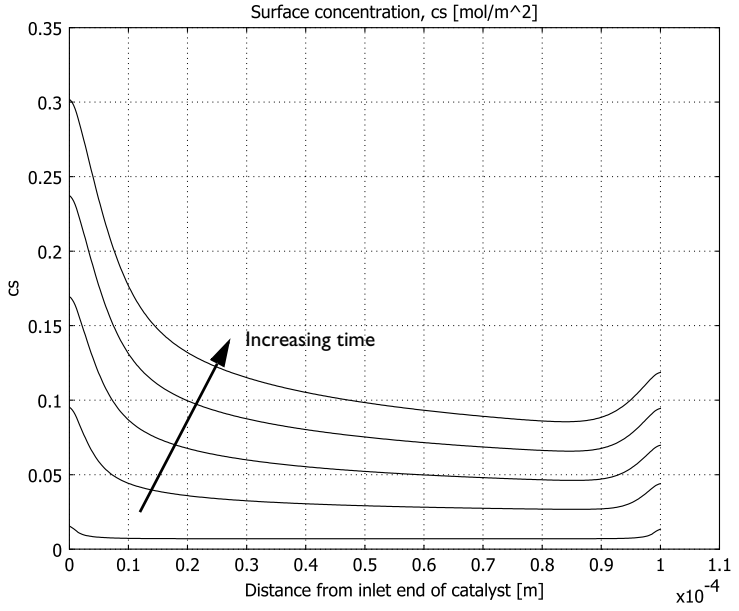


Figure 3-3: The concentration of adsorbed species increases with time. The edge effect appears at both edges due to the increased supply of reactants. This figure displays the concentration after 0.05, 0.5, 1.0, 1.5, and 2.0 s.

The concentration of reacting species decreases while the surface concentration of the adsorbed species increases with time. This implies that the surface reaction rate decreases with time. You can see this effect in Figure 3-4, which also shows that after 0.5 s the reaction rate almost reaches steady-state. The upper curve shows the reaction rate after 0.05 s, while the lower curve represents the curves for 0.5, 1.0, 1.5, and 2.0 s, which are all on top of each other.

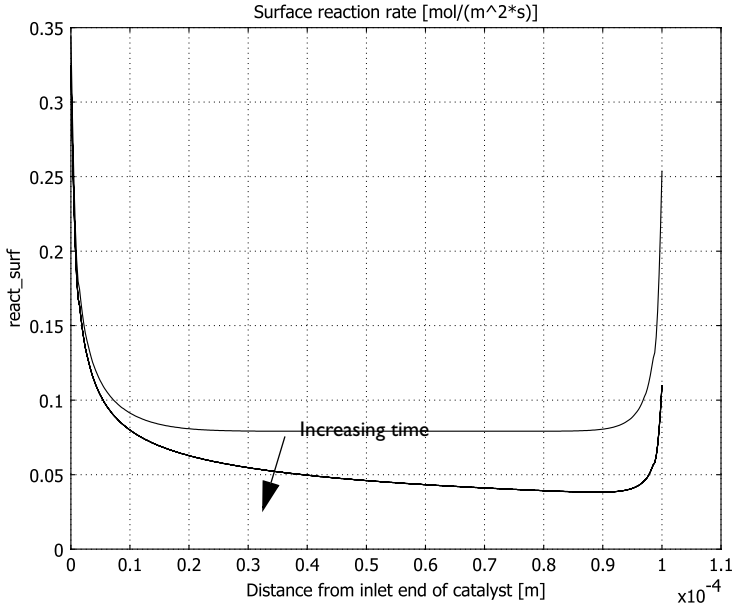


Figure 3-4: Surface reaction rate at the active surface. The largest reaction rate is obtained initially and is at the edges of the active surface. The reaction process almost reaches steady state at 0.5 s.

Model Library path: `COMSOL_Multiphysics/Chemical_Engineering/adsorption`

Modeling Using the Graphical User Interface

The following pages describe how to solve this problem using the graphical user interface.

MODEL NAVIGATOR

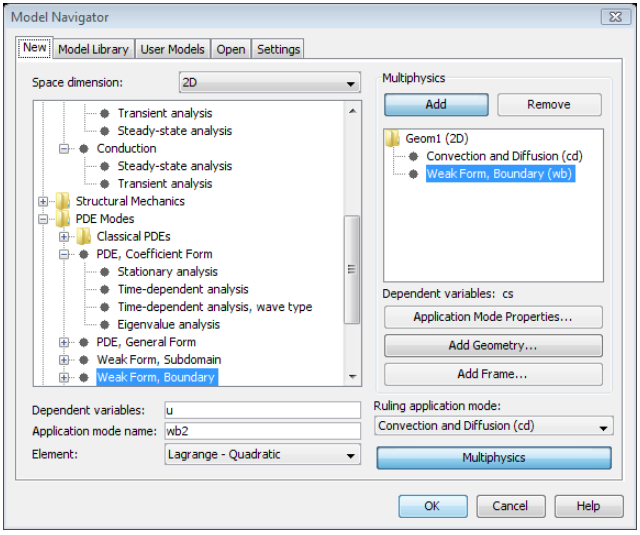
1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click the **Multiphysics** button and select **2D** in the **Space dimension** list.

3 Highlight the application mode **COMSOL Multiphysics>Convection and Diffusion>Convection and Diffusion>Transient analysis**. Click the **Add** button.

4 Select the application mode **COMSOL Multiphysics>PDE Modes>Weak Form, Boundary**. Type `cs` in the **Dependent variables** edit field. Click the **Add** button.

5 Click **OK**.



OPTIONS AND SETTINGS

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

2 Define the following constants in the **Constants** dialog box:

NAME	EXPRESSION	DESCRIPTION
c0	1000[mol/m^3]	Initial concentration
kads	1e-6[m^3/(mol*s)]	Forward rate constant
kdes	1e-9[1/s]	Backward rate constant
theta0	1000[mol/m^2]	Active site concentration
Ds	1e-11[m^2/s]	Surface diffusivity
D	1e-9[m^2/s]	Gas diffusivity

NAME	EXPRESSION	DESCRIPTION
v_max	1[mm/s]	Maximum velocity
delta	0.1[mm]	Channel width

3 Click **OK**.

4 Open the **Axes/Grid Settings** dialog box from the **Options** menu. Specify the following settings and click **OK**.

POSITION	X-Y LIMITS
x min	-15e-5
x max	25e-5
y min	-15e-5
y max	25e-5

GEOMETRY MODELING

1 Hold down the shift key and click the **Rectangle/Square** button on the Draw toolbar. Enter the values listed below in the corresponding edit fields and click **OK**.

EDIT FIELD	VALUE
Width	1e-4
Height	3e-4
x	0
y	-1e-4

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

3 Click the **Point** button and click on the coordinate (1e-4, 0) in the drawing area. Click the **Point** button again and click on (1e-4, 1e-4).

PHYSICS SETTINGS

Expression Variables

1 On the **Options** menu, point to **Expressions** and then click **Boundary Expressions**.

2 Select Boundary 5 in the **Boundary selection** list and enter the following expression.

NAME	EXPRESSION
react_surf	kads*c*(theta0-cs)-kdes*cs

3 Click **OK**.

4 On the **Options** menu, select **Expressions** and then click **Subdomain Expressions**.

5 Select Subdomain 1 in the **Subdomain selection** list and enter the following expression.

NAME	EXPRESSION
v_lam	v_max*(1-((x-0.5*delta)/(0.5*delta))^2)

6 Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Convection and Diffusion (cd)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 Enter boundary conditions according to the following table:

SETTINGS	BOUNDARIES 1, 4, 6	BOUNDARY 2	BOUNDARY 3	BOUNDARY 5
Type	Insulation/ Symmetry	Concentration	Convective flux	Flux
c_0		c0		
N_0				-react_surf

4 Click **OK**.

Subdomain Settings

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

2 Select Subdomain 1 in the **Subdomain Settings** dialog box.

3 Specify the settings as in the following table:

QUANTITY	VALUE/EXPRESSION
δ_{ts}	1
D (isotropic)	D
R	0
u	0
v	v_lam

4 Click the **Init** tab and type c0 in the **Concentration, c** edit field (**c(t_0)**).

5 Click **OK**.

Boundary Conditions

Perform this step to specify the transport equation stated in Equation 3-1. Do so in the **Boundary Settings** dialog box because the catalytic surface is a boundary of the 2D geometry.

1 In the **Multiphysics** menu, select **2 Weak Form, Boundary (wb)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 Select the **Select by group** check box, then click in the **Boundary selection** list to select all boundaries (Boundaries 1–6). Clear the **Active in this domain** check box.

4 Clear the **Select by group** check box, then select Boundary 5. Check the **Active in this domain** check box to enable the weak form application mode only on this boundary.

5 Click the **Init** tab and then type `0` in the **cs(t_0)** edit field.

6 Click the **Weak** tab. Make the following specifications:

TERM	VALUE/EXPRESSION
weak	`Ds*(-test(csTx)*csTx-test(csTy)*csTy)+ test(cs)*(react_surf-cst)`
dweak	0
constr	0

7 Click **OK**.

By adding `T` to all the weak variables you get the tangential components discussed in the section "Modeling in COMSOL Multiphysics" on page 35. The lowercase `t` indicates the derivative with respect to time.

Point Settings

To enforce the boundary condition in Equation on the surface equation you must open the **Point Settings** dialog box from the **Physics** menu and select Points 4 and 5. In this case the default settings are correct, that is, the **weak**, **dweak**, and **constr** edit fields should all contain 0, so just leave them as is.

MESH GENERATION

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

2 In the **Free Mesh Parameters** dialog box, click the **Boundary** tab and select Boundary 5 from the list.

3 Type `1.5e-6` in the **Maximum element size** edit field.

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

COMPUTING THE SOLUTION

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

2 Select **Time dependent** in the **Solver** list.

3 In the **Time stepping** area, type `range(0,0.05,2)` in the **Times** edit field.

4 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

To generate the right plot in Figure 3-2:

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

2 Go to the **General** tab and click the **Line/Extrusion plot** button. Select **2** in the **Solutions to use** list. Customize the plot with text labels by clicking the **Title/Axis** button.

3 Click the **Line/Extrusion** tab and then select **Convection and Diffusion (cd)> Concentration, c** from the **Predefined quantities** list.

4 From the **Boundary selection** list select Boundary 5.

5 Under **x-axis data**, click the upper option button. Select **y** from the adjacent list.

6 Click **OK**.

To generate Figure 3-3, repeat the previous operations but with these changes:

1 On the **General** page, go to the **Solutions to use** list and hold down the Ctrl key to select the times 0.05, 0.5, 1.0, 1.5, and 2.0.

2 Click the **Line/Extrusion** tab and then select **Weak Form, Boundary (wb)>cs** from the **Predefined quantities** list.

To generate Figure 3-4, repeat the previous operations but with this change:

On the **Line/Extrusion** tab, type `react_surf` in the **Expression** edit field.

Tubular Reactor

Introduction

This example studies an elementary, exothermic, 2nd-order reversible reaction

$$A + B \Leftrightarrow 2C \tag{3-4}$$

in a tubular reactor (liquid phase, laminar flow regime). The reactor is equipped with a cooling jacket to limit the temperature increase due to the exothermic nature of the reaction and avoid an explosion. The model is described by the material balances for the species involved and the energy balances for the reactor and the cooling jacket.

Additional background to this model is available in Section 8.9 of the Fourth Edition of *Elements of Chemical Reaction Engineering* by H.S. Fogler.

Model Definition

Figure 3-5 illustrates the reactor geometry. By assuming that the variations in the angular direction around the centerline are negligible, you can use a 2D axisymmetric model.

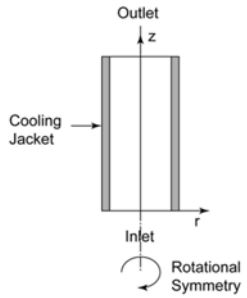


Figure 3-5: Geometry for the 2-dimensional rotationally symmetric models.

The model geometry consists of an inlet boundary, an outlet boundary, a reactor wall facing the cooling jacket, and the symmetry axis r =0. The reactor's radius is R = 8 cm its length L = 1 m.

Assuming the diffusivities for the three species to be identical, you can model the reactor using three differential equations:

- A material-balance partial differential equation (PDE) for one of the species. As noted in the next section, separate material-balance equations are not necessary for the other two species if the diffusivities are identical.
- An energy-balance PDE for the reactor core.
- An energy-balance ordinary differential equation (ODE) for the cooling jacket. Under the assumptions that the coolant flow is turbulent and that turbulent mixing eliminates any temperature differences in the radial direction, only axial temperature variations are present in the cooling jacket. For this reason, the cooling jacket is not included in the model geometry.

The material and energy balances in the reactor are automatically set up in COMSOL Multiphysics by selecting the proper application modes. The ordinary differential equation that describes the energy balance in the cooling jacket is manually defined as a boundary equation.

The material balance and energy balances for the reactor are described by the equations

$$\begin{aligned} \nabla \cdot (-D\nabla c_{\mathrm{A}} + \mathbf{u}c_{\mathrm{A}}) &= r_{\mathrm{A}} \\ \nabla \cdot (-k\nabla T + \mathbf{u}\rho C_p T) &= \Delta H_{Rx} r_{\mathrm{A}} \end{aligned} \tag{3-5}$$

In the material-balance equation for c_A (mol/m^3), the concentration of species A, D (m^2/s) denotes the diffusion coefficient, $\mathbf{u}$ (m/s) the flow velocity, and r_{A} (mol/(m^3·s)) the reaction rate. In the energy-balance equation for the reactor temperature, T (K), the additional parameters are the thermal conductivity, k (W/(m·K)), the fluid density, ρ (kg/m^3), the specific heat capacity, C_p (J/(kg·K)), and the reaction enthalpy ΔH_{Rx} (J/mol).

The boundary conditions for Equations 3-5 are as follows (see Figure 3-5 for the appropriate references):

$$\begin{aligned} c_A(r,0) = c_{A0} \quad & \frac{\partial c_A}{\partial r}(R,z) = \frac{\partial c_A}{\partial r}(0,z) = 0 \quad \frac{\partial c_A}{\partial z}(r,L) = 0 \\ T(r,0) = T_0 \quad & \frac{\partial T}{\partial r}(R,z) = \frac{\partial T}{\partial r}(0,z) = 0 \quad \frac{\partial T}{\partial z}(r,L) = 0 \end{aligned} \tag{3-6}$$

Here c_{A0} and T_0 denote the initial concentration and temperature, respectively.

For the flow velocity, assume a laminar profile:

$$u = u_{\max}\left(1-\left(\frac{r}{R}\right)^2\right) \tag{3-7}$$

Here $u_{\max} = 2u_0$, where the average velocity, u_0 (m/s), is calculated as the ratio between the total volume flow rate, v_0 (m^3/s), and the reactor's cross-sectional area, πR^2.

In this model, assume that the species A, B, and C have the same diffusivity. This implies that you only need to solve one material balance, because you can find the other species' concentrations through stoichiometry. Specifically, assuming the initial concentration for species C to be zero, the concentrations are given by

$$c_A = (1-x_A)c_{A0} \qquad c_B = c_{B0}-x_A c_{A0} \qquad c_C = 2x_A c_{A0} \tag{3-8}$$

where x_A is the conversion of species A.

In the COMSOL Multiphysics Chemical Engineering Module, you could have modeled all three species using their true multicomponent diffusivities. These assumptions give the reaction-rate expression

$$r_A = -A\exp\left(\frac{E}{R_g T}\right)\left(c_A c_B - \frac{c_C^2}{K_{eq}}\right) \tag{3-9}$$

where A (m^3/(mol·s)) refers to the rate constant, E (J/mol) is the activation energy, R_g =8.314 J/(mol·K) denotes the ideal gas constant, T (K) is the temperature, and the equilibrium constant is

$$K_{eq} = K_{eq0}\exp\left(\Delta H_{Rx} R_g\left(\frac{1}{303\ \text{K}}-\frac{1}{T}\right)\right) \tag{3-10}$$

The energy-balance ODE for the coolant reads

$$\frac{\partial T_c}{\partial z} = \frac{2\pi R U_k (T - T_c)}{C_{pc} m_c} \tag{3-11}$$

where T_c is the coolant temperature (K), U_k (W/(m^2·K)) is the total heat-transfer coefficient between the reactor and the cooling jacket, rate, C_{pc} (J/(kg·K)) is the coolant's specific heat capacity, and m_c (kg/s) represents its mass flow. You can neglect the heat conduction in the cooling jacket and thus assume that heat transport takes place only through convection.

As a boundary condition, set the temperature of the incoming cooling fluid:

$$T_c(0) = T_{c0} . \quad (3\text{-}12)$$

Table 3-1 summarizes the relevant input data.

TABLE 3-1: MODEL INPUT DATA

PROPERTY	VALUE
D	10^{-9} m^2/s
k	0.559 W/(m·K)
ρ	1000 kg/m^3
C_p	4180 J/(kg·K)
ΔH_{Rx}	-83,680 J/mol
T_0	320 K
c_{A0}	500 mol/m^3
c_{B0}	500 mol/m^3
v_0	$5 \cdot 10^{-4}$ m^3/s
A	$1.65 \cdot 10^{11}$ m^3/(mol·s)
E	95,238 J/mol
K_{eq0}	10^3
U_k	1300 W/(m^2·K)
C_{pc}	4180 J/(kg·K)
m_c	0.01 kg/s
T_{c0}	298 K

Results

From the plots in Figure 3-6 you can see how the conversion and temperature vary inside the reactor. Due to a larger residence time, you find the highest conversion close to the wall (right side). Also, the cooling effect of the wall is evident from the temperature plot. Nevertheless, the temperature maximum is located close to the wall because the temperature depends strongly on the relation between the convected heat and the heat produced in the reaction. Due to the laminar-flow velocity profile, the

fluid close to the reactor wall but not in contact with the cooling jacket is heated during a longer time by the exothermic reactions.

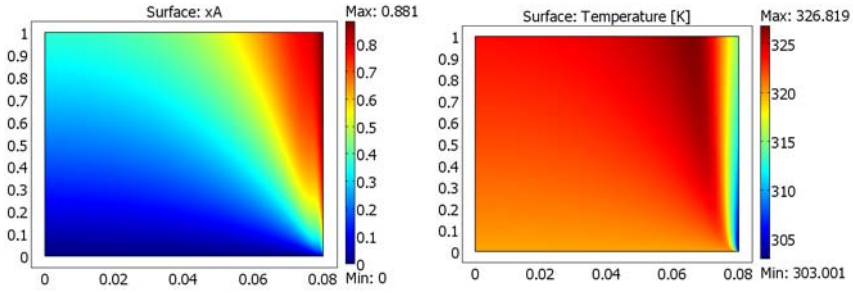


Figure 3-6: Conversion (left) and temperature (right) in the reactor.

Figure 3-7 shows how the coolant temperature increases along the length of the reactor. The temperature increases rapidly close to the inlet, but as the reaction rate decreases due to the depletion of reactants so does the rate of temperature increase.

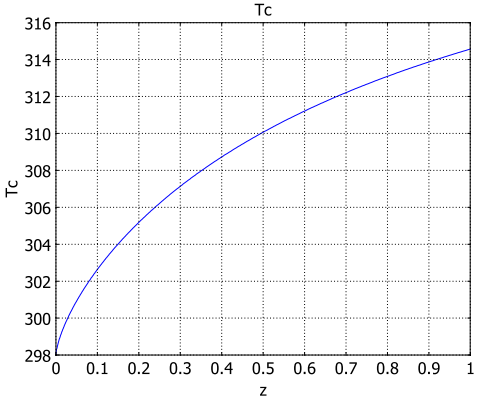


Figure 3-7: Coolant temperature along the length of the reactor.

Model Library path:
`COMSOL_Multiphysics/Chemical_Engineering/tubular_reactor`

MODEL NAVIGATOR

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

2 Click the **Multiphysics** button in the lower-right corner.

3 Open the **COMSOL Multiphysics** folder and select the **Convection and Diffusion** application mode from the **Convection and Diffusion** folder.

4 In the **Dependent variables** edit field, type `cA`. Click **Add**.

5 Add the **Convection and Conduction** application mode from the **Heat Transfer** folder.

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

7 Open the **COMSOL Multiphysics>PDE Modes** folder and select **Weak Form, Boundary**.

8 Change the name of the dependent variable to `Tc`, then click **Add**.

9 Click **OK**.

OPTIONS AND SETTINGS

1 Go to the **Options** menu and choose **Constants**.

2 Make the following entries in the **Constants** dialog box and then click **OK**.

NAME	EXPRESSION	DESCRIPTION
D	1e-9[m^2/s]	Diffusivity
k	0.559[W/(m*K)]	Thermal conductivity, reactor
rho	1000[kg/m^3]	Fluid density, reactor
Cp	4180[J/(kg*K)]	Specific heat capacity, reactor
dHRx	-83680[J/mol]	Reaction enthalpy
T0	320[K]	Initial temperature, reactor
cA0	500[mol/m^3]	Initial concentration, species A
cB0	500[mol/m^3]	Initial concentration, species B
R	8[cm]	Reactor radius
v0	0.0005[m^3/s]	Total flow rate, reactor
u0	v0/(pi*R^2)	Mean axial flow velocity
E	95238[J/mol]	Activation energy
A	1.65e11[m^3/(mol*s)]	Rate constant frequency factor
Rg	8.314[J/(mol*K)]	Ideal gas constant
Keq0	1000	Equilibrium constant at 303 K
Uk	1300[W/(m^2*K)]	Heat transfer coefficient

NAME	EXPRESSION	DESCRIPTION
Tc0	298[K]	Coolant temperature, inlet
Cpc	4180[J/(kg*K)]	Specific heat capacity, coolant
mc	0.01[kg/s]	Total mass-flow rate, coolant

3 Go to the **Options** menu and choose **Expressions>Scalar Expressions**.

4 Make the following entries in the **Scalar Expressions** dialog box; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
uz	2*u0*(1-(r/R)^2)	Axial flow velocity
xA	(cA0-cA)/cA0	Conversion, species A
cB	cB0-cA0*xA	Concentration, species B
cC	2*cA0*xA	Concentration, species C
rA	-A*exp(-E/(Rg*T)) *(cA*cB-cC^2/Keq)	Reaction rate
Keq	Keq0*exp(dHRx/Rg *(1/303[K]-1/T))	Equilibrium constant
Q	(-rA)*(-dHRx)	Heat production

GEOMETRY MODELING

1 Go to the **Draw** menu and select **Specify Objects>Rectangle**.

2 Type 0.08 in the **Width** edit field and 1 in the **Height** edit field. Click **OK**.

3 Click **Zoom Extents** to center the geometry.

PHYSICS SETTINGS

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, select **Convection and Diffusion (cd)**.

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

3 In the **Subdomain Settings** dialog box, select Subdomain 1 and type D in the **Diffusion coefficient** edit field.

4 In the **Reaction rate** edit field, type rA.

5 In the **z-velocity** edit field, type uz.

6 Still in the **Subdomain Settings** dialog box, click the **Init** tab.

7 In the edit field for **cA(t_0)**, enter the initial value cA0.

8 Click **OK**.

Boundary Conditions—Convection and Diffusion

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

2 In the **Boundary Conditions** dialog box enter the following boundary conditions.

SETTINGS	BOUNDARIES 1, 4	BOUNDARY 2	BOUNDARY 3
Type	Insulation/Symmetry	Concentration	Convective flux
cA_0	-	cA0	-

3 Click **OK**.

Subdomain Settings—Convection and Conduction

1 From the **Multiphysics** menu, choose **Convection and Conduction (cc)**.

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

3 In the **Thermal conductivity** edit field, type `k`.

4 In the **Density** edit field, type `rho`.

5 In the **Heat capacity at constant pressure** edit field, type `Cp`.

6 In the **Heat source** edit field, type `Q`.

7 In the *z* component (right) edit field for the **Velocity field**, type `uz`.

8 Still in the **Subdomain Settings** dialog box, click the **Init** tab.

9 In the edit field for **$T(t_0)$**, enter the initial value `T0`.

10 Click **OK**.

Boundary Conditions—Convection and Conduction

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

2 In the **Boundary Conditions** dialog box enter the following boundary conditions.

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY 4
Type	Axial symmetry	Temperature	Convective flux	Heat flux
q_0	-	T0	-	-Uk*(T-Tc)

Because `Tc` is the dependent variable of a PDE application mode, it does not have an associated unit. Therefore, if the **Highlight unexpected units** check box is selected in your modeling session, the **Unit** label for the **q_0** edit field appears in red. Provided you specify the boundary condition for `Tc` using the chosen base unit system (specified under **Physics>Model Settings**; the default choice is **SI**), you can safely ignore this warning.

3 Click **OK**.

Boundary Conditions—Weak Form, Boundary

1. From the **Multiphysics** menu, choose **Weak Form, Boundary (wb)**.
2. From the **Physics** menu, choose **Boundary Settings**.
3. Select Boundaries 1–3 in the **Boundary selection** list and clear the **Active in this domain** check box.
4. Select Boundary 4 and click the **Weak** tab.
5. In the **weak** edit field, type `Tc_test*(TcTz-2*pi*R*Uk*(T-Tc)/(Cpc*mc))`.
6. Click **OK**.
7. From the **Physics** menu, choose **Point Settings**.
8. Select Point 3 from the **Point selection** list.
9. Set the inlet temperature of the cooling water by typing `Tc-Tc0` in the **constr** edit field.
10. Click **OK**.

MESH GENERATION

1. From the **Mesh** menu, choose **Mapped Mesh Parameters**.
2. Click the **Boundary** tab.
3. Select Boundaries 1 and 4 from the **Boundary selection** list by left-clicking and holding down the Ctrl-key.
4. Select the **Constrained edge element distribution** check box, then set the **Number of edge elements** to 100. In the **Distribution** area, set the **Element ratio** to 15 and select **Exponential** as the **Distribution method**.
5. Select Boundaries 2 and 3 from the **Boundary selection** list.
6. Select the **Constrained edge element distribution** check box, then set the **Number of edge elements** to 60. In the **Distribution** area, set the **Element ratio** to 40, select **Exponential** as the **Distribution method**, and select the **Reverse direction** check box.
7. Click **Remesh**. When the mesher has finished, click **OK**.

The generated mesh is dense both close to the cooling wall to resolve the large gradients in temperature and close to the reactor inlet to resolve the large gradients in composition.

COMPUTING THE SOLUTION

1. Click the **Solver Parameters** button on the Main toolbar.
2. Make sure the **Stationary** solver is selected.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar to start the simulation.

POSTPROCESSING AND VISUALIZATION

The default plot displays the concentration profile.

To see the resulting conversion or temperature profiles, follow these steps:

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

2 To see the conversion or temperature profile, go to the **Surface** page and type `xA` (for the conversion) or `T` (for the temperature) in the **Expression** edit field.

3 Click **OK** to close the **Plot Parameters** dialog box.

4 Use the **Zoom Window** tool on the Main toolbar to get a closer look at the results (see Figure 3-6).

To plot the coolant temperature throughout the length of the reactor (see Figure 3-7), follow these steps:

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

2 Click the **Line/Extrusion** tab and select Boundary 4 from the **Boundary selection** list.

3 From the **Predefined quantities** list, select **Weak Form, Boundary (wb)>Tc**.

4 From the **x-axis data** list, select **z**.

5 Click **OK**.

To investigate the average outlet conversion, concentration, and temperature follow the steps below:

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

2 Select Boundary 3 in the **Boundary selection** list.

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

4 Type `1` in the **Expression** edit field to get the cross-sectional area of the reactor.

5 Click **Apply**. The value of the integral (roughly $0.0201\ \mathrm{m}^2$) appears in the message log at the bottom of the user interface.

6 Type `xA` in the **Expression** edit field, then click **OK**. To get the average outlet conversion, divide the result with the reactor's cross-sectional area.

7 Follow the same procedure using the expressions `cA` and `T` to find the average outlet concentration and temperature, respectively.

4

Electromagnetics Models

This chapter contains a few electromagnetics models—more comprehensive sets are available in the model libraries that comes with the AC/DC Module and RF Module. For introductory electromagnetics models and information about the application modes for electromagnetics, see "Electromagnetics" on page 77 in the *COMSOL Multiphysics Modeling Guide*.

Several physical quantities are fundamental to electromagnetics. They are:

- *Electric field intensity*, **E**
- *Electric flux density* or *electric displacement*, **D**
- *Magnetic flux density*, **B**
- *Magnetic field intensity*, **H**
- *Current density*, **J**
- *Electric charge density*, ρ

The governing partial differential equations for all macroscopic electromagnetic problems are well known—they are the four *Maxwell's equations*. Of these relationships, the first three are *Faraday's law*, *Ampère's circuital law*, and *Gauss' Law*. The fourth equation states that isolated magnetic charges (monopoles) do not exist in nature.

In electromagnetics, *constitutive relations* specify material-dependent interactions between fundamental physical quantities such as **E** and **D**. The definition of boundary conditions, taken together with Maxwell's equations and the constitutive relations, make it possible to describe any macroscopic electromagnetic problem. For an introduction to the theory of electromagnetics, see the section "Fundamentals of Electromagnetics" on page 79 in the *COMSOL Multiphysics Modeling Guide*.

Electrostatic Potential Between Cylinders

This example model demonstrates each step in building and solving a 3D electrostatics model. The analysis shows the electric potential between two cylinders in a vacuum.

Model Definition

The first step is to define the overall model and draw its geometry. This model consists of two cylinders with opposite electrostatic potentials. The potential difference between them induces an electric field in the vacuum. The electrostatic scalar potential V is related to an electric field as $\mathbf{E} = -\nabla V$. Gauss' law, $\nabla \cdot (\varepsilon \mathbf{E}) = \rho$, gives $-\nabla \cdot (\varepsilon \nabla V) = \rho$.

This equation includes a material property and a source term:

- ε is the permittivity.
- ρ is the space charge density.

To simulate the vacuum chamber, create a box in which there is no atmosphere or gas of any kind. In addition, assume that the potential is zero on the bottom boundary and that there is no electric field normal to the other exterior boundaries.

Results

The plot in Figure 4-1 on page 58 combines a surface plot of the potential with a streamline plot of the electric field. The surface plot shows the electric potential on the cylinder and box faces. As expected, the electric field lines run from cylinder to cylinder and from the cylinders to the grounded bottom plate. The electric field does not penetrate the top and side walls.

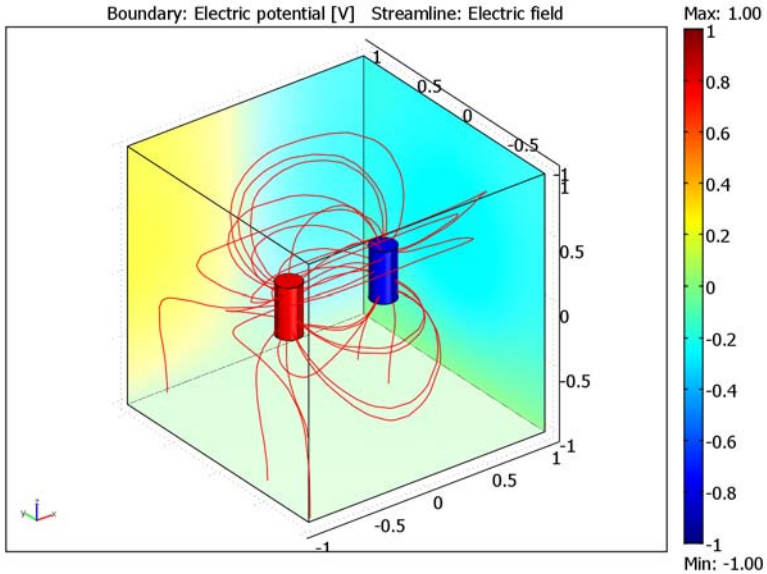


Figure 4-1: The electric potential (surface) and the electric field (streamlines).

Modeling Using the Graphical User Interface

Start COMSOL Multiphysics using the procedure for the operating system on your computer. On Windows double-click the **COMSOL Multiphysics** icon to start COMSOL Multiphysics and open the **Model Navigator**.

Model Library path: `COMSOL_Multiphysics/Electromagnetics/potential_between_cylinders`

MODEL NAVIGATOR

For this model use the Electrostatics application mode.

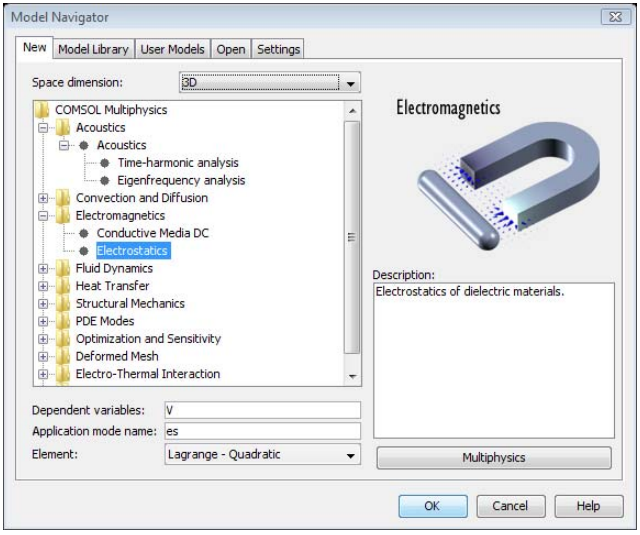
1 In the **Model Navigator** click on the **New** tab.

2 Select **3D** in the **Space dimension** list.

3 In the list of application modes, open the **COMSOL Multiphysics** folder and then the **Electromagnetics** folder. Select **Electrostatics** from the list of electromagnetics application modes.

4 Accept the default element type (quadratic Lagrange elements), which is suitable for most cases.

5 Click **OK**.



The Electrostatics application mode provides predefined equations and boundary conditions that make it easy to create this model, but you must still attend to a few details.

OPTIONS AND SETTINGS

In this model the permittivity of free space, ε_0, defines the permittivity in the domain. It is not necessary to enter this variable because it is a predefined application scalar variable in the Electrostatics application mode. If you prefer to use another value rather than the standard SI unit value, choose **Scalar Variables** from the **Physics** menu. Doing so, however, changes the underlying formulation for electrostatics, so we recommend that you use the predefined value.

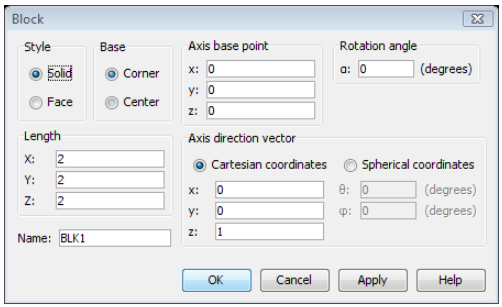
GEOMETRY MODELING

Next define the model geometry. For this example, create a box measuring 2-by-2-by-2 meters, and then place two cylinders inside that box. When you exit the

Model Navigator to begin setting up a model, COMSOL Multiphysics enters Draw mode with access to the drawing tools.

To define the model geometry, begin with the box:

1. Open the **Block** dialog box by clicking on the appropriate symbol on the Draw toolbar.
2. In that dialog box, go to the **Base** area and click the **Center** button to use centered base coordinates.
3. In the **Length** area, type `2` in the **X**, **Y**, and **Z** edit fields as the length for all three dimensions.
4. Click **OK** to create the block.



5. To ensure that the full geometry is visible, click the **Zoom Extents** button on the Main toolbar.

Now move on to the two cylinders. To create these 3D objects on a 2D screen, work in a 2D work plane. The method to follow in creating the cylinders is simple: draw two circles in 2D and then extrude them in the *z* direction to form 3D objects.

1. Go to the **Draw** menu and choose **Work-Plane Settings** to define a new work plane.
2. Click the **Quick** tab and make sure that the **x-y** button is selected (the default).
3. Type `-0.2` in the **z** edit field.
4. Click **OK** to enter the 2D work plane.

Now draw the cylinder cross sections in the work plane:

1. Click on the **Zoom In** button several times until the grid spacing equals 0.2 in both the *x* and *y* directions.
2. Go to the **Options** menu and choose **Axes/Grid Settings**.
3. In the **Axes/Grid Settings** dialog box, click the **Grid** tab.

4 Clear the **Auto** check box and type `0.1` in the **y spacing** edit field.

5 Click **OK**. You can now create circles with a radius of 0.1.

6 Click on the **Ellipse/Circle (Centered)** button in the Draw toolbar.

7 Place the crosshairs at the coordinates (–0.4, 0). Then click on the right mouse button and drag up or down until you create a circle with radius of 0.1.

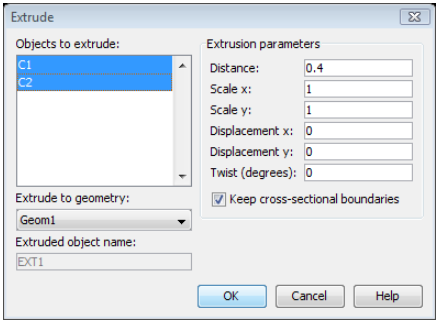
8 Repeat the process to draw a second circle of the same size centered at (0.4, 0).

Create the cylinders:

1 Press Ctrl+A to select both circles.

2 Go to the **Draw** menu and choose **Extrude**.

3 In the **Extrude** dialog box define the height of the cylinders by typing `0.4` in the **Distance** edit field. The resulting cylinders extend from –0.2 to 0.2 in the z direction.



4 Click **OK** to close the dialog box.

COMSOL Multiphysics now returns to the 3D environment where the cylinders are present. The cylinders have become extruded geometry objects with the names EXT1 and EXT2.

To complete the geometry, subtract the two cylinders from within the box using a Boolean operation:

1 Click the **Create Composite Object** button in the Draw toolbar.

2 Type the Boolean expression `BLK1-EXT1-EXT2` in the **Set formula** edit field.

3 Click **OK**.

The resulting geometry is a new composite object with the default label CO1.

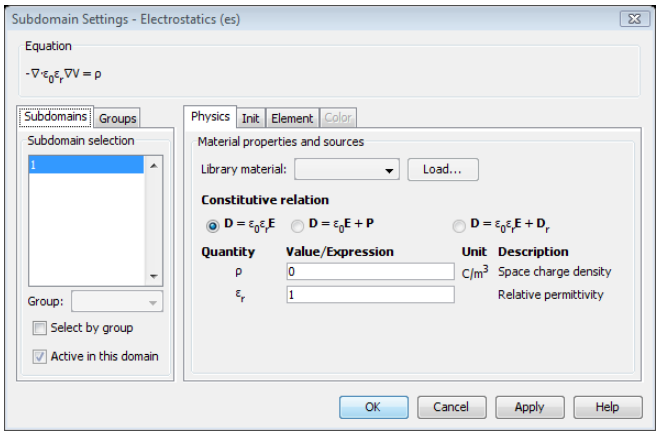
PHYSICS MODELING

The next task is to define the physics through material properties on the domain and conditions on the boundaries.

Subdomain Settings

First, specify the material properties in the modeling domain.

Open the **Subdomain Settings** dialog box from the **Physics** menu. COMSOL Multiphysics then switches to Subdomain mode where you can specify material properties for each subdomain.



In this example, ε equals the permittivity of free space $\varepsilon_0 = 8.854 \cdot 10^{12}$ F/m, a value predefined in COMSOL Multiphysics. The relative permittivity ε_r then equals 1.

SETTINGS	SUBDOMAIN 1
ε_r	1
ρ	0

The space charge density option specifies the distribution of a space charge in a subdomain. Here there is none, so the value of ρ equals zero.

Now set the value for the permittivity in the model:

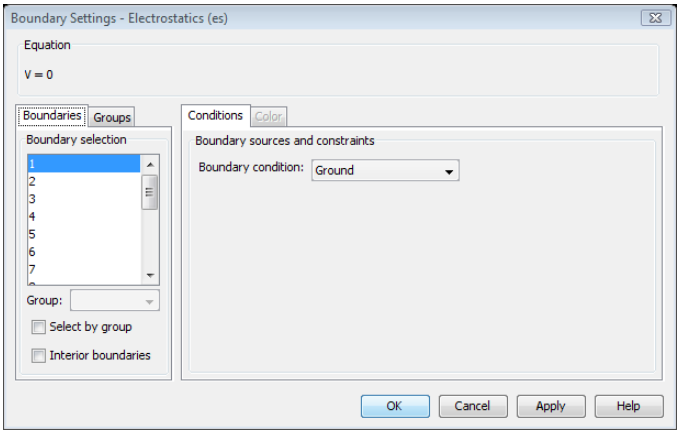
1. This model consists of only one subdomain. Make certain that Subdomain 1 is selected in the **Subdomain selection** list.
2. Go to **Constitutive relation** and make certain that the default $\mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}$ is selected.
3. Click **OK**.

For time-dependent and nonlinear analyses you might find it necessary to set initial conditions. That step is not necessary for this linear electrostatics problem.

Boundary Conditions

To set boundary conditions, go to the **Physics** menu and choose **Boundary Settings** to open up the corresponding dialog box. Here you select boundaries and specify the boundary conditions.

When you select a specific boundary, the program allows you to choose from a list of available boundary conditions.



To speed up the modeling process even with a relatively simple 3D model, you can select several faces with one mouse click. To learn more about the various selection methods see "Object Selection Methods in 3D" on page 127 in the *COMSOL Multiphysics User's Guide*.

The following table summarizes the boundaries in this model and their values:

SETTINGS	BOUNDARIES 6–11	BOUNDARIES 12–17	BOUNDARIES 1, 2, 4, 5, 18	BOUNDARY 3
Type	Electric potential	Electric potential	Zero charge/Symmetry	Ground
V_0	1	-1		

- Boundaries 6–11 define the left cylinder where the electric potential is 1 V.
- The second cylinder consists of Boundaries 12–17 and has an electric potential of –1 V.
- The third set of boundaries defines the box, except the bottom boundary.
- The last set (Boundary 3) is the grounded bottom plate.

To enter these boundary values into the model, follow these steps:

1. To enable object selection with the mouse you must first deselect the orbit/pan/zoom function. To do so, click the **Orbit/Pan/Zoom** button.
2. Draw a rubber-band box around one of the cylinders.
3. When its faces are highlighted, select **Electric potential** from the **Boundary condition** list.
4. Type 1 in the V_0 edit field.
5. Repeat the procedure for the second cylinder, but this time type –1 in the V_0 edit field.
6. Select the **Select by group** check box.
7. Select Boundary 1. The group selection then also selects all other exterior boundaries.
8. Select **Zero charge/Symmetry** from the **Boundary condition** list.
9. To select the bottom face, first click to clear the **Select by group** check box and then select Boundary 3.
10. Select **Ground** from the **Boundary condition** list.
11. Click **OK**.

MESH GENERATION

Generating the mesh is usually quite simple: just click one of the mesh buttons on the Main toolbar. In cases with special requirements you can also use commands in the **Mesh** menu. In this case, use a predefined setting for creating a coarse mesh, which makes the solution process faster than the default mesh-size settings.

1. From the **Mesh** menu, choose **Free Mesh Parameters**.
2. In the **Free Mesh Parameters** dialog box, select **Coarser** from the **Predefined mesh sizes** list.
3. Click **OK**.
4. Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

At this point you can either accept the default settings for the solver COMSOL Multiphysics should use, or you can interactively select the solver and its operating parameters. In most cases, though, you only need to click on the **Solve** button in the Main toolbar.

To reduce the time and memory requirements for the solution process, it is wise to make a few changes to the solver parameters. The default settings for 3D electrostatics models specify an *iterative solver*. These solvers generally use less memory than direct solvers and are often faster.

Iterative solvers work with a set of *preconditioners*, and the *algebraic multigrid* (*AMG*) preconditioner works best for scalar elliptic PDEs such as Laplace's equation and Poisson's equations. It is the default preconditioner for the 3D Electrostatics application mode.

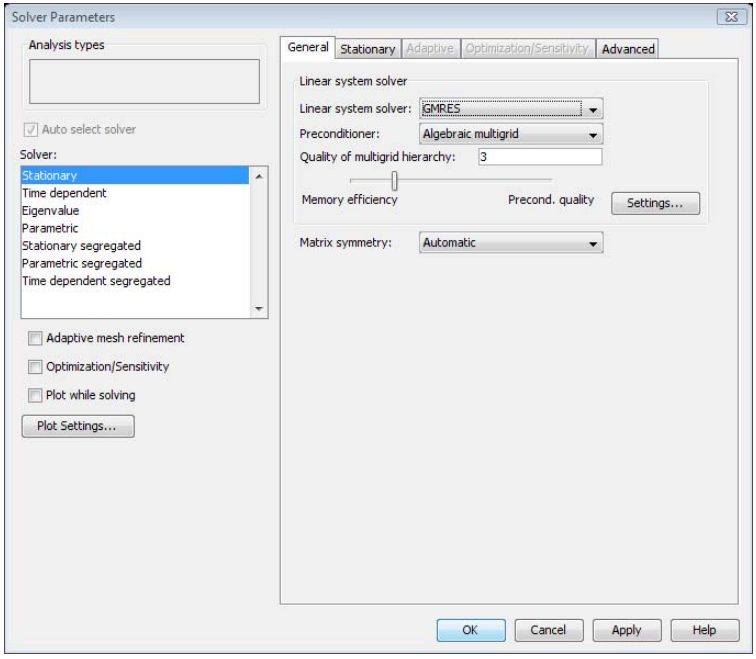
1 From the **Solve** menu, open the **Solver Parameters** dialog box.

2 Click the **General** tab.

3 Choose a linear system solver. Select **GMRES** from the **Linear system solver** list.

4 Choose a preconditioner. Select **Algebraic multigrid** from the **Preconditioner** list.

5 Click **OK**.



6 Start the solution process by clicking the **Solve** button on the Main toolbar. The results might take a few seconds to compute depending on the problem's complexity.

POSTPROCESSING AND VISUALIZATION

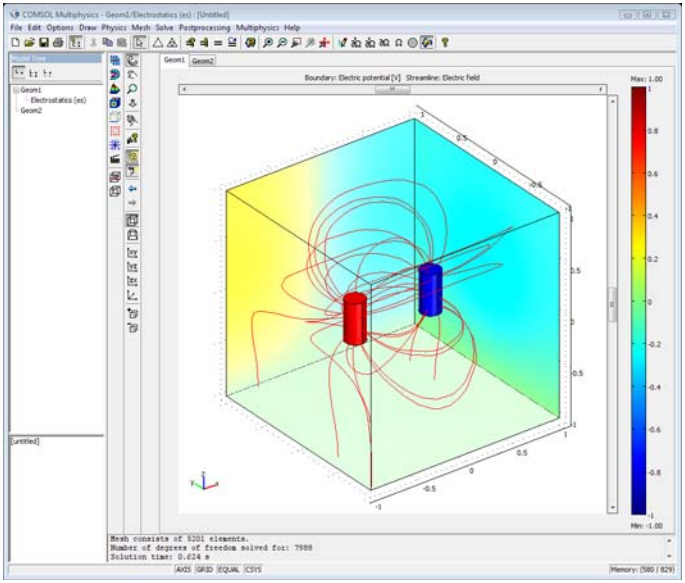
After solving the problem, COMSOL Multiphysics shifts to its postprocessing mode and shows a slice plot of the electric potential V. This plot, however, might not offer much immediately useful information, but COMSOL Multiphysics provides a variety of color plots and animations that help you more quickly spot trends and regions of interest. To better examine the solution for an electrostatic problem, for instance, you might want to view a surface or contour plot, and as the variable of interest you can select the electrostatic potential, the electric field, the electric displacement field, or the polarization field. Further, for arrow or streamline plots it is possible to select the x, y, or z components of most of those parameters.

To combine a surface plot with a flow plot, follow these steps:

1. Choose **Plot Parameters** from the **Postprocessing** menu.
2. On the **General** page, clear the **Slice** check box to deactivate the slice plot.
3. Select the **Boundary** and **Streamline** check boxes to activate these features.
4. Click the **Streamline** tab.
5. Type 30 in the **Number of start points** edit field on the **Start Points** tab.
6. Click **OK**.

The surface plot obstructs the view, making it impossible to see inside the box. To remove the rendering of the front faces, use the ability of COMSOL Multiphysics to suppress boundaries.

1. In the **Options** menu, point to **Suppress** and then click **Suppress Boundaries**.
2. While holding down the Ctrl key, select Boundaries 1, 2, and 4 in the **Boundary selection** list.
3. Click **OK** to close the dialog box and render all boundaries except 1, 2, and 4.
4. To add lighting to the model, click the **Scene Light** and **Headlight** buttons on the Camera toolbar.
5. Click the **Postprocessing Mod**e button on the Main toolbar.


File Edit Options Draw Physics Mesh Solve Postprocessing Multiphysics Help
Geom1
Geom2
Boundary: Electric potential [V] Streamline: Electric field
Max: 1.00
Min: -1.00
Mesh consists of 5201 elements.
Number of degrees of freedom solved for: 7988
Solution time: 0.624 s

Pacemaker Electrode

This model illustrates the use of COMSOL Multiphysics for modeling of ionic current distribution problems in electrolytes, in this case in human tissue. The problem is exemplified on a pacemaker electrode, but it can be applied in electrochemical cells like fuel cells, batteries, corrosion protection, or any other process where ionic conduction takes place in the absence of concentration gradients.

Introduction

The modeled device is a pacemaker electrode that is placed inside the heart and helps the patient's heart to keep a normal rhythm. The device is referred to as an electrode, but it actually consists of two electrodes: a cathode and an anode.

Figure 4-2 shows a schematic drawing of two pair of electrodes placed inside the heart. The electrodes are supplied with current from the pulse generator unit, which is also implanted in the patient.

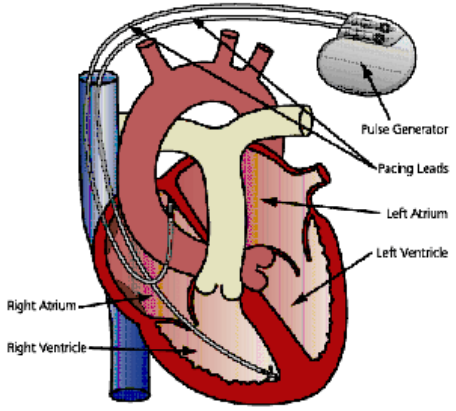


Figure 4-2: Schematic drawing of the heart with two pairs of pacemaker electrodes.

This model deals with the current and potential distribution around one pair of electrodes.

Model Definition

The model domain consists of the blood and tissue surrounding the electrode pair. The actual electrodes and the electrode support are boundaries to the modeled domain. Figure 4-3 shows the electrode in a darker shade, while the surrounding modeling domain is shown in a lighter shade.

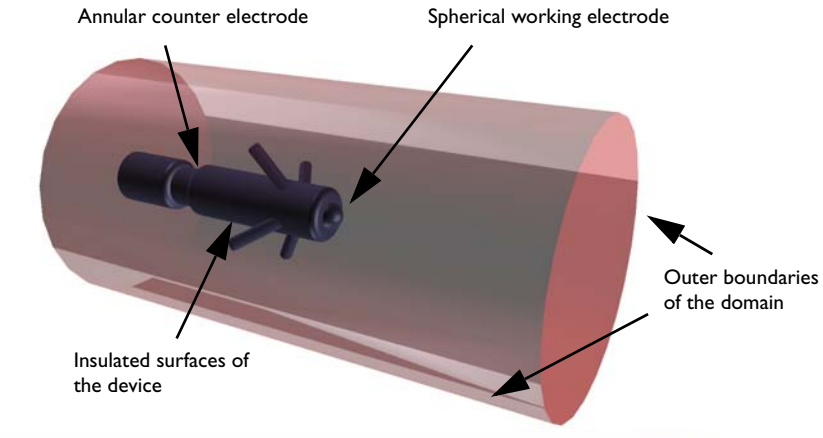


Figure 4-3: Modeling domain and boundaries.

The working electrode consists of a a hemisphere placed on the tip of the supporting cylindrical structure. The counter electrode is placed in the "waist" of this structure. All other surfaces of the supporting structure are insulated. The outer boundaries are placed far enough from the electrode to give a small impact on the current and potential distribution.

In COMSOL Multiphysics, use the 3D Conductive Media DC application mode for the analysis of the electrode. This application mode is useful for modeling conductive materials where a current flows due to an applied electric field.

DOMAIN EQUATIONS

The current in the domain is controlled by the continuity equation, which follows from the Maxwell's equations:

$$-\nabla \cdot (\sigma \nabla V) = 0$$

where σ is the conductivity of the human heart. This equation uses the following relations between the electric potential and the fields.

$$\mathbf{E} = -\nabla V$$
$$\mathbf{J} = \sigma\mathbf{E}$$

BOUNDARY CONDITIONS

Ground potential boundary conditions are applied on the thinner waist of the electrode. The tip of the electrode has a fixed potential of 1 V. All other boundaries are electrically insulated.

$$\mathbf{n} \cdot \mathbf{J} = 0$$

Results and Discussion

This simulation gives you the potential distribution on the surface of the electrode and the streamlines of the current distribution inside the human heart. This plot appears in Figure 4-4.

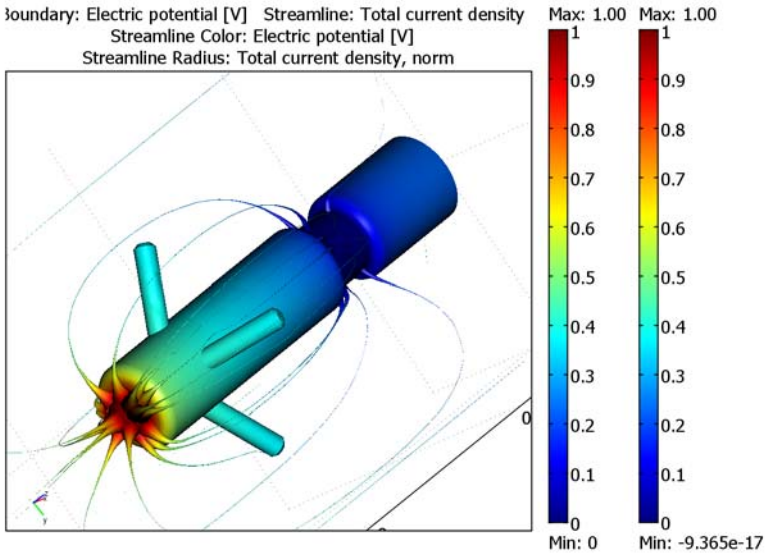


Figure 4-4: The plot shows the electrostatic potential distributed on the surface of the electrode. The total current density is shown as streamlines.

As expected, the current density is highest at the small hemisphere, which is the one that causes the excitation of the heart. The current density is fairly uniform on the

working electrode. The counter electrode is larger and there are also larger variations in current density on its surface. Mainly, the current is lower with the distance from the working electrode. The model shows that the anchoring arms of the device have little influence on the current density distribution.

Model Library path: `COMSOL_Multiphysics/Electromagnetics/pacemaker_electrode`

Modeling Using the Graphical User Interface

1 In the **Model Navigator**, select **3D** from the **Space dimension** list.

2 In the **COMSOL Multiphysics>Electromagnetics** folder, select **Conductive Media DC**. Make sure **Lagrange - Quadratic** is selected in the **Element** list.

3 Click **OK**.

GEOMETRY MODELING

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

2 Click the **y-z** button and then click **OK**.

3 From the **Draw** menu, select **Specify Objects>Rectangle**. In the **Rectangle** dialog box, enter `2.1e-3` in the **Width** edit field, `5.5e-3` in the **Height** edit field, and enter the corner coordinates (0, 14.5e-3) in the edit fields **x** and **y**. Make sure that **Corner** is selected in the **Base** list. Click **OK**.

4 Select **Fillet/Chamfer** from the **Draw** menu. Expand R1 and select point number 2. Enter `5e-4` in the **Radius** edit field. Click **OK**.

5 Create a rectangle with width `1.6e-3`, height `2e-3`, and corner position at (0, 12.5e-3).

6 Create a rectangle with width `2.1e-3`, height `12.5e-3`, and corner position at (0, 0).

7 Select **Fillet/Chamfer** from the **Draw** menu. Expand R2 and select point number 2 and 3. Enter `5e-4` in the **Radius** edit field. Click **OK**.

8 From the **Draw** menu, select **Specify Objects>Circle**. Enter `1e-3` in the **Radius** edit field. Click **OK**.

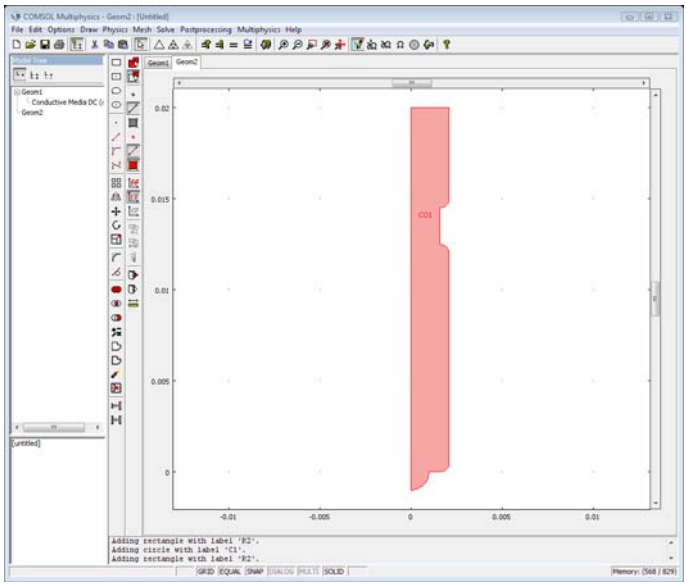
9 Create a rectangle with width `2e-3`, height `2e-3`, and corner position at (–2e-3, –1e-3).

10 Select **Create Composite Object** from the **Draw** menu. In the dialog box, type the formula `C1-R2` in the **Set formula** edit field. Click **OK**.

11 Select all objects by pressing Ctrl+A. Click on the **Union** toolbar button located to the left side.

12 Click the **Delete Interior Boundaries** toolbar button on the same toolbar.

13 Click the **Zoom Extents** button on the Main toolbar. You should have a window similar to the figure below.



14 Select **Revolve** from the **Draw** menu. Click **OK**.

15 Click the **Zoom Extents** button to see the revolved geometry.

These steps created the electrode, but the electrode also has some hooks that hold it in place.

1 Go back to the work plane by clicking on the **Geom2** tab.

2 Create a rectangle with width `5e-4`, height `5.2e-3`, and corner position at (`0`, `3.5e-3`).

3 Select **Fillet/Chamfer** from the **Draw** menu. Expand R1 and select point number 3. Click the **Chamfer** radio button, and enter `2e-4` in the **Distance** edit field. Click **OK**.

4 Select **Revolve** from the **Draw** menu. Click **OK**.

5 Click the **Rotate** toolbar button and enter `60` in the edit field for the rotation angle. Define the point and axis for the rotation by specifying the coordinate (`0`, `0`, `2.5e-3`) in the **Point on rotation axis** frame, and the direction (`1`, `0`, `0`) in the **Rotation axis direction vector** frame. Click **OK**.

6 Press Ctrl+C to copy the object. Press Ctrl+V to paste it directly. In the **Paste** dialog box, leave all displacement fields set to zero. Click **OK**.

7 Click the **Rotate** toolbar button and set the rotation angle to `90`. Click **OK**.

8 Press Ctrl+V again and click **OK** (zero displacements).

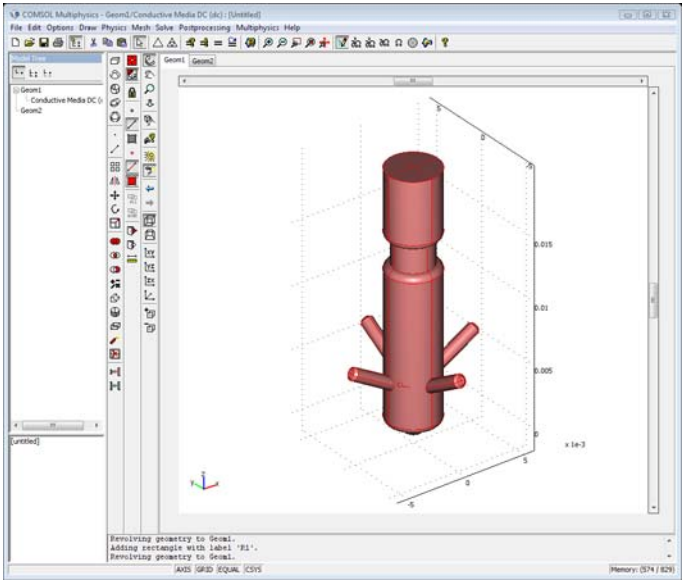
9 Click the **Rotate** toolbar button and set the rotation angle to 180. Click **OK**.

10 Press Ctrl+V and click **OK** (zero displacements).

11 Click on the **Rotate** toolbar button and set the rotation angle to 270. Click **OK**.

12 Press Ctrl+A to select all objects. Click on the **Union** toolbar button and then click on the **Delete Interior Boundaries** toolbar button.

13 Click the **Zoom Extents** and the **Headlight** toolbar buttons to see geometry in the following figure.



Finally, you need to define the volume surrounding the electrode. The simulation only takes place in this volume, where the boundaries of the electrode influence the result.

1 Click the **Cylinder** toolbar button. In the **Cylinder** dialog box, enter `10e-3` in the **Radius** edit field, `40e-3` in the **Height** edit field, and the coordinate (`0`, `0`, `-20e-3`) in the edit fields of the **Axis base point** frame. Click **OK**.

2 Choose **Create Composite Object** from the **Draw** menu. In the dialog box, type the formula `CYL1-C02` in the **Set formula** edit field. Click **OK**.

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

PHYSICS SETTINGS

Boundary Conditions

The thin waist of the electrode is grounded, and a positive potential is applied to the lower half sphere. All other boundaries are kept electrically insulated.

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

2 Define the boundary condition according to the following table. Click **OK**.

SETTINGS	BOUNDARIES 29, 30, 58, AND 63	BOUNDARIES 31, 32, 59, AND 60	ALL OTHER BOUNDARIES
Boundary condition	Ground	Electric potential	Electric insulation
V_0		1	

Subdomain Settings

The electrode is inserted into the human heart, so you must define the conductivity for the heart tissue.

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Select Subdomain 1, then click in the σ edit field. In the pop-up window that opens, type `5000` in the active upper-left edit field to set the isotropic electric conductivity.

3 Click **OK**.

MESH GENERATION

Use the default mesh settings. Click the **Initialize Mesh** button on the Main toolbar to generate the mesh.

COMPUTING THE SOLUTION

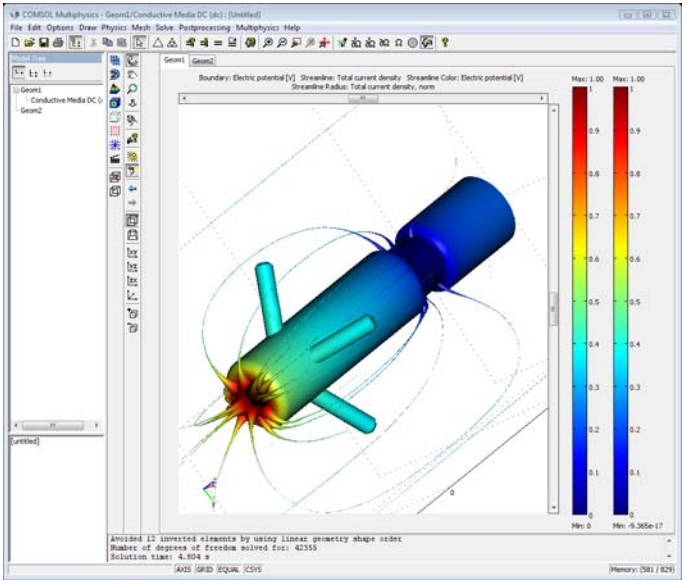
Use the default solver parameters—the stationary solver using the conjugate gradients iterative solver—and algebraic multigrid as the preconditioner.

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

POSTPROCESSING AND VISUALIZATION

The potential distribution on the electrode boundary is used together with a streamline plot of the total current density to visualize the result of the simulation.

1. Start by suppressing some boundaries not to be used for visualization. On the **Options** menu, point to **Suppress**, and then choose **Suppress Boundaries**.
2. In the **Suppress Boundaries** dialog box, select Boundaries 1, 2, 3, 4, 45, and 74. Click **OK**.
3. Choose **Plot Parameters** from the **Postprocessing** menu. In the **Plot Parameters** dialog box under the **General** tab, clear the **Slice** check box and select the **Boundary** and **Streamline** check boxes.
4. Click the **Boundary** tab and make sure that **Electric potential** is selected as boundary data.
5. Click the **Streamline** tab and then select **Total current density** from the **Predefined quantities** list. Click the **Line Color** tab, and then click the **Use expression** radio button. Use the default expression—the electric potential.
6. Select **Tube** from the **Line type** list. Click the **Tube Radius** button. In the **Tube Radius Parameters** dialog box, select the **Radius data** check box, and choose **Total current density, norm** from the **Predefined quantities** list. Click **OK** twice. You should now see something similar to the figure below after proper rotation and zoom operations.



Skin Effect in a Circular Wire

Introduction

This model demonstrates the *skin effect*, that is, the phenomenon that electrons tend to move along the surface when an AC current flows through a conductor. Changes in the current's amplitude and direction induce a magnetic field that pushes the electrons toward the wire's exterior. The effect increases with frequency and conductor size.

Engineers working at microwave frequencies take advantage of these effects by designing hollow waveguides because at these frequencies, the core of a conductor does not carry current anyway.

In solid conductors, the skin effect can have important implications even at powerline frequencies. For instance, utilities can replace expensive, heavy copper wire with aluminum cables clad with a copper skin without appreciably increasing power losses. As proof of this claim, this model first computes the current distribution at 50 Hertz in an unusually large copper cable (20 cm diameter). It then goes on to compute the current distribution and compare resistive losses in a like-sized copper-clad cable that consists of 90% aluminum.

Model Definition

Copper specifies a conductivity σ of $5.99 \cdot 10^7$ S/m and permeability μ of $4\pi \cdot 10^{-7}$ H/m. For aluminum the values are $3.77 \cdot 10^7$ S/m and $4\pi \cdot 10^{-7}$ H/m, respectively. The materials' dielectric properties have no influence on the fields at low frequencies as in this case. You can therefore set $\varepsilon = \varepsilon_0 = 8.854 \cdot 10^{-12}$ F/m.

Using the AC Power Electromagnetics application mode, the equation that COMSOL Multiphysics solves is a complex-valued Helmholtz equation for the amplitude of the magnetic potential:

$$-\nabla \cdot \left(\frac{1}{\mu}\nabla A_z\right) + k^2 A_z = 0$$

$$k = \sqrt{j\omega\sigma - \omega^2\varepsilon}$$

Here ω is the angular frequency, in this case $2\pi \cdot 50$ rad/s. For good conductors, such as copper and aluminum, $\sigma >> \omega\varepsilon$. So, for engineering purposes the approximation $k = \sqrt{j\omega\sigma}$ is close enough.

The boundary conditions require some careful consideration. From a mathematical point of view, it is necessary to specify either the magnetic potential A_z (corresponding to a Dirichlet type condition) or the normal derivative of the same field (a Neumann condition) on the outer surface. These quantities, however, have little or no significance in applied engineering. In COMSOL Multiphysics the Neumann type condition on the A_z field is implemented by specifying a surface current equal to the negative of the tangential magnetic field at the boundary. The current might not be physically real. On exterior boundaries you can interpret it as the surface current necessary to make the magnetic field **H** vanish outside the domain.

Even better from the pure engineering point of view is to specify the total current throughput, which is rather straightforward in this case. Making the magnetic field disappear everywhere outside the circular domain requires that the total current through the domain equals zero. One way of achieving this is by adding a "virtual" surface current of opposite sign to the "real" current inside the conductor. Because the problem is rotationally symmetric, you can write the necessary virtual surface current density

$$J_s = -\frac{I_{\text{tot}}}{2\pi R}$$

where I_{tot} is the total real current throughput, and R is the radius of the wire.

Results

Figure 4-5 shows the real part of the total current density through a cross section of the wire. Because of the time lag between the surface and the interior, the solution of the AC power electromagnetics equation is complex valued. You can plot various properties of the complex solution by typing expressions such as `imag(Jz_qa)` or `abs(Jz_qa)` in an **Expression** edit field in the **Plot Parameters** dialog box.

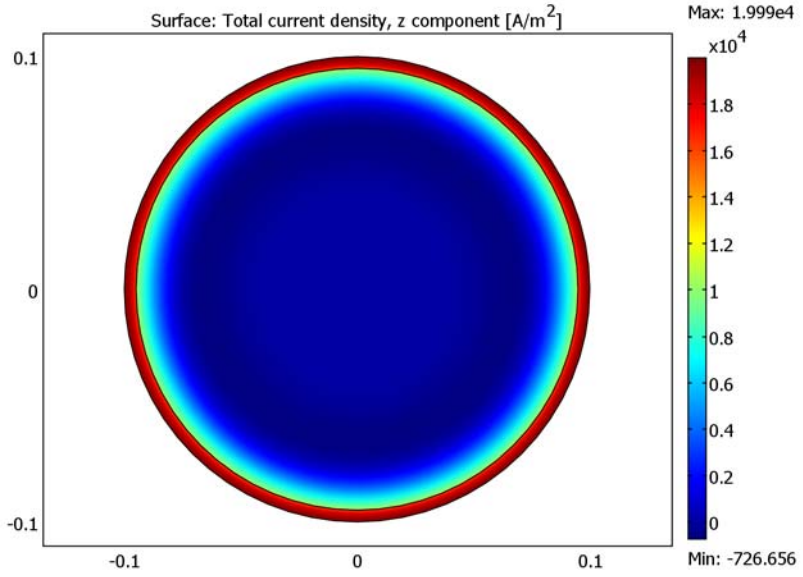


Figure 4-5: Total current density through a wire carrying an AC current.

Model Library path: `COMSOL_Multiphysics/Electromagnetics/skin_effect`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **2D** from the **Space dimension** list.

2 In the list of application modes, open the **COMSOL Multiphysics** folder and then the **Electromagnetics** folder. Select **AC Power Electromagnetics** from the list of electromagnetics application modes.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 Set axis and grid settings according to the following table. On the **Grid** page, clear the **Auto** check box to enter the grid spacings manually.

AXIS		GRID	
x min	-0.15	x spacing	0.1
x max	0.15	Extra x	
y min	-0.1	y spacing	0.1
y max	0.1	Extra y	

3 Click **OK**.

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

5 Enter the following constants (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
sigma_Cu	5.99e7[S/m]	Electrical conductivity, copper
sigma_Al	3.77e7[S/m]	Electrical conductivity, aluminum
I_tot	100[A]	Total current

6 Click **OK**.

GEOMETRY MODELING

The cross section of the conductor is represented by a circle with radius 0.1. The aluminum core is drawn as a circle with radius 0.0949.

1 Draw a circle centered at (0, 0) with a radius of 0.1.

2 Draw one more circle centered at (0, 0) with a radius of 0.1.

3 Double-click the last circle and enter a new radius of 0.0949.

PHYSICS SETTINGS

Boundary Conditions

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

2 Enter boundary coefficients according to the following table. When done, click **OK**.

BOUNDARY	ALL
Type	Surface current
J_{sz}	-I_tot/(2*pi*0.1[m])

Subdomain Settings

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

2 Click the **Electric Parameters** tab.

3 Enter the subdomain settings (material property) according to the following table. When done, click **OK**.

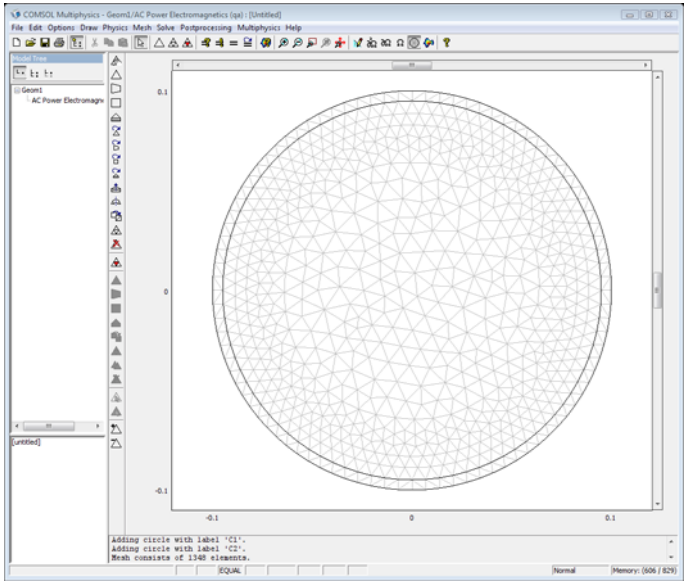
SETTING	SUBDOMAINS 1, 2
σ	`sigma_Cu`

MESH GENERATION

The small gap between the concentric circles gives you a fine mesh close to the boundaries, where the solution is expected to vary fastest. If you decrease the element growth rate, the mesh becomes smoother.

1 In the **Free Mesh Parameters** dialog box, click the **Custom mesh size** button and type `1.1` in the **Element growth rate** edit field. Click **OK**.

2 Initialize the mesh.



COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

Due to the skin effect, the current density at the surface is much higher than that within the interior of the conductor. Plotting the current density J_z clearly shows this effect.

1. Open the **Plot Parameters** dialog box.
2. Click the **Surface** tab.
3. On the **Surface Data** tab, select **Total current density, z component** from the **Predefined quantities** list.
4. Click **OK**.

The resistance per meter is defined as $R = P/I^2$, where P is the power loss per meter of wire, and I is the current through the power line. You can compute both the power and the current with integrations over the cross section:

$$P = \int Q dA$$

$$I = \int J_z dA$$

where $Q = \sigma|\mathbf{E}|^2$. The value of the second integral is known a priori, because the total current is part of the boundary conditions.

1. From the **Postprocessing** menu, open the **Subdomain Integration** dialog box. Select both subdomains and choose the **Total current density, z component** from the **Predefined quantities** list. Click **Apply** and note that the total current is very close to 100 A, as expected.
2. Change the integration expression to **Resistive heating, time average** and click **OK**.
3. You can now compute the resistance per meter from $R = P/I^2$.

Modeling a Wire with an Aluminum Core

Next, replace almost all copper with aluminum, leaving only a thin copper shell, and compare the results.

SUBDOMAIN SETTINGS

Change the conductivity in Subdomain 2 to `sigma_Al`.

COMPUTING THE SOLUTION

Solve the problem.

POSTPROCESSING

Now calculate the resistance per meter in the modified design.

1. From the **Postprocessing** menu, open the **Subdomain Integration** dialog box.
2. Select both subdomains and select **Resistive heating, time average** from the **Predefined quantities** list.
3. Click **OK**.
4. Calculate the resistance per meter as before.

For a given current the combined copper/aluminum wire suffers approximately 10% more resistance compared to pure copper. On the other hand it weighs only one third and is considerably less expensive.

Quadrupole Lens

Introduction

Just like optical lenses focus light, electric and magnetic lenses can focus beams of charged particles. Systems of magnetic quadrupole lenses find a common use in focusing both ion and particle beams in accelerators at nuclear and particle physics centers such as CERN, SLAC, and ISIS. This COMSOL Multiphysics model shows the path of B^{5+} ions going through three consecutive magnetic quadrupole lenses. The model is set up in a cross section of the geometry. You can find a full 3D version in the AC/DC Module Model Library.

Model Definition

The quadrupole consists of an assembly of four permanent magnets, as seen in Figure 4-6 below, where the magnets work together to give a good approximation of a quadrupole field. To strengthen the field and keep it contained within the system, the magnets are set in an iron cylinder.

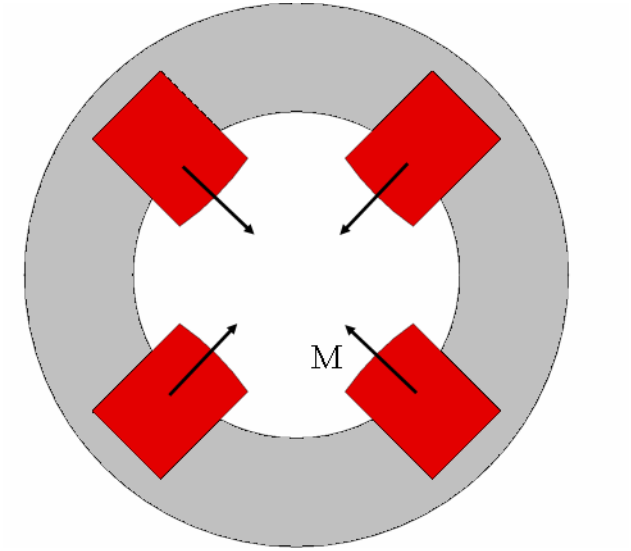


Figure 4-6: Cross-sectional view of one of the magnetic quadrupoles used in the lens.

The ions are sent through a system of three consecutive quadrupole assemblies. The middle one is twice as long as the other ones, and is rotated by 90 degrees around the central axis. This means the polarity of its magnets is reversed. Figure 4-7 gives a full view of the magnetic quadrupole lens.

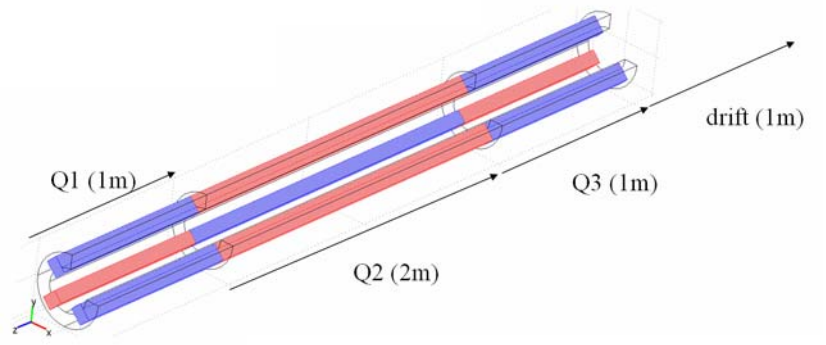


Figure 4-7: Cutout of the quadrupole lens. The second quadrupole (Q2) has its polarities reversed compared to Q1 and Q2. After traveling through the lens, the ions are left to drift 1 m.

An accelerator feeds the system with ions traveling with the velocity $0.01c$ along the the central axis. To study the focusing effect of the quadrupoles, track a number of ions starting out from a distance of 3 cm from the central axis, evenly distributed along the circumference of a circle in the transverse plane. They are all assumed to have a zero initial transverse velocity. Each quadrupole focuses the ion beam along one of the transverse axes and defocuses it along the other one. The net effect after traveling through the system of the three quadrupoles and the drift length is focusing in all directions. As the ions exit the system, they are all contained within a 1 cm radius in the transverse plane.

The model is set up in a 2D cross section of any of the two identical quadrupoles Q1 and Q3. Neglecting fringe fields, the transverse magnetic field at a given point in a transverse plane in Q2 will automatically have the same magnitude as the corresponding in Q1 and Q3, but point in the opposite direction. It is therefore sufficient to model the fields in one of the quadrupoles.

DOMAIN EQUATIONS

The magnetic field is described using the Magnetostatics equation, solving for the z component of the magnetic potential $\mathbf{A}$ (Wb/m):

$$\nabla \times (\mu_0^{-1}(\nabla \times A_z - \mathbf{M})) - \sigma \mathbf{v} \times (\nabla \times A_z) = \sigma \Delta V/L + J_z^{\mathrm{e}}$$

Here $\mu_0 = 4\pi \cdot 10^{-7}$ H/m denotes the permeability of vacuum, $\mathbf{M}$ is the magnetization (A/m), σ the conductivity (S/m), and $\mathbf{v}$ the velocity of the medium (m/s). In this model, the medium is not moving. The right-hand side of the equation holds an imposed current, specified in terms of either ΔV (V) and L (m), or an external current density J_z^{e} (A/m^2). No currents are imposed in this model. The iron subdomain uses a slightly different formulation of the same equation:

$$\left(\nabla \times \frac{1}{\mu_0 \mu_{\mathrm{r}}} \nabla \times A_z\right) - \sigma \mathbf{v} \times (\nabla \times A_z) = \sigma \Delta V/L + J_z^{\mathrm{e}},$$

where $\mu_{\mathrm{r}} = 4000$ is the relative permeability. The magnetic potential is everywhere defined so that $\mathbf{B} = \nabla \times \mathbf{A}$.

BOUNDARY CONDITIONS

The magnetic field is approximately parallel to the exterior boundary of the iron cylinder. To enforce this, use the *magnetic insulation* boundary condition, stating that $A_z = 0$.

The magnetic field density and flowlines in a cross section of Q1 or Q3 appear in Figure 4-8 below.

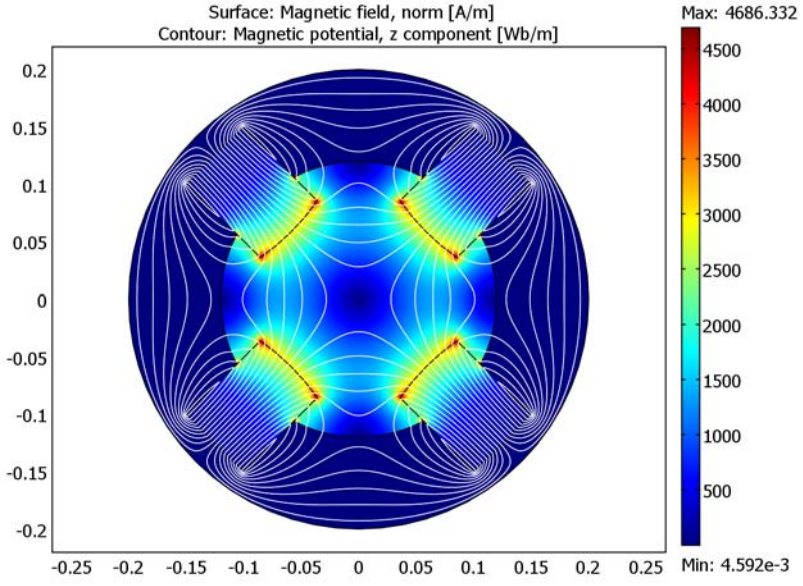


Figure 4-8: The magnetic field density and flowlines in the center of one of the quadrupole magnets.

Each ion passing through the assembly experiences a Maxwell force equal to $\mathbf{F} = q\,\mathbf{v}\times\mathbf{B}$, where $\mathbf{v}$ (m/s) is the ion's velocity. Next, assume that the z component of the velocity is constant and much larger than the x and y (transverse) components. Thus consider only the force contributions from the z component of the velocity. To find the transverse position as a function of time, you need to solve Newton's second law for each ion, $q\,\mathbf{v}\times\mathbf{B} = m\,\mathbf{a}$, where m is the ion mass (kg), and $\mathbf{a}$ denotes its acceleration (m/s^2). If the computed magnetic flux density in Q1 equals $\mathbf{B}'$, and the length of quadrupole i is L_i (m), the flux density that the ion experiences is given by

$$\mathbf{B} = \begin{cases} \mathbf{B}' \text{ if } t < \dfrac{L_1}{v_z} \\ -\mathbf{B}' \text{ if } \dfrac{L_1}{v_z} < t < \dfrac{L_1 + L_2}{v_z} \\ \mathbf{B}' \text{ if } \dfrac{L_1 + L_2}{v_z} < t < \dfrac{L_1 + L_2 + L_3}{v_z} \\ 0 \text{ if } t > \dfrac{L_1 + L_2 + L_3}{v_z} \end{cases}$$

where t (s) is the time of flight. This dependency of the magnetic flux density on the time of flight is fed to the particle-tracing algorithm as a logical expression. Figure 4-9 below shows how the ions travel in the transverse plane.

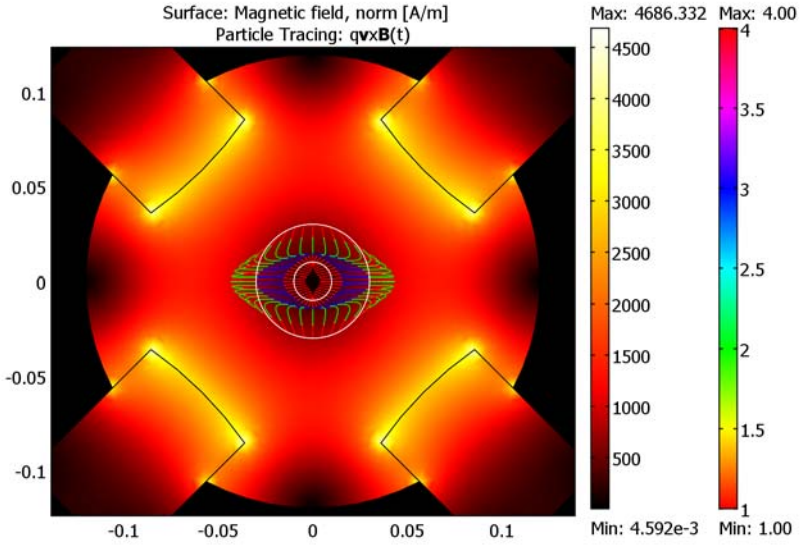


Figure 4-9: As the ions enter Q1, they start out evenly distributed around the larger circle, 3 cm from the z-axis. Q1 focuses along the x-axis and defocuses along the y-axis. The force on each ion is approximately proportional to its distance from the z-axis, so as the ions enter Q2, those that are far out on the x-axis rapidly turn around and move toward the center. Q3 stabilizes the motion and gets all ions on the right track. Finally the ions are left to drift toward a waist situated a little bit more than 1 m beyond Q3.

Model Library path: `COMSOL_Multiphysics/Electromagnetics/quadrupole`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, select **COMSOL Multiphysics>Electromagnetics>Magnetostatics** from the list of application modes.

2 Click **OK** to close the dialog box.

OPTIONS AND SETTINGS

1 Enter the following constant names and expressions in the **Constants** dialog box (units and descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
M	11	Ion mass number
Z	5	Ion charge number
L1	1[m]	Length of first quadrupole
L2	2[m]	Length of second quadrupole
L3	1[m]	Length of third quadrupole
vz	0.01*3e8[m/s]	Ion velocity
mp	1.672e-27[kg]	Proton mass
Ze	1.602e-19[C]	Proton charge
m	M*mp	Ion mass
q	Z*Ze	Ion charge
MQ	5.8e3[A/m]	Quadrupole magnetization

2 Click **OK** to close the dialog box.

GEOMETRY MODELING

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

2 Specify a rectangle with the following properties; when done, click **OK**.

PROPERTY	EXPRESSION
Width	0.177
Height	0.07

PROPERTY	EXPRESSION
Position: Base	Corner
Position: x	0
Position: y	-0.035

3 Click the **Rotate** button on the Draw toolbar. Rotate the rectangle by 45 degrees around the origin.

4 Click the **Ellipse/Circle (Centered)** button on the Draw toolbar.

5 Specify a circle with the following properties; when done, click **OK**.

PROPERTY	EXPRESSION
Radius	0.2
Position: Base	Center
Position: x	0.2
Position: y	0.2

6 Select both the circle and the rectangle, then click the **Intersection** button on the Draw toolbar.

7 Make a copy of your composed object (CO1) and paste it at the same location, that is with zero displacements.

8 Rotate the copied object (CO2) by 90 degrees around the origin.

9 Paste two more copies of CO1 at the same location, and rotate them by 180 and 270 degrees respectively.

10 Create a circle centered at the origin with a radius of 0.2 m.

11 Create another circle centered at the origin, with a radius of 0.12 m.

12 Click the **Create Composite Object** button and create an object using the formula C1+C2-(CO1+CO2+CO3+CO4).

13 Draw a circle centered at the origin with a radius of 0.2 m.

The geometry should now look like that in the figure below.

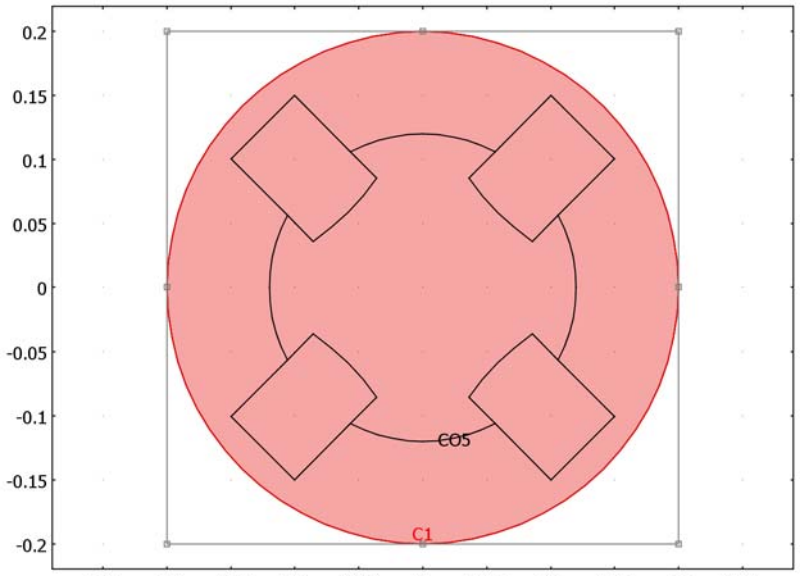


Figure 4-10: The COMSOL Multiphysics geometry of the quadrupole lens.

PHYSICS SETTINGS

Boundary Conditions

Use the default condition **Magnetic insulation** at all exterior boundaries.

Subdomain Settings

1. From the **Physics** menu, select **Subdomain Settings**. Select Subdomain 1.
2. Click the **Load** button. In the **Materials/Coefficients Library** dialog box that appears, select **Basic Material Properties>Iron** in the **Materials** area.
3. Leave the default settings in Subdomain 4.
4. In all the other subdomains, set the constitutive relation to $\mathbf{B} = \mu_0\mathbf{H} + \mu_0\mathbf{M}$ and specify the magnetization components according to the table below.

PROPERTY	SUBDOMAIN 2	SUBDOMAIN 3	SUBDOMAIN 5	SUBDOMAIN 6
M (x component)	`MQ/sqrt(2)`	`-MQ/sqrt(2)`	`MQ/sqrt(2)`	`-MQ/sqrt(2)`
M (y component)	`MQ/sqrt(2)`	`MQ/sqrt(2)`	`-MQ/sqrt(2)`	`-MQ/sqrt(2)`

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** to close the dialog box.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the norm of the magnetic flux density. Follow the instructions to view the magnetic field.

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

2 On the **Surface** page, select **Magnetic field, norm** from the **Predefined quantities** list.

3 On the **Contour** page, select the **Contour plot** check box. From the **Predefined quantities** list, select **Magnetic potential, z component**.

4 In the **Contour color** area, click first the **Uniform color** option button and then the **Color** button. Select a white color, then click **OK**. Clear the **Color legend** check box.

5 Click **Apply** to see the magnetic field. The magnetic field lines follow the same pattern as the magnetic potential contour lines (see Figure 4-8 on page 86).

To see how the ions travel through the system of quadrupoles, do the following:

6 On the **Surface** page, change the **Color table** to **Thermal**.

7 On the **Particle Tracing** page, select the **Particle tracing plot** check box and apply the following settings:

PROPERTY	EXPRESSION
Mass	`m`
Fx	`-q*vz*By_qa*(1-2*(partt>L1/vz)+2*(partt>(L1+L2)/vz) -(partt>(L1+L2+L3)/vz))`
Fy	`q*vz*Bx_qa*(1-2*(partt>L1/vz)+2*(partt>(L1+L2)/vz) -(partt>(L1+L2+L3)/vz))`
Start Points, x	`0.03*cos(range(0,0.05*pi,2*pi))`
Start Points, y	`0.03*sin(range(0,0.05*pi,2*pi))`

8 On the **Line Color** page, click the **Use expression** option button.

9 Click the **Color Expression** button. Set the **Color table** to **Cyclic** and the expression to `1+(partt>L1/vz)+(partt>(L1+L2)/vz)+(partt>(L1+L2+L3)/vz)`. Click **OK**.

10 Click the **Advanced** button. Set the **Relative tolerance** to `1e-6`, the **End time for static flow fields** to `5/3e6`, and the **Maximum number of steps** to `1e5`. Click **OK**.

11 On the **Contour** page, set the **Expression** to `sqrt(x^2+y^2)`. For **Contour levels**, select **Vector with isolevels** and enter `0.01 0.03`.

12 Click the **General** tab. To create a suitable plot title, click the **Title** button, and then click the option button for a user-defined title. In the edit field for the title, type:

```
Surface: Magnetic field, norm [A/m]  Particle Tracing: q<b>v</
b>x<b>B</b>(t)
```

13 Click **OK**.

14 Click **OK** in the **Plot Parameters** dialog box to close it and generate the plot.

15 Click the **Zoom In** button on the Main toolbar to zoom in on the center of the model geometry as in Figure 4-9 on page 87.

Spherical Capacitor

Introduction

This example is a study of a capacitor consisting of two spherical copper conductors separated by glass.

You can compute the capacitance of a capacitor in two ways. By definition, the capacitance is given by the expression

$$C = \frac{Q}{V_{12}}$$

where V_{12} is the voltage difference between the two conductors and Q is the charge of the two conductors, positive and negative, respectively, when connected in a DC circuit.

The energy required to charge a capacitor is given by the expression

$$W_e = \frac{Q^2}{2C}$$

The energy defined above should equal the energy of the electrostatic field:

$$W_e = \int_{\Omega} \mathbf{D} \cdot \mathbf{E}\, dV$$

Because this integral is readily available in the Electrostatics application mode, the capacitance is obtained from the expression

$$C = \frac{Q^2}{2W_e}$$

With the second method, an analytical expression for the capacitance is calculated and used for a comparison with the numerical solution. Thus, assume charges $+Q$ and $-Q$ on the inner and outer spherical conductor, respectively. Denote the radii of the two spheres by R_i and R_o, respectively. Applying Gauss's law to a spherical surface with radius R ($R_\mathrm{i} < R < R_\mathrm{o}$) gives

$$\mathbf{E} = \frac{Q}{4\pi\varepsilon R^2}\mathbf{e}_r$$

The potential difference between the spheres is then

$$V = -\int_{R_o}^{R_i} \mathbf{E} \cdot \mathbf{e}_r \, dR = \frac{Q}{4\pi\varepsilon}\left(\frac{1}{R_\mathrm{i}} - \frac{1}{R_\mathrm{o}}\right)$$

Hence, the analytical expression for the capacitance is

$$C = \frac{Q}{V} = 4\pi\varepsilon / \left(\frac{1}{R_\mathrm{i}} - \frac{1}{R_\mathrm{o}}\right)$$

Model Definition

In COMSOL Multiphysics, you solve the spherical capacitor problem using the axisymmetric 2D Electrostatics application mode. It is easy to compute the capacitance from the COMSOL Multiphysics user interface using the available integration tools.

DOMAIN EQUATIONS

The electric scalar potential V, must obey Poisson's equation,

$$-\nabla \cdot (\varepsilon_0 \varepsilon_\mathrm{r} \nabla V) = \rho$$

where ε_0 is the permittivity of free space, ε_r is the relative permittivity and ρ is the space charge density. The electric field and displacement are obtained from the gradient of V

$$\mathbf{E} = -\nabla V$$
$$\mathbf{D} = \varepsilon_0 \varepsilon_\mathrm{r} \mathbf{E}$$

BOUNDARY CONDITIONS

A ground potential boundary condition describes the condition at the outer electrode. At the inner electrode, the boundary condition gives the surface charge:

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s$$

A symmetry boundary condition describes the condition at the symmetry axis.

Model Library path: `COMSOL_Multiphysics/Electromagnetics/spherical_capacitor`

MODEL NAVIGATOR

1. Select **Axial symmetry (2D)** from the **Space dimension** list.
2. In the list of application modes, select **COMSOL Multiphysics>Electromagnetics>Electrostatics**.
3. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, choose **Axes/Grid Settings**.
2. Set axis and grid settings according to the following table. To enter the settings on the **Grid** page, first clear the **Auto** check box. When done, click **OK**.

AXIS		GRID	
r min	-0.2	r spacing	0.05
r max	0.3	Extra r	0.19
z min	-0.2	z spacing	0.05
z max	0.2	Extra z	

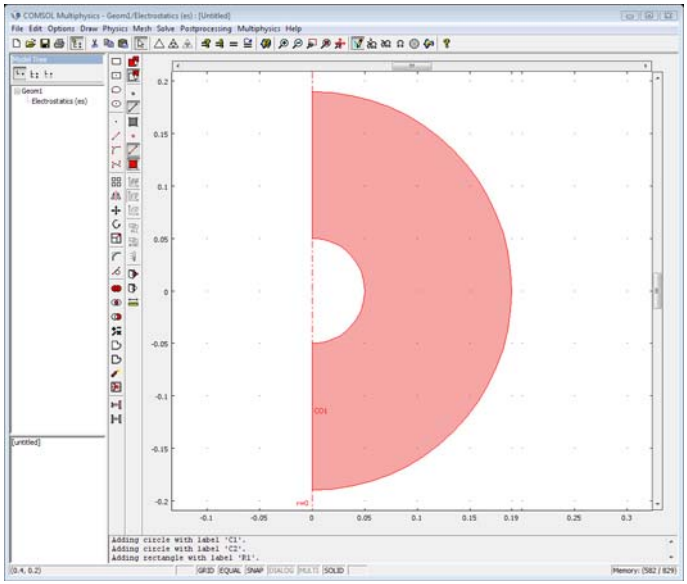
3. In the **Constants** dialog box, enter the following variable name and expression, and then click **OK**.

NAME	EXPRESSION
Q0	5e-12

GEOMETRY MODELING

1. Draw a circle C1 with radius 0.19 centered at (0, 0).
2. Draw a circle C2 with radius 0.05 centered at (0, 0).
3. Draw a rectangle with opposite corners at (–0.2, –0.2) and (0, 0.2).
4. Open the **Create Composite Object** dialog box from the Draw toolbar or the **Draw** menu.
5. Form a composite object by typing `C1-(C2+R1)` in the **Set formula** edit field.

6 Click **OK** to close the dialog box, then click the **Zoom Extents** button on the Main toolbar.



PHYSICS SETTINGS

Boundary Conditions

From the **Physics** menu, choose **Boundary Settings**. Enter boundary conditions according to the following table and then click **OK**.

SETTINGS	BOUNDARIES 1, 2	BOUNDARIES 4, 5	BOUNDARIES 3, 6
Type	Axial symmetry	Surface charge	Ground
ρ_s		`Q0/(4*pi*0.05^2)`	

Subdomain Settings

In this model, use the materials library for defining the material properties:

1 Open the **Subdomain Settings** dialog box, and select Subdomain 1.

2 Click the **Load** button to open the **Materials/Coefficients Library** dialog box.

3 Open the **Basic Material Properties** folder and select **Glass (quartz)** from the list of materials and click **OK**.

4 Now the defined material's relative permittivity is used in the subdomain settings. Click **OK**.

MESH GENERATION

1 Initialize the mesh by clicking the **Initialize Mesh** button on the Main toolbar.

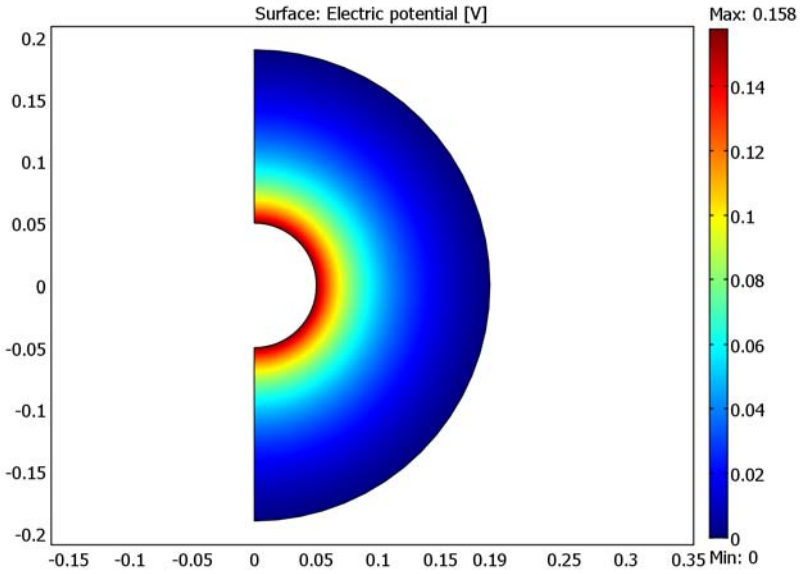
2 Click the **Refine Mesh** button on the Main toolbar to refine the mesh once.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

The resulting electrostatic potential is zero at the outer conductor and positive and constant at the inner conductor as shown in the default surface plot of *V*.



Capacitance Calculation

You can compute the capacitance of the capacitor using the available postprocessing functionality in COMSOL Multiphysics:

1 Choose **Boundary Integration** from the **Postprocessing** menu and integrate the expression `V/(0.05*pi)` for Boundaries 4 and 5. This gives an average value of 0.157676 for the potential on the inner conductor.

2 Choose **Subdomain Integration** from the **Postprocessing** menu, select the **Compute volume integral (for axisymmetric modes)** check box, and choose **Electrostatics (es)>Electric energy density** from the **Predefined quantities** list to compute volume

integral of the electric energy density, `We_es`. This gives a value of $3.94188 \cdot 10^{-13}$ joule for the total electric energy. It is now possible to compute the capacitance in two different ways:

```
C1 = Q/V
```

which gives the result

```
C1 = 3.17106e-011
```

and

```
C2 = Q^2/(2*We)
```

which gives the result

```
C2 = 3.17107e-11
```

Compare this to the analytical result

```
C0 = 4.2*4*pi*epsilon0_es/(1/0.05-1/0.19)
```

which gives the result

```
C0 = 3.171053e-11
```

Clearly, both numerical results are in good agreement with the analytical expression.

5

Equation-Based Models

This chapter contains models using the COMSOL Multiphysics PDE language to solve partial differential equations.

The Black-Scholes Equation

Introduction

There are different types of stock options:

- A *call option* is the right to buy a security at a specified price (called the exercise or strike price) during a specified period of time.
- A *put option* is the right to sell a security at a specified price during a specified period of time.

American options can be exercised at any time up to and including the day the option expires. European options can be exercised only on the day the option expires.

The famous Black-Scholes equation computes the cost u of a European stock option

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sigma^2 x^2 \frac{\partial^2 u}{\partial x^2} + rx\frac{\partial u}{\partial x} = ru$$

with the following parameters:

- x, the underlying asset price
- r, the continuous compounding rate of interest
- σ, the standard deviation of the asset's rate of return (also known as volatility)

A put option's value on the exercise day is

$$u(T, x) = \max(K - x, 0),$$

where K is the strike price. The problem domain is infinite and consists of the entire real axis across the time domain $0 \le t \le T$.

The assumptions made in deriving the Black-Scholes equation are:

- The underlying stock pays no dividends.
- The price of the stock, one period ahead, has a log-normal distribution with mean and standard deviation that are constant over the life of the option.
- The existence of a risk-free interest rate which is constant over the life of the option.
- You can lend and borrow at the risk-free interest rate.

Black and Scholes derived an analytical expression for the solution to the above problem. However, the formula works only for certain cases. For instance, you cannot use it when σ and r are functions of x and t. Using the PDE formulation, you can determine the price for such cases.

Model Definition

Because you must work within a finite domain $0 \le x \le X$, it becomes necessary to specify not only the boundary conditions for $t = T$ but also for $x = 0$ and $x = X$. It is therefore necessary to analyze the problem's characteristics to determine the location of the input and output boundaries.

EQUATION DEFINITION

To put the equation in coefficient form, rewrite the equation as

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}\sigma^2 x^2 \frac{\partial u}{\partial x}\right) + \left(rx - \frac{\partial}{\partial x}\left(\frac{1}{2}\sigma^2 x^2\right)\right)\frac{\partial u}{\partial x} - rc = 0.$$

In the following, denote

$$\bar{r} = rx - \frac{\partial}{\partial x}\left(\frac{1}{2}\sigma^2 x^2\right).$$

To reduce the problems with inflow boundaries, start by considering a put option: Study the value of a put option at a strike price $K = 40$ with $\sigma = 0.3$ and $r = 0.12$.

BOUNDARY CONDITIONS AND INITIAL CONDITIONS

Make the domain be $0 \le x \le 80$ with time running from 12 to 0. Then the initial condition at $t = 12$ and $x = 80$ is 0 based on the put option's value. The initial condition in the region $0 \le x \le 40$ varies linearly from 0 to 40. At the end of the simulation domain, the boundary is free (use a homogeneous boundary condition).

Modeling in COMSOL Multiphysics

Model the Black-Scholes equation using the following approach:

- Create a 1D time-dependent model, using the time-stepping algorithm to solve for c as a function of x and t, the time. The time steps go backward in time. Using a variable substitution to reverse the sign of the time, the d_a coefficient becomes –1.
- To model the initial condition, use the logical expression `(x<40)*(40-x)`. This means that in the areas where $x > 40$, the initial value is zero.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/black_scholes_put`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **1D** in the **Space dimension** list.

2 In the application mode list, open **COMSOL Multiphysics>PDE Modes** and then **PDE, Coefficient Form**.

3 Select **Time-dependent analysis**. Make sure **Lagrange - Quadratic** elements are selected.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

2 In the **x min** and **x max** edit fields, type `-1` and `81`, respectively.

3 Click **OK**.

4 From the **Options** menu, open the **Constants** dialog box.

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

NAME	EXPRESSION
r	0.12
sigma	0.3

GEOMETRY MODELING

Draw a line from 0 to 80:

1 On the **Draw** menu, point to **Specify Objects** and then click **Line**.

2 In the **x** edit field, type `0 80`.

3 Click **OK**.

PHYSICS MODELING

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Select Subdomain 1 and enter the PDE coefficients as follows:

COEFFICIENT	VALUE
c	`1/2*sigma^2*x^2`
a	`r`
f	`0`
d_a	`-1`
e_a	`0`
β	`(-r+sigma^2)*x`

3 Click the **Init** tab and type `(x<40)*(40-x)` in the **u(t_0)** edit field. Click **OK**.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Select the left boundary and click the **Neumann boundary condition** button.

Use the default zero Dirichlet condition on the right boundary.

3 Click **OK**.

MESH GENERATION

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

2 On the **Global** page, type 2 in the **Maximum element size** edit field.

3 Click **OK**.

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

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box.

2 Enter `range(12,-0.5,0)` in the **Times** edit field to step backward in time from 12 to 0 with 0.5 decrement.

3 Click **OK** to close the dialog box.

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

Optimizing a Flywheel Profile

Introduction

Note: This model requires the Optimization Lab.

The radial stress component in an axially symmetric and homogeneous flywheel of constant thickness exhibits a sharp peak near the inner radius. From there, it decreases monotonously until it reaches zero at the flywheel's outer rim; see Figure 5-1. The uneven stress distribution—apparent also for the azimuthal component—reveals a design that does not make optimal use of the material available.

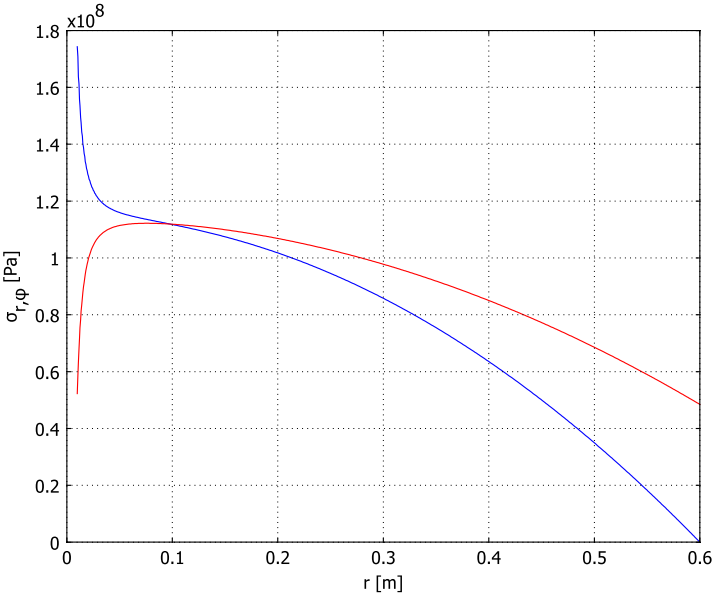


Figure 5-1: Radial (blue) and azimuthal (red) stress components in a homogeneous flywheel of constant thickness.

This model solves the problem of finding the thickness profile that results in a radial stress distribution that is as even as possible for given values of the flywheel's mass and moment of inertia. The model was inspired by Ref. 1.

Model Definition

Before describing the optimization problem, this section derives the dynamical equations, which you implement using a PDE, General Form application mode in 1D.

STRESSES IN A ROTATING FLYWHEEL

In a rotating flywheel, stresses due to the flywheel's weight are typically very small compared to dynamically induced stresses; therefore this model neglects gravitational stress. Expressed in terms of $U \equiv u/r$, where u is the local radial displacement (m) and r is the radial coordinate, the stress components along the radial and azimuthal directions in a rotationally symmetric disk made of a homogeneous, isotropic, and elastic material with Young's modulus E (N/m^2) and Poisson's ratio ν read:

$$\begin{aligned} \sigma_r &= \frac{E}{1-\nu^2}\left[r\frac{dU}{dr} + (1+\nu)U\right] \\ \sigma_\varphi &= \frac{E}{1-\nu^2}\left[\nu r\frac{dU}{dr} + (1+\nu)U\right] \end{aligned} \tag{5-1}$$

Inserting these expressions in the equation of motion for an infinitesimal mass element, results in the second-order ordinary differential equation (ODE)

$$-r^2\frac{d^2U}{dr^2} - (3+\Phi)r\frac{dU}{dr} + (1-(1+\nu)\Phi)U = \frac{1-v^2}{E}\rho\omega^2 r^2 \qquad r_0 < r < r_1 \tag{5-2}$$

valid for a centrally bored flywheel with inner radius r_0 (m) and outer radius r_1 (m) rotating with the angular velocity ω (rad/s). In this equation, the flywheel's thickness, H, which can be a function of r, enters through the dimensionless function

$$\Phi \equiv \frac{r}{H}\frac{dH}{dr} = r\frac{d}{dr}\log\left(\frac{H}{H_0}\right) \tag{5-3}$$

At the inner radius the displacement is zero and at the outer radius the radial stress component vanishes, which corresponds to the following boundary conditions:

$$U|_{r=r_0} = 0, \qquad r\frac{dU}{dr} + (1+v)U|_{r=r_1} = 0 \tag{5-4}$$

Given the function Φ, Equation 5-2 together with Equations 5-4 form a well-posed ODE problem. With the solution $U = U(r)$ at hand, you can then determine the stress components through the Equations 5-1.

THE OPTIMIZATION PROBLEM

For the special case of constant flywheel thickness, $H(r) = H_0$, the function Φ is identically zero. As Figure 5-1 shows and you verify later, this shape results in an uneven stress distribution, with a maximum for σ_r at $r = r_0$.

This model concerns optimizing the flywheel's profile to obtain a radial stress distribution that is as even as possible under the design requirements of specified flywheel mass and moment of inertia. To formulate the task in mathematical terms, tentatively introduce the objective function

$$Q_{\text{stress}}[H] = \int_{r_0}^{r_1} \frac{(\sigma_r - \sigma_{r,\,\text{mean}})^2}{\sigma_0^{\,2}} dr \tag{5-5}$$

where $\sigma_{r,\text{mean}}$ denotes the average radial stress value along the flywheel's radial extension, and σ_0 is a normalization constant. The latter is introduced to make the integrand dimensionless and its value is chosen to be roughly an order of magnitude smaller than σ_r to give Q_{stress} a suitable magnitude. The optimization problem is then to find the shape $H = H(r)$ that minimizes Q_{stress} under the additional constraints

$$m \equiv 2\pi\rho \int_{r_0}^{r_1} H r dr = m_0$$

and

$$I \equiv \pi\rho \int_{r_0}^{r_1} H r^3 dr = I_0$$

where m_0 and I_0 are the desired mass and moment of inertia, respectively.

However, Equation 5-5 alone does not give a reasonable result; suppressing profiles where dH/dr is not smooth requires a second term in the objective function:

$$Q_{\text{smoothness}}[H] = A \int_{r_0}^{r_1} \left(\frac{dH}{dr}\right)^2 dr \tag{5-6}$$

Here A is a normalization constant to be chosen such that $Q_{\text{smoothness}}$ and Q_{stress} are comparable in magnitude; as long as this condition is satisfied, the model is fairly insensitive to the value of A.

MODEL DATA

Table 5-1 gives the input data for the model. As the initial design, take a flywheel of constant thickness H_0. The material properties correspond to those of steel.

TABLE 5-1: MODEL DATA

PROPERTY	VALUE	DESCRIPTION
r_0	0.01 m	Inner flywheel radius
r_1	0.60 m	Outer flywheel radius
H_0	0.03 m	Initial flywheel thickness
E	$2.1 \cdot 10^{11}$ N/m^2	Young's modulus
ν	0.3	Poisson's parameter
ρ	7800 kg/m^3	Density
ω	$2\pi \cdot 50$ rad/s	Angular velocity
σ_0	10^7 Pa	Normalization constant, stress term
A	1	Normalization constant, smoothness term

Figure 5-2 shows the optimized flywheel profile (black lines) with the original flat flywheel of the same mass and moment of inertia included for comparison (gray lines).

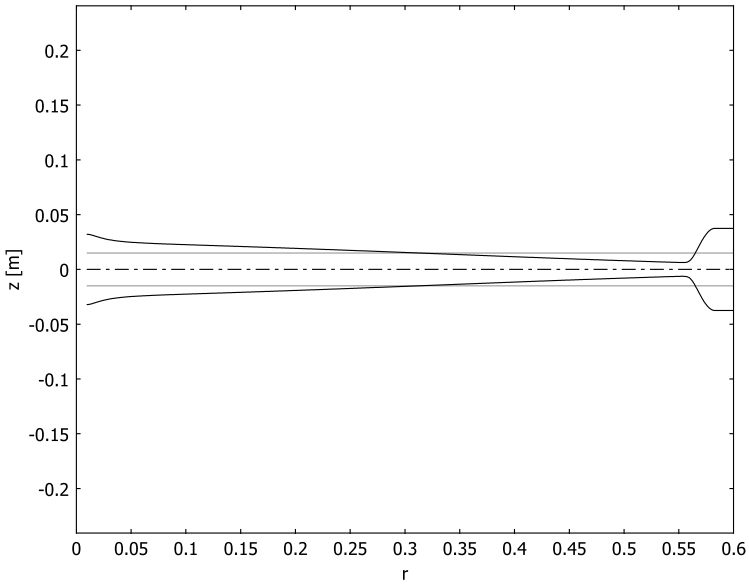


Figure 5-2: Optimized thickness profile.

Figure 5-3 displays the radial and azimuthal stress components for both the initial and the optimized flywheel profile. In the optimized flywheel, the stress components are almost equal and nearly constant for most of the radial cross-section. The maximal stress, which occurs in the radial direction at the inner radius, is roughly 102 MPa for

the optimized profile compared to 174 MPa for the flat flywheel—a reduction by more than 40%.

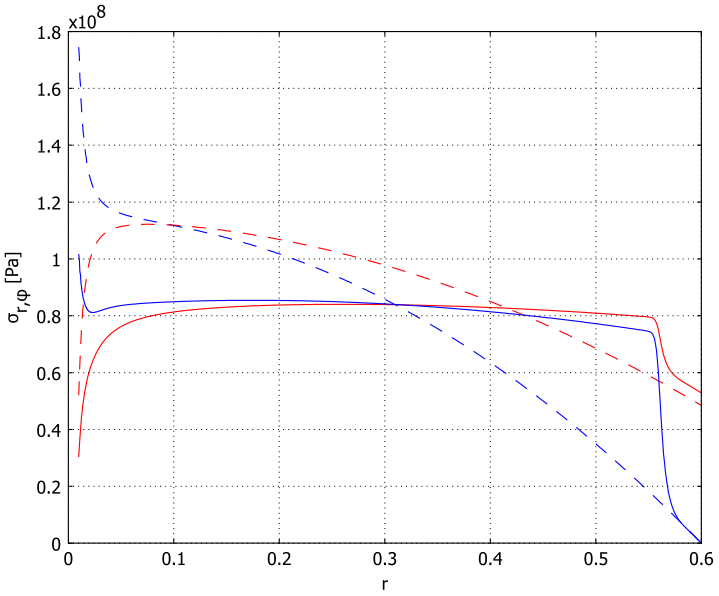


Figure 5-3: Radial (blue) and azimuthal (red) stress components for initial (dashed) and optimized (solid) flywheel profiles.

Reference

1. G.R. Kress, "Shape Optimization of a Flywheel," *Struct. Multidisc. Optim.*, vol. 19, pp. 74–81, 2000.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/flywheel_profile`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click **Multiphysics**, then click **Add Geometry**.

3 In the **Add Geometry** dialog box, set the **Space dimension** to **1D**.

4 Enter the **Independent variables** `r phi z` and set the **Unit system** to **None**. Click **OK**.

5 From the **Application Modes** tree, select **COMSOL Multiphysics>PDE Modes>PDE, General Form**.

6 In the **Dependent variables** edit field, type `U`, then click **Add**.

7 From the **Application Modes** tree, select **COMSOL Multiphysics>Optimization and Sensitivity>Optimization**, then click **Add**.

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

GEOMETRY MODELING

1 Shift-click the **Line** button on the Draw toolbar to open the **Line** dialog box.

2 In the **Coordinates** area, type `0.01 0.60` in the **r** edit field.

3 Click **OK**.

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

OPTIONS AND SETTINGS

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

2 Define constants according to the following table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
r0	0.01	Inner flywheel radius (m)
r1	0.60	Outer flywheel radius (m)
H0	0.03	Initial flywheel thickness (m)
E	2.1e11	Young's modulus (N/m^2)
nu	0.3	Poisson's ratio
C	E/(1-nu^2)	Constant in ODE and stress equations
rho	7.8e3	Density (kg/m^3)
omega	2*pi*50	Angular velocity (rad/s)
sigma0	1e7	Normalization constant, stress term (Pa)
A	1	Normalization constant, smoothness term

SCALAR EXPRESSIONS

1 From the **Options** menu, select **Expressions>Scalar Expressions**.

2 Define the following scalar expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
sigma_r	C*(r*Ur+(1+nu)*U)	Stress, r-component
sigma_phi	C*(nu*r*Ur+(1+nu)*U)	Stress, phi-component
Phi	(r/H)*Hr	Expression in ODE
q_stress	(sigma_r-sigma_r_mean)^2/ sigma0^2	Objective function, stress term
q_smoothness	A*Hr^2	Objective function, smoothness term

The function $\Phi \equiv (r/H)dH/dr$ appears in the source term for the ODE. Because it is proportional to dH/dr, it is zero for the flat flywheel.

INTEGRATION COUPLING VARIABLES

1 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**.

2 Select Subdomain 1. Define the integration coupling variables specified in the following table (use the default settings for **Integration order** and **Global destination**):

NAME	EXPRESSION
R	1
sigma_r_mean	sigma_r/R
m0	2*pi*rho*H0*r
m	2*pi*rho*H*r
I0	pi*rho*H0*r^3
I	pi*rho*H*r^3

3 Click **OK**.

PHYSICS SETTINGS

First, define the PDE for $U \equiv u/r$.

Subdomain Settings—PDE, General Form

1 From the **Multiphysics** menu, select **1 PDE, General Form (g)**.

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

3 Specify the PDE coefficients for Subdomain 1 according to the following table:

PROPERTY	VALUE
Γ	-r^2*Ur-(1+nu)*r*U
F	rho*omega^2*r^2/C-(nu-Phi)*r*Ur-(1+nu)*(1-Phi)*U

4 Click **OK**.

Boundary Conditions—PDE, General Form

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

2 Specify the following boundary conditions; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 2
Type	Dirichlet	Neumann
G	0	0
R	-U	

Next, define the design variable, objective function, and constraints for the optimization problem.

Subdomain Settings–Optimization

1 From the **Multiphysics** menu, select **2 Optimization (opt)**.

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

3 Select Subdomain 1.

4 On the **Objective** page, type `q_stress+q_smoothness` in the $\mathbf{q_1}$ edit field.

5 On the **Pointwise Constraints** page, specify the following constraint:

LB	EXPRESSION	UB	CONSTRAINT ORDER
0.25*H0	H	2.5*H0	1

6 On the **Variables** page, specify the optimization variable as in the following table:

VARIABLE	INIT	ELEMENT
H	H0	Lagrange - Linear

The model involves only the first-order derivative dH/dr, so linear Lagrange elements suffice for H.

7 Click **OK**.

Scalar Settings–Optimization

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

2 On the **Scalar Constraints** page, define the constraints for mass and moment of inertia according to the following table:

LB	EXPRESSION	UB
0	m-m0	0
0	I-I0	0

3 Click **OK**.

MESH GENERATION

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

2 On the **Global** page, set the **Maximum element size** to `2.5e-3`.

3 Click the **Boundary** tab.

4 From the **Boundary selection** list, select **1**, then set the **Maximum element size** to `1e-3`.

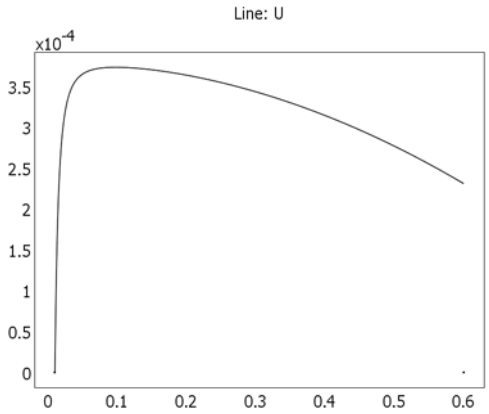
5 From the **Boundary selection** list, select **2**, then set the **Maximum element size** to `5e-4`.

6 Click **OK**.

COMPUTING THE SOLUTION—CONSTANT THICKNESS

Click the **Solve** button on the Main toolbar to solve the PDE problem for U for the case of constant flywheel thickness.

The default solution plot of U should resemble that in figure below.



Local radial displacement, u, over radial coordinate, r, for constant flywheel thickness.

POSTPROCESSING AND VISUALIZATION—CONSTANT THICKNESS

First inspect the maximal radial-stress value for the flat flywheel:

1 From the **Postprocessing** menu, select **Point Evaluation**.

2 From the **Point selection** list, select **1**.

3 In the **Expression** edit field, type `sigma_r`, then click **OK**.

The result—roughly 1.74e8, that is, 174 MPa—appears in the message log at the bottom of the user interface.

Reproduce the plots in Figure 5-1 of the stress components σ_r and σ_φ with the following steps.

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

2 On the **General** page, select the **Keep current plot** check box.

3 Click the **Line/Extrusion** tab. Make sure Subdomain 1 is selected.

4 Find the **y-axis data** area, and in the **Expression** edit field, type `sigma_r`.

5 Click **Apply** to generate the first graph.

6 Change the **Expression** to `sigma_phi`.

7 Click the **Line Settings** button.

8 From the **Line color** list, select **Color**. Click **OK**.

9 Click **OK** to generate the second graph.

10 In the figure window, click the **Edit Plot** toolbar button.

11 Find the **Title** area, and adjust the title and axis labels as appropriate (enclose subscript text with the tags `<sub>` and `</sub>`, and type `\phi` to write φ).

12 Click **OK**.

Leave the figure window open.

COMPUTING THE SOLUTION—OPTIMIZATION PROBLEM

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

2 Select the **Optimization/Sensitivity** check box.

3 Select the **Plot while solving** check box. Although optional, this setting is very useful because it lets you follow the optimization solver's progress by displaying after each model evaluation an updated plot as defined by the current settings in the **Plot Parameters** dialog box. In addition, the value of the objective function appears above the plot.

4 Click the **Optimization/Sensitivity** tab.

5 From the **Analysis** list, select **Optimization**.

6 In the **Tolerances** area, set the **Optimality tolerance** to `1e-4`.

7 Click **OK**.

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

The solution time is roughly 1 minute.

POSTPROCESSING AND VISUALIZATION—OPTIMIZATION PROBLEM

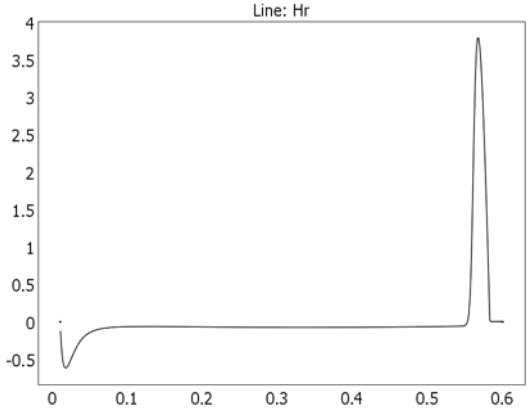
Begin by verifying that the relative normalization between the two terms in the objective function has a suitable value by plotting the derivative dH/dr.

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

2 Click the **Line** tab.

3 From the **Predefined quantities** list, select **Optimization (opt)>Hr**.

4 Click **OK** to generate the following plot.



dH/dr as a function of r for the optimized flywheel profile.

The smooth nature of the plot, shows that the normalization constant A is sufficiently large to suppress short-scale variations in the thickness, H. Conversely, if you were to specify a significantly lower A value and re-solve the optimization problem, you would notice sharp features in the dH/dr curve, indicating that you should not lower A further.

Having concluded that the solution is sound, proceed to inspect the maximal radial-stress value for the optimized flywheel profile:

1 From the **Postprocessing** menu, select **Point Evaluation**.

2 Make sure that Point 1 is still selected, then click **OK**.

The result in the message log should be close to 102 MPa.

Reproduce the plots in Figure 5-3 by first adding the optimized results for the stress components to the figure-window plot you created earlier and then adjusting line styles, title, and axis labels.

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

2 Click **Apply** to generate the graph for the azimuthal stress component.

3 Change the **Expression** in the **y-axis data** area to `sigma_r`.

4 Click the **Line Settings** button.

5 From the **Line color** list, select **Cycle**. Click **OK**.

6 Click **OK** to generate the graph for the radial stress.

7 In the figure window, click the **Edit Plot** toolbar button.

8 In the **Axes** tree, select the first **Line** object. From the **Line style** list select **Dashed line**.

9 Repeat the previous step for the second **Line** object.

10 Select **Axes** to activate the **Axis** page.

11 In the **Title** area, adjust the title and *y*-axis label as appropriate, then click **OK**.

To reproduce the profile plot in Figure 5-2, follow these instructions:

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

2 Click the **General** tab. From the **Plot in** list, select **New figure**. Leave the **Keep current plot** check box selected.

3 Click the **Line/Extrusion** tab. In the **Expression** edit field in the **y-axis data** area, type `0`.

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 black, then click **OK**.

5 From the **Line style** list, select **Dash-dot line**.

6 Click **OK** to close the **Line Settings** dialog box.

7 In the **Domain Plot Parameters** dialog box, click **Apply** to generate the first line.

8 Change the **Expression** to `H0/2`, then click the **Line Settings** button.

9 Click the **Color** button. Select a gray shade, then click **OK**.

10 Change the **Line style** to **Solid line**, then click **OK**.

11 Click **Apply**.

12 Change the **Expression** to `-H0/2`, then click **Apply**.

13 Change the **Expression** to `-H/2`, then click the **Line Settings** button.

14 Click the **Color** button. Select black, then click **OK** to close the **Line Color** dialog box.

15 Click **OK** to close the **Line Settings** dialog box.

16 Click **Apply**.

17 Change the **Expression** to `H/2`, then click **OK**.

18 In the second figure window, click the **Edit Plot** toolbar button.

19 On the **Grid** page, clear the **Show grid** check box, then return to the **Axis** page.

20 Select the **Axis equal** check box, adjust title and axis labels, and then click **OK**.

Finally, to change the plot in the main user interface to the one you see when you open the model in the Model Library, do as follows:

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

2 Click the **Line** tab.

3 In the **Expression** edit field, type `H/2`.

4 Click **OK**.

Electrical Signals in a Heart

This model is kindly provided by Prof. Simonetta Filippi and Dr. Christian Cherubini from Università Campus Biomedico di Roma, Italy.

Introduction

Modeling the electrical activity in cardiac tissue is an important step in understanding the patterns of contractions and dilations in the heart. The heart produces rhythmic electrical pulses, initiated from a point known as the sinus node. The electrical pulses, in turn, trigger the mechanical contractions of the muscle. In a healthy heart these electrical pulses are damped out, but a number of heart conditions involve an elevated risk of re-entry of the signals. This means that the normal steady pulse is disturbed, a severe and acute condition which is often referred to as arrhythmia.

This section presents two mathematical models describing different aspects of electrical signal propagation in cardiac tissue: the *FitzHugh-Nagumo* equations and the *Complex Ginzburg-Landau* equations, both of which are solved on the same geometry. Interesting patterns emerging from these types of models are, for example, spiral waves, which, in the context of cardiac electrical signals, can produce effects similar to those observed in cardiac arrhythmia.

EXCITABLE MEDIA AND THE FITZHUGH-NAGUMO EQUATIONS

It has been shown that many important characteristics of electrical signal propagation in cardiac tissue can be reproduced by a class of equations which describe *excitable media*, that is, materials consisting of elementary segments or cells with the following basic characteristics:

- Well-defined rest state
- Threshold for excitation
- A diffusive-type coupling to its nearest neighbors

Excitable media is a rather general concept, which is useful for modeling of (in addition to the electrical signals in cardiac tissue) a number of different phenomena, including nerve pulses, the spreading of forest fires, and certain types of chemical reactions. One of the most important qualitative characteristics displayed by excitable media, and equally a common denominator between the diversity of phenomena mentioned

above, is the almost immediate damping out of signals below a certain threshold. On the other hand, signals exceeding this threshold propagate without damping.

The heart works by passing ionic current inside the muscle, thus triggering the rhythmic contractions that pump blood in and out. The ions move through small pores or *gates* in the cellular membrane, which can be either open (excitation state) or closed (rest state).

In nerve cells and cardiac cells the three abstract characteristics of excitable media are manifested as

- Rest cell membrane potential
- Threshold for opening the ionic gates in the cellular membrane
- The diffusive spreading of the electrical signals

The state of the membrane gates is random on a microscopic scale, but the probability of a given state can be modelled as a continuous function of the voltage, thus allowing an averaged macroscopic continuum description of the current flow.

The *FitzHugh-Nagumo* equations for excitable media describe the simplest physiological model with two variables, an *activator* and an *inhibitor*. In these heart models the activator variable corresponds to the electric potential, and the inhibitor is a variable that describes the voltage-dependent probability of the pores in the membrane being open and ready to transmit ionic current.

CHAOTIC DYNAMICS AND THE COMPLEX LANDAU-GINZBURG EQUATIONS

The *complex Landau-Ginzburg* equations provide a relatively simple way of modeling some aspects of the transition, displayed by many dynamical systems under the influence of strong external stimulus, from periodic oscillatory behavior into a chaotic state with gradually increasing amplitude of oscillations and decreasing periodicity.

Although their first use was to describe the theory of superconductivity, the complex Landau-Ginzburg equations are also generic in their nature (as are the FitzHugh-Nagumo equations), and examples of dynamical systems which you can model successfully using these equations are:

- The formation of vortices behind a slender obstacle in transversal fluid flow
- Oscillating chemical reactions of the Belousov-Zhabotinsky type

In this model the complex Landau-Ginzburg equations simulate the dynamics of the spiral waves in excitable media.

Model Definition

The geometry here is a simplified 3D model of a heart with two chambers, represented with semispherical cavities[1].

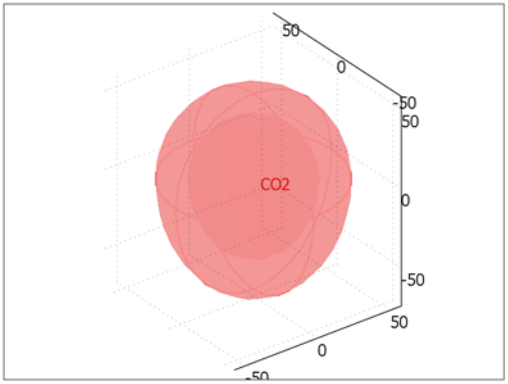


Figure 5-4: Model geometry.

THE FITZHUGH-NAGUMO EQUATIONS

The equations are the following:

$$\frac{\partial u_1}{\partial t} = \Delta u + (\alpha - u_1)(u_1 - 1)u_1 + (-u_2)$$

$$\frac{\partial u_2}{\partial t} = \varepsilon(\beta u_1 - \gamma u_2 - \delta)$$

Here u_1 is an *action potential* (the activator variable), and u_2 is a *gate variable* (the inhibitor variable). The parameter α represents the threshold for excitation, ε represents the excitability, and β, γ, and δ are parameters that affect the rest state and dynamics of the system.

The boundary conditions for u_1 are insulating, using the assumption that no current is flowing into or out of the heart. The initial condition defines an initial potential distribution u_1 where one quadrant of the heart is at a constant, elevated potential V_0, while the rest remains at zero. The adjacent quadrant has instead an elevated value ν_0 for the inhibitor u_2. It is convenient to implement this initial distribution using the following logical expressions, where TRUE evaluates to 1 and FALSE to 0:

1. Note that it is possible to import more realistic human/animal heart geometries, with anisotropies and inhomogenities as well as proper dimensions, into COMSOL Multiphysics using the CAD import capabilities.

$$u_1(0,x,y,z) = V_0((x+d)>0)\cdot((z+d)>0)$$
$$u_2(0,x,y,z) = v_2((-x+d)>0)\cdot((z+d)>0)$$

Here d is equal to 10^{-5}, and it is included in the expressions to shift the elevated potential slightly off the main axes.

THE COMPLEX LANDAU-GINZBURG EQUATIONS

The complex Landau-Ginzburg equations are:

$$\frac{\partial u_1}{\partial t} - \Delta(u_1 - c_1 u_2) = u_1 - (u_1 - c_3 u_2)(u_1^2 + u_2^2)$$
$$\frac{\partial u_2}{\partial t} - \Delta(c_1 u_1 + u_2) = u_2 - (c_3 u_1 + u_2)(u_1^2 + u_2^2)$$

The two variables u_1 and u_2 are the activator and inhibitor, respectively. The constants c_1 and c_2 are parameters reflecting the properties of the material. These constants also determine the existence and nature of the stable solutions.

As in the previous model, the boundary conditions are kept insulating. The initial condition, which gives a smooth transition step near $z = 0$, are the following:

$$u_1(0,x,y,z) = \tanh(z)$$
$$u_2(0,x,y,z) = -\tanh(z)$$

Modeling in COMSOL Multiphysics

The simplified geometry is quite straightforward to create using the drawing tools in COMSOL Multiphysics. The FitzHugh-Nagumo and Landau-Ginzburg equations are also readily entered in one of the PDE-based application modes[2].

It is important to note that these equations are strongly nonlinear. It is therefore necessary (especially in full 3D models like these) to use a much finer mesh or use higher element order than in these examples to get results with some degree of reliability for the time intervals of interest. This is particularly important in solving the complex Landau-Ginzburg equations, which describe inherently chaotic phenomena. They are highly sensitive to perturbations in the initial value and similarly to numerical errors during the course of the time-dependent solution. We recommend the use of the fourth-order Hermite element for the complex Landau-Ginzburg equation.

2. With this stage completed, it would also be straightforward to replace the rather simple FitzHugh-Nagumo equations with a physiologically more realistic mathematical model.

For the reasons above, the results presented here are only intended as a first rough estimate of the qualitative behavior that you can expect the system to show under a given stimulus. Consequently, higher-order elements, finer meshing, and smaller relative and absolute time dependent tolerances clearly give quantitatively more correct simulation results. These improvements may require several hours of computational time to solve the equations, while the rough model described here should solve within around 20 minutes on a standard PC. When attempting these types of large models we strongly recommend the use of 64-bit platforms.

Results

THE FITZHUGH-NAGUMO EQUATIONS

The plots in Figure 5-5 below show the action potential u_1. To visualize the solution on the inside, a quarter of the outside shell of the heart and one of the chamber surfaces are suppressed in the plot.

The parameters used in the model along with the initial pulse lead to a reentrant wave which travels around the tissue without damping in a characteristic spiral pattern.

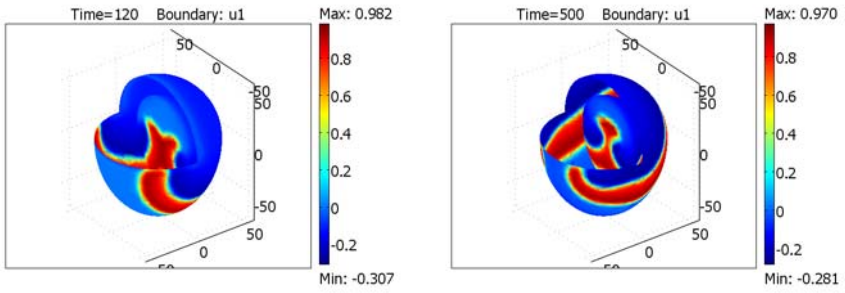


Figure 5-5: Solution to the FitzHugh-Nagumo equations at times t = 120 s (left plot) and t = 500 s (right plot).

THE LANDAU-GINZBURG EQUATIONS

Figure 5-6 below shows the species u_1 at different times.

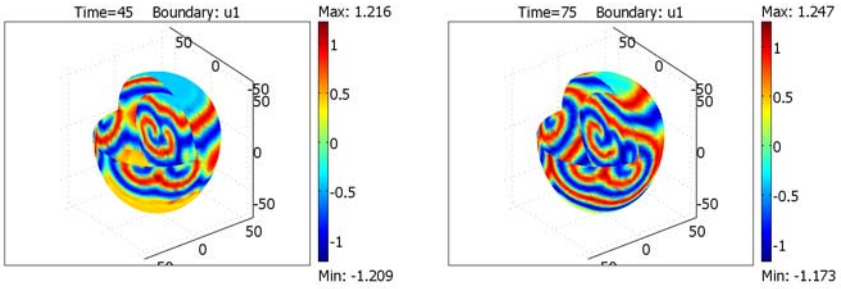


Figure 5-6: Solution to the Complex Landau-Ginzburg equations at times t = 45 s (left) and t = 75 s (right).

The equation parameters and initial condition used here lead the diffusing species (u_1) to display characteristic spiral patterns with growing complexity over time.

Modeling Using the Graphical User Interface

The instructions below describe how to create the model containing the FitzHugh-Nagumo equations for excitable media. To create the model containing the complex Landau-Ginzburg equations, follow the instructions from the beginning until you have completed the "Geometry Modeling" section. Then jump to the section called "Modifications."

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/heart_electrical_fhn`

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, select **3D** from the **Space dimension** list.
3. Expand the **COMSOL Multiphysics** folder, then expand the **PDE Modes** subfolder, and finally select the **PDE, General Form** application mode.
4. Enter the dependent variables u_1 and u_2 by typing `u1 u2` in the **Dependent variables** edit field at the bottom of the window.

5 Click **OK** to confirm and close the **Model Navigator**.

GEOMETRY MODELING

1 Click the **Sphere** button on the Draw toolbar on the left. Enter a **Radius** of 54 for the sphere, then click **OK**.

2 Click the **Ellipsoid** button on the Draw toolbar. Enter 54, 54, and 70 for the x-, y-, and z-semiaxes, respectively. Click **OK**.

Next create the egg-shaped solid by fusing the top half of the sphere with the bottom half of the ellipsoid. As a first step, divide the two solids across the middle by using a work plane.

3 To create a work plane, select **Draw>Work-Plane Settings**. In the **Work-Plane Settings** dialog box, click the **Vertices** tab. Expand the **ELP1** folder in the **Vertex selection** area on the left, select Vertex 1, and then click the **>>** button to add it to the **Selected vertices** area. In the same manner, add Vertices 2 and 6 to the **Selected vertices**. When done, click **OK**.

4 In the 2D **Geom2** geometry, click **Zoom Extents** on the Main toolbar at the top of the main user interface and draw a rectangle that completely covers the blue circle by using the **Rectangle** button on the Draw toolbar. (Note that the blue curves show the contours of the 3D geometry in the 2D plane.) Select **Draw>Embed**, then click **OK**.

The rectangular surface should now have been added to the 3D geometry, splitting both the sphere and the ellipse in two halves.

5 To create the separated geometry objects for the halves, select the rectangular surface, confirm the selection by right-clicking, and then similarly select and confirm the spherical solid. With both the spherical solid and the rectangular surface selected, click the **Coerce to Solid** button on the Draw toolbar, then click the **Split object** button. Finally, remove the bottom half of the sphere by clicking on it to select it and press the Delete button on the keyboard.

6 Go back to the 2D geometry and select the rectangle, then choose **Draw>Embed**, and then click **OK**. Repeat Step 5 for the elliptical solid instead of the sphere. Note that this time you need to remove the top half of the elliptic solid (for the sphere it was the bottom half).

7 Select both objects by pressing Ctrl+A and go to **Draw>Create Composite Object**. Make sure that the **Keep interior boundaries** check box is cleared and click the **Union** button. Click **OK**.

8 To create the cavity inside the heart, press first Ctrl+C and then Ctrl+V. In the **Paste** dialog box, click **OK** to create a copy of the egg-shaped solid (leave the **x**, **y**, and **z displacements** at zero). Then choose **Modify>Scale** from the **Draw** menu. In the **Scale factor** area, type `2/3` in the **x**, **y**, and **z** edit fields. Click **OK**.

9 Open the **Create Composite Object** dialog box again (choose **Draw>Create Composite Object**). Enter the expression `C01-C02` in the **Set formula** edit field, then click **OK** to subtract the smaller solid from the larger one. To see the cavities inside the solid you can click the **Increase Transparency** button on the Draw toolbar a couple of times.

10 To create the wall separating the two chambers click the **Cylinder** button on the Draw toolbar and enter `45` for the radius and `10` for the height. Type the values `-5`, `0`, and `-5` respectively in the **x**, **y**, and **z** edit fields in the **Axis base point** frame. Enter `1`, `0`, and `0` as the **x**, **y**, and **z** values in the **Axis direction vector** frame. Click **OK**.

11 Once again, open the **Create Composite Object** dialog box from the **Draw** menu. Select both geometry objects, make sure the **Keep interior boundaries** check box is not selected, and then click the **Union** button. Click **OK**.

The final geometry should look as shown in Figure 5-4 on page 120.

VARIABLES AND EXPRESSIONS

1 Choose **Options>Constants**.

2 In the **Constants** dialog box, enter the following constants; when done, click **OK**.

NAME	VALUE	DESCRIPTION
alpha	0.1	Excitation threshold
beta	0.5	System parameter
gamma	1	System parameter
delta	0	System parameter
epsilon	0.01	Excitability
V0	1	Elevated potential value
nu0	0.3	Elevated inhibitor value
d	1e-5	Off-axis shift distance

PHYSICS SETTINGS

Subdomain Settings

1 Choose **Physics>Subdomain Settings**.

2 Enter the subdomain settings according to the following table:

SETTINGS	SUBDOMAIN 1
F (row 1)	`(alpha-u1)*(u1-1)*u1-u2`
F (row2)	`epsilon*(beta*u1-gamma*u2-delta)`
Γ (row 1)	`-u1x -u1y -u1z`
Γ (row2)	`0 0 0`

3 On the **Init** page, enter the following initial conditions:

DEPENDENT VARIABLE	INITIAL CONDITION EXPRESSION
$u1(t_0)$	`V0*((x+d)>0)*((z+d)>0)`
$u2(t_0)$	`nu0*((-x+d)>0)*((z+d)>0)`

4 If you can afford the increase in memory usage and solution time needed for better accuracy, click the **Element** tab and select **Hermite - Quartic** from the **Predefined elements** list. Otherwise skip this step and use the default second-order Lagrange elements.

5 Click **OK**.

Boundary Conditions

1 Choose **Physics>Boundary Settings**.

2 Select all boundaries by pressing Ctrl+A.

3 On the **Type** page, click the **Neumann boundary condition** button.

Leave the **G coefficient** components at their default zero values.

4 Click **OK**.

COMPUTING THE SOLUTION

1 Choose **Solve>Solver Parameters**.

2 From the **Solver** list, select **Time dependent**. In the **Time stepping** area on the **General** page, type `range(0,5,500)` in the **Times** edit field.

3 In the **Linear system solver** list, select **GMRES**. Make sure that the **Preconditioner** is set to **Incomplete LU**, then click **OK**.

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

POSTPROCESSING AND VISUALIZATION

1. To create the right plot in Figure 5-5 on page 122, choose **Postprocessing>Plot Parameters** and select the **Boundary** check box on the **General** page. Clear all other check boxes in the **Plot type** area, then click **OK**.
2. Choose **Options>Suppress>Suppress Boundaries**. Select Boundaries 2 and 4–9, then click **OK** to hide these boundaries.
3. Click the **Postprocessing Mode** button on the Main toolbar to see the plot.
4. To create the left plot in Figure 5-5 on page 122, choose **Postprocessing>Plot Parameters**, select **125** from the **Solution at time** list on the **General** page, and then click **OK**.

MODIFICATIONS FOR USING COMPLEX LANDAU-GINZBURG EQUATIONS

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/heart_electrical_clg`

Follow the steps under the sections "Model Navigator" and "Geometry Modeling" just described. Then proceed with the following instructions.

Variables and Expressions

1. Choose **Options>Constants**.
2. In the **Constants** dialog box, specify the following constants; when done, click **OK**.

NAME	VALUE	DESCRIPTION
c1	2	PDE parameter
c3	-0.2	PDE parameter

Subdomain Settings

1. Choose **Physics>Subdomain Settings**.
2. Enter the following expressions for the PDE coefficient Γ:

DEPENDENT VARIABLE	Γ_x	Γ_y	Γ_z
u1	-u1x+c1*u2x	-u1y+c1*u2y	-u1z+c1*u2z
u2	-c1*u1x-u2x	-c1*u1y-u2y	-c1*u1z-u2z

3 Enter the following for the source term **F**:

DEPENDENT VARIABLE	F
u1	`u1-(u1-c3*u2)*(u1^2+u2^2)`
u2	`u2-(c3*u1+u2)*(u1^2+u2^2)`

4 Click the **Init** tab, then enter the following initial values; when done, click **OK**.

DEPENDENT VARIABLE	INITIAL VALUE
$u1(t_0)$	`tanh(z)`
$u2(t_0)$	`-tanh(z)`

Boundary Conditions

Follow the instructions under "Boundary Conditions" on page 126 (the boundary conditions are the same for both equations).

Computing the Solution

Follow the steps under "Computing the Solution" on page 126 with the following modifications:

- In the **Time stepping** area on the **General** page, enter the **Times** `range(0,5,75)`.
- Set both the **Relative tolerance** and the **Absolute tolerance** to `1e-7`.

Postprocessing and Visualization

Follow the steps under "Postprocessing and Visualization" on page 127 to produce the corresponding plots for the Landau-Ginzburg equations. Note that to produce the plot on the left in Figure 5-6 on page 123 you need to select `50` from the **Solution at time** list on the **General** page.

References

2. F.H. Fenton, E.M. Cherry, H.M. Hastings, and S.J. Evans, "Real-time computer simulations of excitable media: JAVA as a scientific language and as a wrapper for C and FORTRAN programs," *BioSystems 64*, pp. 73–96, 2002.

3. Y. Kuramoto, *Chemical Oscillations, Waves and Turbulence*, Dover Publications, 2003.

4. J. Keener and J. Sneyd, *Mathematical Physiology*, Springer, 1998.

An Integro-Partial Differential Equation[3]

Introduction

This example investigates how to solve the integro-partial differential equation

$$\frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right) - \frac{4D_\mathrm{i}}{{D_\mathrm{o}}^2 - {D_\mathrm{i}}^2}\varepsilon\sigma T^4 + \frac{4D_\mathrm{i}}{{D_\mathrm{o}}^2 - {D_\mathrm{i}}^2}\varepsilon\sigma\int_0^L k(x,x')T(x')^4\cdot\frac{dx'}{D_\mathrm{i}} = \rho C_p\frac{\partial T}{\partial t}$$

where ρ is the density, C_p is the heat capacity, κ is the thermal conductivity, σ is Stefan's constant (the Stefan-Boltzmann constant), ε is the emissivity, and $k(x,x')$ is the kernel corresponding to the radiation view factor. This equation arises in the physical description of 1D heat conduction and radiation along a pipe. Figure 5-7 shows the model geometry.

Before setting up the model, make the following assumptions:

- Inside the tube, neglect convection and consider only radiation and conduction.
- Assume blackbody radiation with $\varepsilon = 1$.
- Model heat transfer only in the x direction (assume θ symmetry).
- The pipe's outer wall is perfectly insulated so that no heat escapes to the outside world by either radiation or conduction.

The definition of the kernel $k(x, x')$ is

$$1 - \frac{2\xi^3 + 3\xi}{2(\xi^2+1)^{3/2}}$$

where $\xi = |x - x'|/D_\mathrm{i}$ as explained in Ref. 1.

3. This model is courtesy of Daniel Smith and Ali Shajii of MKS Instruments, Wilmington, Mass., USA.

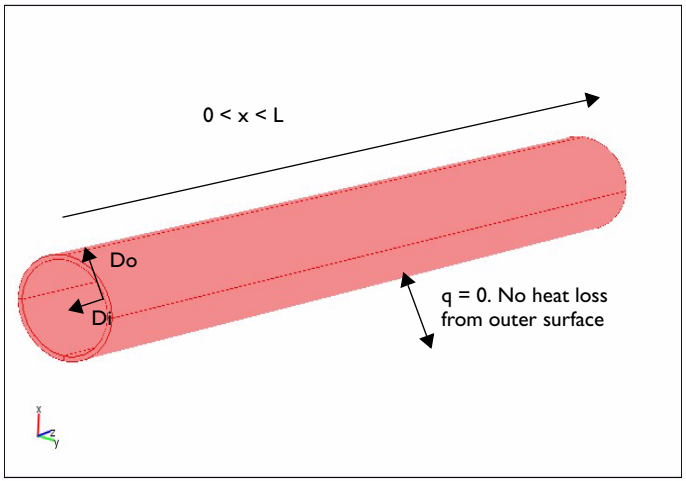


Figure 5-7: Model geometry and boundary conditions.

Also consider the following boundary conditions and initial condition:

$$T(0, t) = 300 + 1200\tanh\left(\frac{t}{1\ \text{min}}\right)\ \text{K}$$

$$T(L, t) = 300\ \text{K}$$

$$T(x, 0) = 300\ \text{K}$$

Modeling in COMSOL Multiphysics

To model the equation, use the Heat Transfer by Conduction application mode. In this application mode you can include the radiation effects in the source term, Q, using an integration-coupling variable.

To enter convolution integrals of the type needed here, use the `dest` operator, which forces COMSOL Multiphysics to evaluate the expression on which it operates on the destination points instead of the source points. In the expression $k(x, x')$, x' is the variable to integrate over, whereas the model does not integrate over x. To specify that x should remain a variable that can take on values from the entire domain, write it as `dest(x)` when defining the integration-coupling variable. In the case of a coupling variable, `dest(f(x))` makes COMSOL Multiphysics evaluate `f(x)` on the destination domain and not the source domain.

Results

The temperature distribution along the length of the pipe at $t = 3600$ s appears in Figure 5-8.

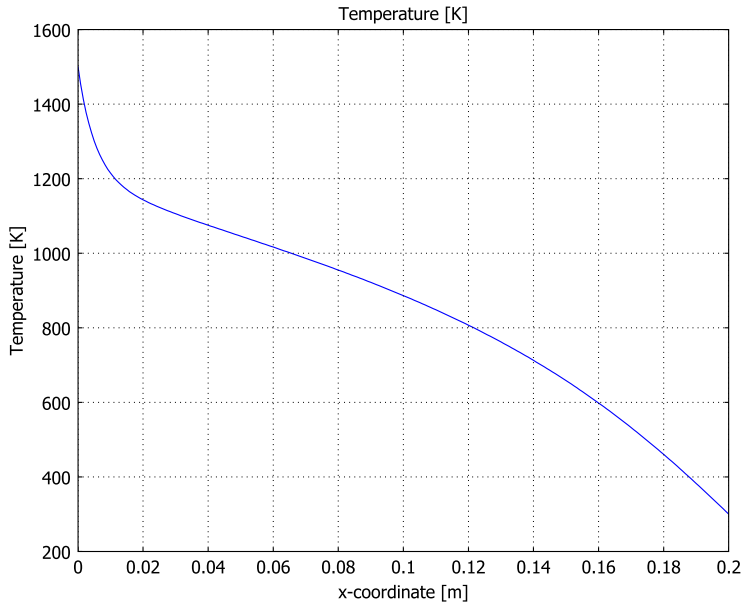


Figure 5-8: Temperature distribution along the pipe at t = 3600 s.

It is easy to make a comparison with a radiation-free model by removing the source term from the heat transfer equation. The equation to solve now becomes

$$\frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right) = \rho C_p\frac{\partial T}{\partial t}\,.$$

Figure 5-9 plots the solutions to both the radiation-free heat transfer and the original PDE with radiation as a heat source.

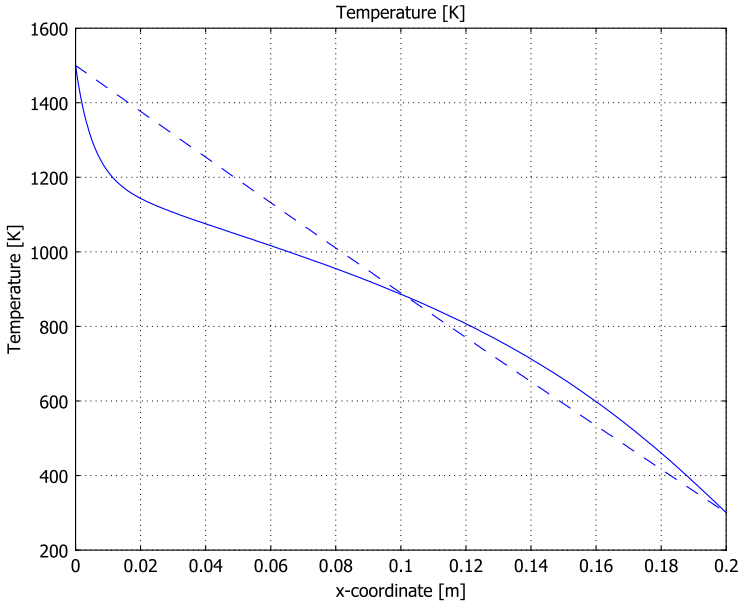


Figure 5-9: The temperature distribution with radiation (solid line) and without radiation (dashed line).

Comparison with the Full 3D Radiation Model

To illustrate the validity of the 1D model, you can set up the entire stationary 3D model using the Heat Transfer Module. Its General Heat Transfer application mode handles surface-to-surface radiation boundary conditions, making it easy to verify the results (Figure 5-10).

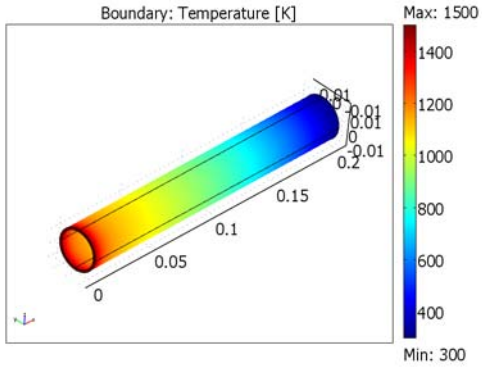


Figure 5-10: 3D temperature distribution in the pipe.

Figure 5-11 compares the temperature distributions along the axial direction for the two models (1D and 3D). Clearly the results are in good agreement.

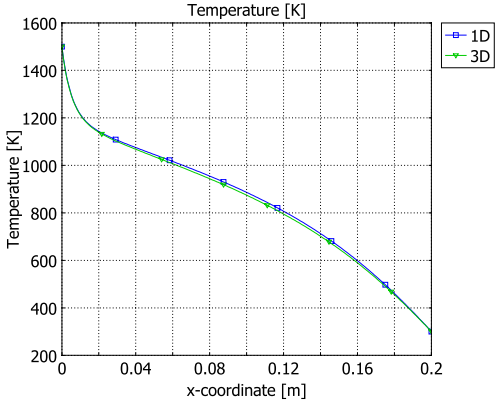


Figure 5-11: The temperature distributions from the 1D model (square markers) and the 3D model (triangle markers).

Reference

1. R. Siegel and J. Howell, *Thermal Radiation Heat Transfer*, 4th ed., Taylor & Francis Group, New York, 2001.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/integro_partial`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **1D** in the **Space dimension** list.

2 In the list of application modes, select **COMSOL Multiphysics>Heat Transfer>Conduction>Transient analysis**.

3 Click **OK**.

GEOMETRY MODELING

1 Draw a line from 0 to 0.2. To do so, press Shift and click the **Line** button on the Draw toolbar. In the **Line** dialog box, enter the coordinates `0 0.2`, then click **OK**.

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

OPTIONS AND SETTINGS

Constants and Expressions

1 From the **Options** menu, select **Constants**. Enter the following names, expressions, and descriptions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
kappa	13[W/(m*K)]	Thermal conductivity
rho	8700[kg/m^3]	Density
C_p	300[J/(kg*K)]	Heat capacity
sigma	5.67e-8[W/(m^2*k^4)]	Stefan's constant
epsilon	1	Emissivity
T_cold	300[K]	Temperature, cold end
DT_max	1200[K]	Maximum temperature difference
T_init	T_cold	Initial temperature
D_i	2.54[cm]	Inner diameter
D_o	D_i*1.1	Outer diameter

2 Go to the **Options** menu and select **Expressions>Subdomain Expressions**. Select Subdomain 1, then enter the following two expressions; when done, click **OK**.

NAME	EXPRESSION
Q_source	4*sigma/(D_o^2-D_i^2)*irrad
Q_loss	-4*D_i/(D_o^2-D_i^2)*sigma*epsilon*T^4

Coupling Variables

1 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**, then enter the following variable (type the complete expression on a single line); when done, click **OK**.

NAME	EXPRESSION
irrad	T^4*(1-(2*(abs(x-dest(x))/D_i)^3+3*(abs(x-dest(x))/D_i))/(2*(((x-dest(x))/D_i)^2+1)^1.5))

This is the integral term in the original equation, which you specify in this way using the `dest` operator. This coupling variable does not have a unit, so for other quantities that include the `irrad` variable (in this case, `Q_source` and the heat source setting that uses `Q_source`), COMSOL Multiphysics indicates inconsistent units.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**, then enter these expressions for the material properties:

NAME	EXPRESSION
κ	kappa
ρ	rho
C_p	C_p
Q	Q_source+Q_loss

2 Click the **Init** tab. In the **$T(t_0)$** edit field type `T_init`, then click **OK**.

Boundary Conditions

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

2 In the **Boundary selection** list, select Boundary 1.

3 In the **Boundary condition** list, select **Temperature**. In the T_0 edit field enter the expression `T_cold+DT_max*tanh(t/1[min])`. Dividing `t` by the time constant `1[min]` makes the input to `tanh` unitless, as is appropriate.

4 Select Boundary 2, and in the **Boundary condition** list select **Temperature**. In the T_0 edit field type `T_cold`, then click **OK**.

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar. Doing so results in 15 elements as you can see in the message log.

2 Click the **Refine Mesh** button on the Main toolbar twice to end up with 60 elements.

COMPUTING THE SOLUTION

1 From the **Solve** menu, select the **Solver Manager**.

2 On the **Initial Value** page, click the **Initial value expression** button. Click **OK**.

3 From the **Solve** menu, select **Solver Parameters**.

4 On the **General** page go to the **Solver** list on the left side of the window and select **Time dependent**. In the **Times** edit field, type `range(0,60,3600)`. Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 5-8, follow these steps:

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

2 On the **General** page, go to the **Solutions to use** area and select the solution for time **3600** only.

3 Click the **Line/Extrusion** tab, then click **Apply** to plot the temperature distribution.

Comparing the Results with a Radiation-Free Model

To compare the temperature distribution in the radiation model with that of a model without radiation, plot the temperature distributions from the two variations in the same figure.

1 Again, choose **Postprocessing>Domain Plot Parameters**. Click the **Line/Extrusion** tab. Click **Apply** to plot the temperature T, then return to the **General** page and select the **Keep current plot** check box at the bottom of the dialog box. Click **OK**.

2 From the **Physics** menu, select **Subdomain Settings**. Click the **Physics** tab. In the **Q** edit field type `0`. Click **OK**. (This step removes the effect of the radiation on the temperature distribution.)

3 Click the **Solve** button.

4 Choose **Postprocessing>Domain Plot Parameters** dialog box.

5 Click the **General** tab. In the **Solutions to use** area, select the solution for time **3600** only.

6 Click the **Line/Extrusion** tab. Click the **Line Settings** button, then select **Dashed line** from the **Line style** list. Click **OK** to close the **Line Settings** dialog box.

7 Back in the **Domain Plot Parameters** dialog box, click **OK**.

The last step plots the temperature T in the same window as the previous temperature distribution, and the result should resemble Figure 5-9.

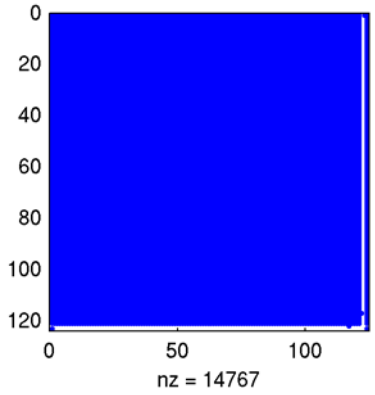
Visualizing the Effect of the Nonlocal Coupling

Note: This step requires that you run COMSOL Multiphysics with MATLAB.

To examine the effect of the nonlocal behavior, first export the model to the workspace (select **File>Export>FEM Structure** or press Ctrl+F), then enter these commands:

```
[K,L,M,N] = assemble(fem,'u',fem.sol,'T',3600);
n = size(N,1);
spy([K,N',L;N,sparse(n,n),M]);
```

The off-diagonal nonzero entries in the sparsity plot reveal that the Jacobian for this problem is a full matrix.



The KdV Equation and Solitons

Introduction

The Korteweg-de Vries (KdV) equation, formulated in 1895 by Korteweg and de Vries, models water waves. It contrasts sharply to the Burgers equation, because it introduces no dissipation and the waves travel seemingly forever. In 1965, Zabusky and Kruskal named such waves as *solitons*.

The KdV equation with boundary conditions and initial value for this model is formulated as

$$\begin{aligned} &u_t + u_{xxx} = 6uu_x \qquad \text{in } \Omega = [-8, 8] \\ &u(-8, t) = u(8, t), \qquad \text{periodic} \\ &u(x, 0) = -6\,\mathrm{sech}^2(x) \end{aligned}$$

The equation models the steepening and dispersion of wavefronts but does not support a train of simple harmonic waves. Such trains comprise the wavecrests normally associated with the ocean: simply a momentary constructive interference of contributing waves moving at different speeds. However, the equation does support solitons, single "humps" that travel without changing shape or speed for unexpectedly long distances.

Indeed, Perry and Schimke (Ref. 2) concluded from shipboard oceanographic measurements that bands of choppy water in the Andaman Sea, which lies east of the Bay of Bengal and west of Burma and Thailand, are associated with large-amplitude oceanic internal waves. Satellite images have since clarified that these waves originate on shallow banks on a layer between warm and cool water. Further, Osborne and Burch (Ref. 1) analyzed oceanographic data in an effort to assess the forces of underwater current fluctuations associated with such waves on offshore drilling rigs. They concluded that the visually observed roughness bands are caused by internal solitons that follow the KdV equation (Ref. 3).

A more recent development is the application of the KdV equation to another type of waves—light waves. Today solitons have their primary practical application in optical fibers. Specifically, a fiber's linear dispersion properties level out a wave while the nonlinear properties give a focusing effect. The result is a very stable, long-lived pulse (Ref. 3). It is amazing that researchers have discovered a formula for such waves:

$$u = \frac{v}{\left[2\cosh^2\left(\frac{1}{2}\sqrt{v}\right)(x - vt - f)\right]}$$

This equation says that the pulse speed is what determines the pulse amplitude and the pulse width. The following simulation illustrates this effect. An initial pulse, which does not conform to the formula, immediately breaks down into two pulses of different amplitudes and speeds. The two new pulses do follow the formula and thus can travel forever. While the formula does not reveal how solitons interact, the simulation shows that they can collide and reappear, seemingly unchanged, just as linear waves do, another counterintuitive observation that is difficult to observe without predictions by computing.

Model Definition

In the model, the term uu_x describes the focusing of a wave and u_{xxx} refers to its dispersion. The balancing of these two terms permits waves to travel with their shape unchanged.

Because COMSOL Multiphysics does not evaluate third derivatives directly, you rewrite the original equation above as a system of two variables to solve it:

$$u_{1t} + u_{2x} = 6u_1u_{1x}$$
$$u_{1xx} = u_2$$

Using the general form PDE, you need to define two dependent variables, `u1` and `u2`, and identify the d_a, Γ, and F coefficients in the following equation:

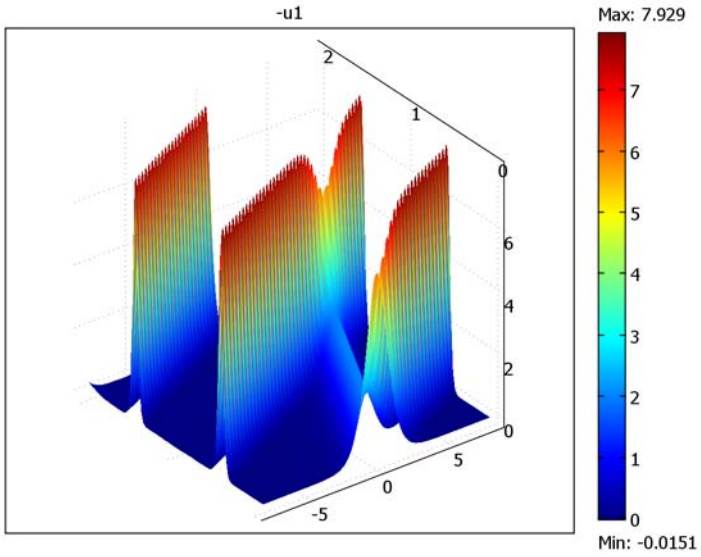
$$d_a\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \Gamma = F$$

- Only the first equation has a time derivative, and it is with respect to u_1, so only $d_a(1,1)$ is 1; the other three components are zero.
- The divergence in this model is a space derivative with respect to x. This means that the Γ component from the first equation is u_2, which you type as `u2`. The Γ component from the second equation is u_{1x}, which you express in COMSOL Multiphysics as `u1x`.
- The F term components are the right-hand side of the equations: F_1 is $6u_1u_{1x}$ (type `6*u1*u1x`), and F_2 is u_2 (type `u2`).

The initial condition for u_1 uses a hyperbolic cosine function to provide an interesting wave form to start with. For u_2, you must provide the second space derivative of this function to provide consistent initial conditions.

Results

The following plot shows how solitons collide and reappear with their shape intact.



References

1. A.R. Osborne and T.L. Burch, "Internal Solitons in the Andaman Sea," *Science*, vol. 208, no. 4443, pp. 451–460, 1980.

2. R.B. Perry and G.R. Schimke, "Large-Amplitude Internal Waves Observed off the Northwest Coast of Sumatra," *J. Geophys. Res.*, vol. 70, no. 10, pp. 2319–2324, 1965.

3. G. Strang, *Applied Mathematics*, Wellesley-Cambridge, 1986.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/kdv_equation`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **1D** in the **Space dimension** list.

2 In the list of application modes, open the **COMSOL Multiphysics>PDE Modes** folder and then **PDE, General Form**. Select **Time-dependent analysis**.

3 Type `u1 u2` (space separated) in the **Dependent variables** edit field to define two dependent variables, u_1 and u_2.

4 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Axes/Grid Settings** dialog box.

2 In the **x limits** area, set **x min** to `-9` and **x max** to `9`.

3 Click **OK** to close the dialog box.

GEOMETRY MODELING

Click the **Line** button on the Draw menu and draw a line from –8 to 8.

PHYSICS MODELING

Periodic Boundary Conditions

1 On the **Physics** menu, point to **Periodic Conditions** and then click **Periodic Boundary Conditions**.

2 On the **Source** page, select Boundary 1 and type `u1` in the **Expression** column.

3 Press Enter. The constraint name **pconstr1** appears in the **Constraint name** column.

4 Click the **Destination** tab.

5 Select destination Boundary 2 and enter destination expression `u1`.

6 Click the **Source Vertices** tab.

7 Select Vertex 1, then click the **>>** button.

8 Click the **Destination Vertices** tab.

9 Select Vertex 2, then click the **>>** button.

10 Click the **Source** tab.

11 Select Boundary 1 and type u2 in the **Expression** column.

12 Press Enter. The constraint name **pconstr2** appears in the **Constraint name** column.

13 Click the **Destination** tab.

14 Select destination Boundary 2 and enter destination expression u2.

15 Click the **Source Vertices** tab.

16 Select Vertex 1 and click the **>>** button.

17 Click the **Destination Vertices** tab.

18 Select Vertex 2 and click the **>>** button.

19 Click **OK**.

Boundary Mode

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

2 Select both boundaries and click the **Neumann boundary condition** button. The default Dirichlet boundary condition would override the periodic boundary conditions.

SETTINGS	BOUNDARIES 1, 2
Type	Neumann
G(1)	0
G(2)	0

3 Click **OK**.

Subdomain Mode

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

2 Select Subdomain 1, then enter the following PDE coefficients:

PROPERTY	VALUE
Γ(1)	u2
Γ(2)	u1x
F(1)	6*u1*u1x
F(2)	u2
d_a(11)	1
d_a(12)	0

PROPERTY	VALUE
$d_a(21)$	0
$d_a(22)$	0

3 Click the **Init** tab.

4 Enter initial conditions.

PROPERTY	VALUE
$u1(t_0)$	`-6*sech(x)^2`
$u2(t_0)$	`-24*sech(x)^2*tanh(x)^2` `+12*sech(x)^2*(1-tanh(x)^2)`

5 Click **OK**.

MESH GENERATION

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

2 Type `0.1` in the **Maximum element size** edit field.

3 Click **OK**.

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

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box.

2 Type `range(0,0.025,2)` in the **Times** edit field. This provides 81 equally spaced time intervals from 0 to 2 seconds.

3 Click the **Time Stepping** tab.

4 Type `2` in the **Maximum BDF order** edit field in the **Advanced** area. This is to ensure stability in the time-stepping algorithm.

5 Click **OK** and then click the **Solve** button.

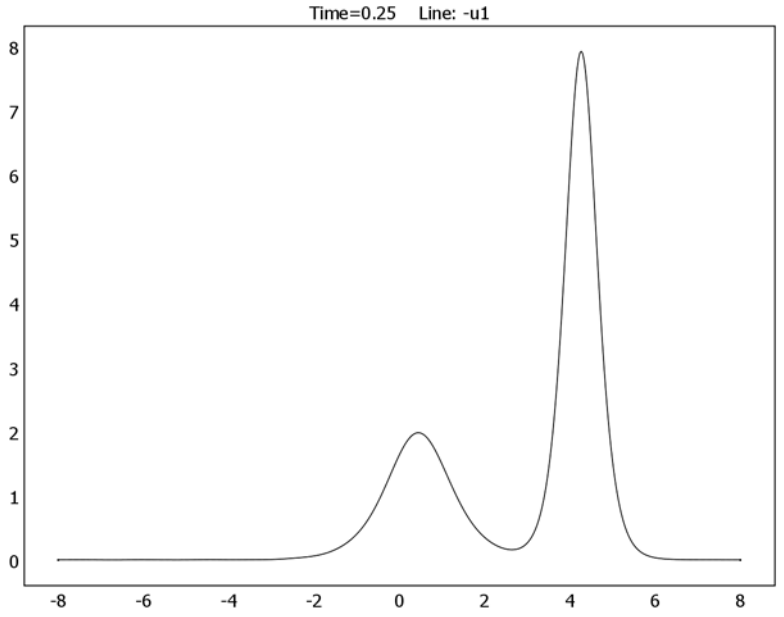


Figure 5-12: The solution to the KdV equation at 0.25 s (plot shows $-u_1$).

POSTPROCESSING AND VISUALIZATION

By default, the software plots the solution at the last time point. The model computes the negated solution, which is positive. The best way to visualize it is to extrude the result along time to create a time-series plot.

1 Open the **Domain Plot Parameters** dialog box.

2 Make sure all time steps are selected in the **Solutions to use** list on the **General** page.

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

4 Click the **Extrusion plot** button.

5 Select Subdomain 1 in **Subdomain selection** list.

6 Type the quantity `-u1` in the **Expression** edit field in the **y-axis data** area.

7 Click **OK**. In the plot window that appears, click the **Go to XY View** button.

Shallow Water Equations

The shallow water equations are frequently used for modeling both oceanographic and atmospheric fluid flow. Models of such systems lead to the prediction of areas eventually affected by pollution, coastal erosion, and polar ice-cap melting.

Comprehensive modeling of such phenomena using physical descriptions such as the Navier-Stokes equations can often be problematic, due to the scale of the modeling domains as well as through resolving free surfaces. The shallow water equations, of which there are a number of representations, provide an easier description of such phenomena.

This 1D model investigates the settling of a wave over a variable bed as a function of time. The initial wave and the shape of the bed are represented by mathematical relations so that it is easy to change parameters such as the wave amplitude or the bed's shape.

Introduction

This example uses the *Saint-Venant's* shallow water equations, which are the following:

$$\frac{\partial z}{\partial t} + \nabla \cdot (zv) = 0$$

and

$$\frac{\partial (zv)}{\partial t} + \nabla \cdot (zvv^T) + gz\nabla z_s - \nu\Delta(zv) = 0$$

where z is the thickness of the water layer (m), v is the velocity (m/s), g is the gravity constant (m/s^2), and ν is the kinematic viscosity (m^2/s). The definition of the

thickness of the water layer, z, is $z_s - z_f$, where z_s and z_f are the measures in Figure 5-13 below. For further details, see Ref. 1.

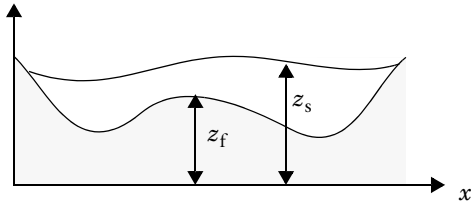


Figure 5-13: Representative vertical section through the fluid domain showing the bed of a lake and the water surface.

Artificial Stabilization

With time, the flow develops discontinuities known as hydraulic jumps. Use artificial stabilization to replace the jumps by steep fronts that can be resolved on the grid. Small amplitude waves on still water of depth z move with velocity $\sqrt{gz}$. The maximal propagation velocity is $v_{\mathrm{phase}} = |v| + \sqrt{gz}$ for water waves.

Stabilize the solution by adding artificial viscosity chosen to make the cell Reynolds number of order unity. To do so, add the term $\mathrm{tune} v_{\mathrm{phase}} h \partial(vz)/\partial x$ to the physical viscous momentum flux $\nu \partial(vz)/\partial x$. Here tune is a O(1) tuning parameter and h is the local element size. You add the contribution to the divergence term of the conservation law so that it does not affect the shock speeds. The modification is first order in element size.

Model Definition

This model studies a simple example of shallow water in a channel with bottom topography shown in Figure 5-14. Notice the difference in scale between the x and y directions.

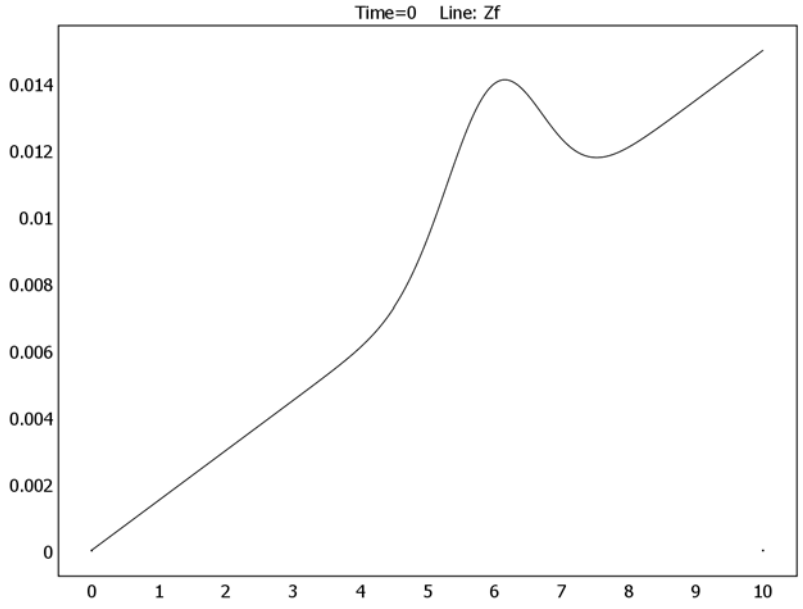


Figure 5-14: Sea bed profile, z_f, used in the model.

Dirichlet boundary conditions ($v = 0$) are implemented at both ends, while the physics are described by the equations above. The initial condition is a wave profile, which the following expression defines:

$$z_0 = 2 \cdot 10^{-2} - z_f + 5 \cdot 10^{-3} e^{\frac{-(x-3)^2}{1^2}}$$

where z_f is the analytical expression for the sea bed profile (see Figure 5-14). The elevation of the water surface is $z + z_f$, while Figure 5-15 shows $z_0 + z_f$.

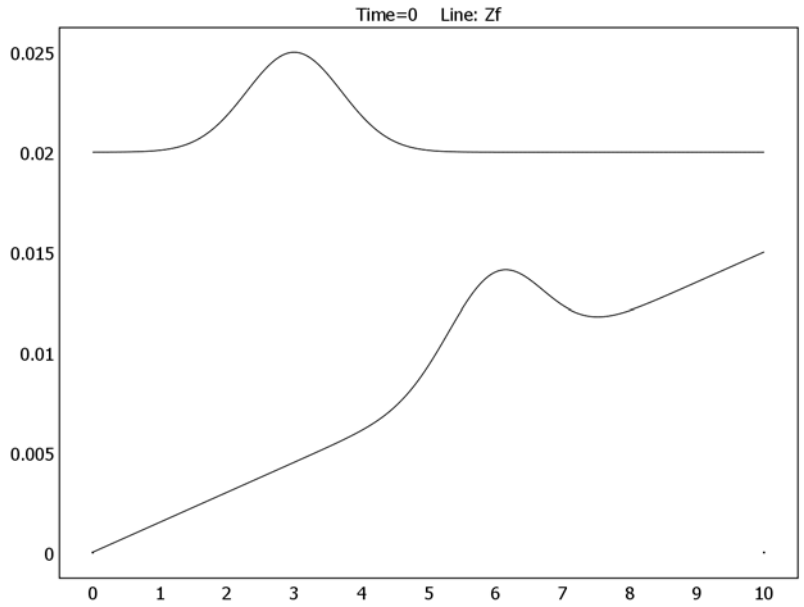


Figure 5-15: The initial water surface profile, $z_0 + z_f$, and the sea bed profile, z_f.

Results and Discussion

The simulation runs for 60 seconds. Figure 5-16 shows the water surface and slope of the sea bed at six output times toward the beginning of the simulation.

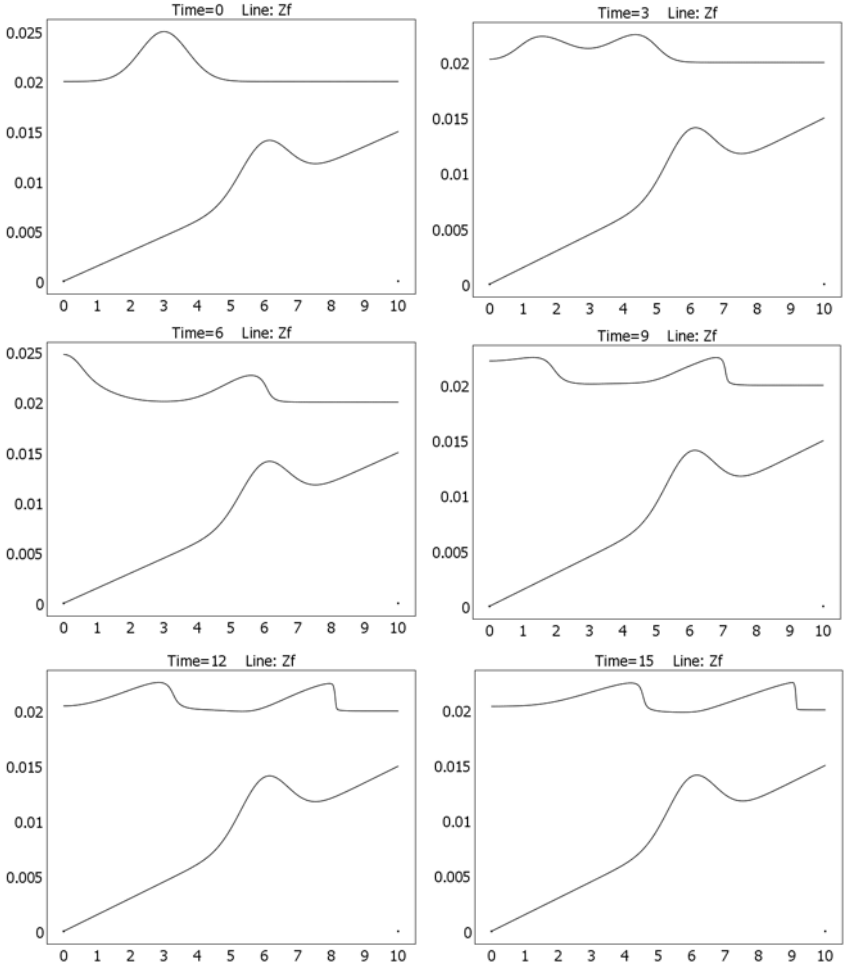


Figure 5-16: The water level and the slope of the sea bed at six output times. Time spans from t = 0 to t = 15 at steps of 3 seconds.

The simulation clearly shows the influence of the topography of the sea bed on the elevation of the water surface. Another interesting visualization of the results is an animation, which is easy to create using COMSOL Multiphysics.

Modeling in COMSOL Multiphysics

The modeling procedure is straightforward using the PDE, General Form application mode with two dependent variables: `Z` and `ZV`. It is easy to define expressions, such as the one that describes the initial wave profile, z_0, in the appropriate dialog box.

Reference

1. O. Pironneau, *Finite Element Methods for Fluids*, John Wiley & Sons, 1989.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/shallow_water`

Modeling Using the Graphical User Interface

1 Double-click the **COMSOL Multiphysics** icon to open the **Model Navigator**.

2 Select **1D** from the **Space dimension** list.

3 Select **COMSOL Multiphysics>PDE Modes>PDE, General Form>Time-dependent analysis**.

4 Type `Z ZV` in the **Dependent variables** edit field.

5 Click **OK**.

OPTIONS AND SETTINGS

1 Select **Constants** in the **Options** menu.

2 Enter the following constants:

NAME	EXPRESSION
nu1	1e-6
ge	9.8
x0	6
a	0.005
k1	0.0015
tune	0.1

3 Click **OK**.

4 Select **Expressions>Scalar Expressions** in the **Options** menu.

5 Enter the following scalar expressions:

NAME	EXPRESSION
Zf	a*exp(-(x-x0)^2)+k1*x
dZfdx	(-2*x+2*x0)*a*exp(-(x-x0)^2)+k1
Zs	Z+Zf
Z0	0.02-Zf+0.005*exp(-(x-3)^2/1^2)
vphase	abs(ZV/Z)+sqrt(ge*Z)
nu	nu1+vphase*h*tune

6 Click **OK**.

GEOMETRY MODELING

1 Select **Specify Objects>Line** in the **Draw** menu.

2 Type `0 10` in the **x** edit field. This creates a line from 0 to 10 along the *x*-axis.

3 Click **OK**.

4 Click the **Zoom Extents** button in the main toolbar.

PHYSICS SETTINGS

Subdomain Settings

1 Select **Subdomain Settings** in the **Physics** menu.

2 Select Subdomain 1 in the **Subdomain selection** list.

3 Type `ZV` in the first edit field (first row) in the **Flux vector** area.

4 Type `ZV*ZV/Z-nu*ZVx` in the second edit field in the **Flux vector** area.

5 Click the **F** tab.

6 Type `0` in the first edit field in the **Source term** area.

7 Type `-ge*Z*(Zx+dZfdx)` in the second edit field in the **Source term** area.

8 Click the **Init** tab to set the initial conditions.

9 Type `Z0` in the **$Z(t_0)$** edit field. Type `0` in all other edit fields.

10 Click **OK**.

Boundary Settings

1 Select **Boundary Settings** from the **Physics** menu.

2 Select both Boundary 1 and Boundary 2 from the **Boundary selection** list.

3 Click the **R** tab.

4 Type `0` in the first edit field (first row).

5 Type `-ZV` in the second edit field.

6 Click **OK**.

MESH GENERATION

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

2 Type `0.05` in the **Maximum element size** edit field.

3 Click **Remesh** and **OK**.

COMPUTING THE SOLUTION

1 Select **Solver Parameters** in the **Solve** menu.

2 In the **Time stepping** area, type `range(0,60)` in the **Times** edit field.

3 Type `1e-5` in the **Relative tolerance** edit field.

4 Type `1e-7` in the **Absolute tolerance** edit field.

5 Click **OK**.

6 Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

The most interesting part of the results is obtained by looking at the scalar expression `Zs`, corresponding to the surface topography, at different times compared to the topography of the bottom.

1 Click the **Plot Parameters** button.

2 Click the **Line** tab.

3 Type `Zs` in the **Expression** edit field; then click **Apply**.

4 Click the **General** page.

5 Select **6** from the **Solution at time** list.

6 Select the **Keep current plot** check box.

7 Click the **Line** tab.

8 Type `Zf` in the **Expression** edit field.

9 Click **OK**.

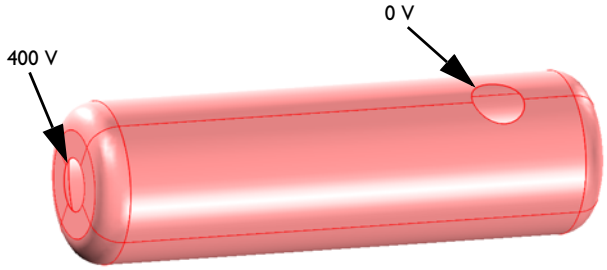
Shell Diffusion

Introduction

A goal for many applications is to predict physics in thin structures, such as shells, without modeling the thickness of the structure. This is because large aspect ratios can cause meshing and geometry analysis problems. The model reported here demonstrates how to use the *tangential derivative variables* in COMSOL Multiphysics to solve partial differential equations in curved 3D shells and 2D boundaries without modeling their thickness.

Model Definition

The steel tank shown below has two pipe connections. One is grounded and the other connects to a dead current source. This model calculates the current density in the tank shell along with the potential distribution across the surface.



EQUATIONS

The fundamental equation to solve is the current conduction, or charge conservation, equation.

$$\nabla \cdot (-\sigma \nabla V) = 0 \tag{5-7}$$

Here, σ is the electric conductivity (S/m) and V is the electric potential (V).

The material is a 1 mm thick steel sheet with a conductivity of $4.032 \cdot 10^6$ S/m. You are working with a surface in 3D so there is no thickness in the model. To account for the charge conservation in Equation 5-7 you must multiply the current flux expression with the shell thickness d:

$$\nabla \cdot (-\sigma d \nabla V) = 0 .$$

Figure 5-17 reveals the potential distribution across the surface.

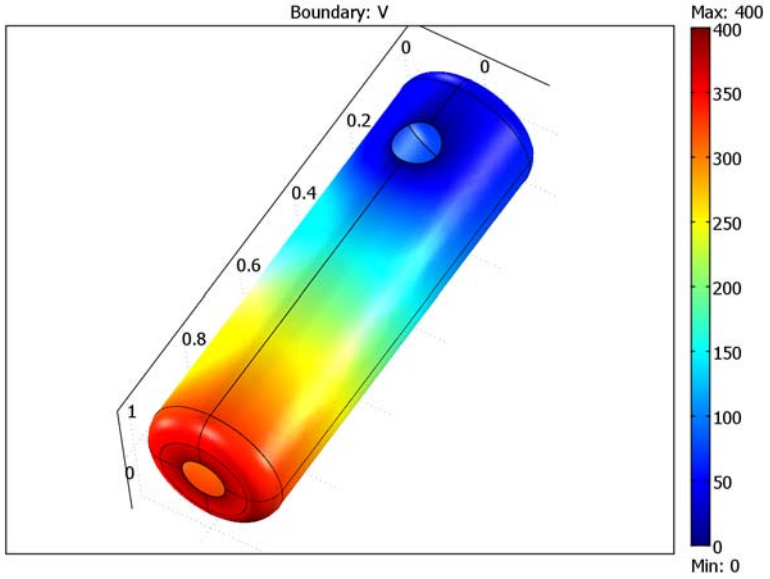


Figure 5-17: Electric potential distribution across the surface (V).

Figure 5-18 adds the current field as an arrow plot, showing clearly how the current collects toward the grounded connection.

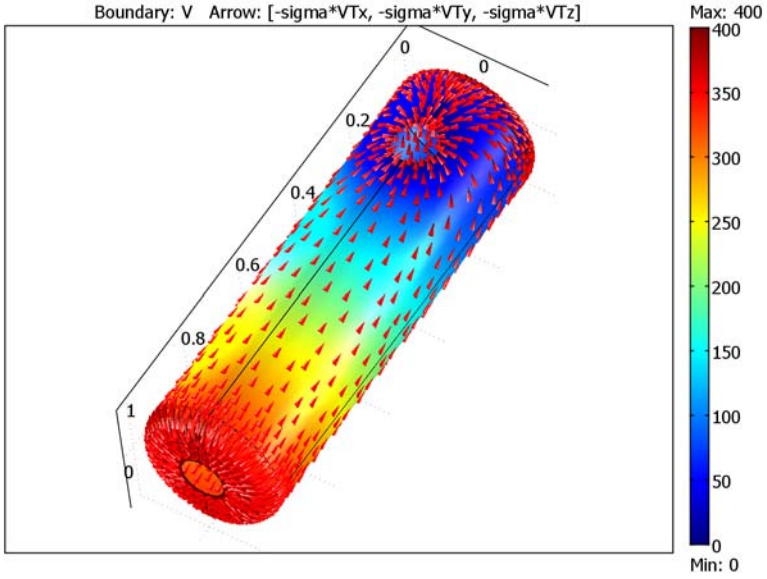


Figure 5-18: Arrow plot of the local current field.

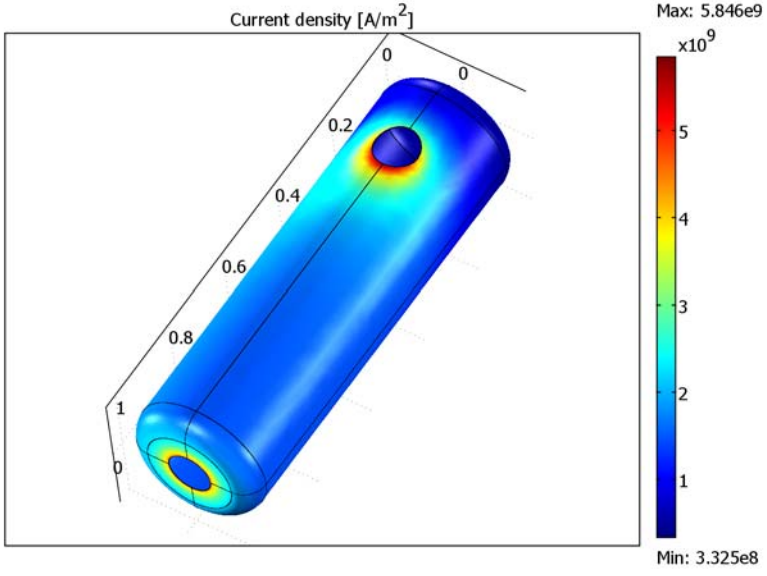


Figure 5-19: Local magnitude of the electric current density (A/m^2).

The plot of the magnitude of the local current density in Figure 5-19 is interesting because you can use it to calculate the resistive heating in the material as an extension to the model.

Modeling in COMSOL Multiphysics

The current conduction equation is modeled here using a Weak Form, Boundary application mode. For example, you can express Poisson's equation, $-\Delta u = F$, in 2D using the weak-term sequence `-ux_test*ux-uy_test*uy+u_test*F`. Tangential derivative variables come into play only in the shell, which you represent as a boundary. To call the tangential derivative variables in COMSOL Multiphysics, add a `T` suffix to the variable name. For example, the tangential derivative corresponding to `ux` is `uTx`. To fully appreciate the weak-level formulation, some knowledge of the weak form in the finite element method is recommended. Further information is available in the section "Theoretical Background" on page 360 in the *COMSOL Multiphysics Modeling Guide*.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/shell_diffusion`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics.
2. In the **Model Navigator**, select **3D** in the **Space dimension** list. In the list of application modes, select **COMSOL Multiphysics>PDE Modes>Weak Form, Boundary**.
3. Type `V` in the **Dependent variables** edit field, then click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, choose **Constants**.
2. Enter the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
sigma	4.032e6	Conductivity (S/m)
d	1e-3	Shell thickness (m)

GEOMETRY MODELING

Create the geometry by drawing the shell's profile of revolution and then subtracting a hole:

1. From the **Draw** menu, choose **Work-Plane Settings**.
2. Click the **Quick** tab and then click the **y-z** button. Click **OK**.
3. In the 2D drawing, double-click **SOLID** on the status bar to disable automatic coercion to solid objects.
4. Shift-click the **Line** button on the Draw toolbar and create an open polygon with corners in (0, 0), (0.15, 0), (0.15, 1), and (0.05, 1) by entering the corresponding x and y coordinates in the **Line** dialog box and then clicking **OK**.
5. Click the **Fillet/Chamfer** button on the Draw toolbar.
6. Open the **BI** folder and select Vertices 1 and 2 (the two corners in the polygon object). Make sure the **Fillet** button is selected and type `0.05` in the **Radius** edit field.
7. Click **OK** to create two fillets with radii of 0.05.
8. Select **Revolve** from the **Draw** menu and use the default settings.
9. Return to the 2D sketch and draw a centered circle centered at (0, 0.2) with a radius of 0.05.
10. Select **Extrude** from the **Draw** menu, type `0.2` in the **Distance** edit field, and click **OK**.
11. Press Ctrl+A to select both objects and then click the **Coerce to Face** button on the Draw toolbar.
12. Double-click on the geometry object with the right mouse button to open up the **Object Properties** dialog box. Select faces 16, 17, 19, 20, and 25–30 in the **Face selection** list and then click **Delete** to remove them. Click **OK**.

BOUNDARY CONDITIONS

1. From the **Physics** menu, choose **Boundary Settings**.
2. Press Ctrl+A to select all boundaries.
3. On the **Weak** page, type `sigma*d*(-VTx_test*VTx-VTy_test*VTy-VTz_test*VTz)` in the **weak** edit field. Click **OK**.

EDGE SETTINGS

1. From the **Physics** menu, choose **Edge Settings**.
2. Select Edges 14, 15, 25, and 29. Type `400-V` in the **constr** edit field.
3. Select Edges 40–43. Type `-V` in the **constr** edit field, then click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

Generate Figure 5-17 on page 154 with the following steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, clear the **Slice** check box and select the **Boundary** check box.
3. On the **Boundary** page, type `V` in the **Expression** edit field in the **Boundary data** area.
4. Click **Apply** to generate the plot.

   To generate Figure 5-18, add an arrow plot:

5. On the **Arrow** page, select the **Arrow plot** check box.
6. Select **Boundaries** from the **Plot arrows on** list. On the **Boundary Data** page, enter the x,- y-, and z-components `-sigma*VTx`, `-sigma*VTy`, and `-sigma*VTz`.
7. In the **Arrow parameters** area, select **Cone** from the **Arrow type** list and **Normalized** from the **Arrow length** list. Clear the **Auto** check box and set the **Scale factor** to **0.7**.
8. Click **Apply** to generate the plot.

   Finally, to generate Figure 5-19 execute the following instructions:

9. Clear the **Arrow plot** check box, then click the **Boundary** tab.
10. Change the **Expression** to `sigma*sqrt(VTx^2+VTy^2+VTz^2)`.
11. On the **General** page, click the **Title** button.
12. In the **Title** dialog box, click the right option button.
13. Enter the **Title** `Current density [A/m<SUP>2</SUP>]`, then click **OK**.
14. Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

Spherically Symmetric Transport

Introduction

Many models of industrial-transport problems allow the assumption that the problem is spherically symmetric. This assumption is of great importance because it eliminates two space coordinates and leaves a 1D problem that is computationally fast and has very small memory requirements. Some applications where spherical symmetry assumptions are useful include:

- Reaction and diffusion in catalytic pellets in chemical reactors
- Heat and mass transfer in the processing of upgraded iron-ore pellets
- Any other process that takes place in beads that are nearly spherical

For spherical symmetry to be valid, the following assumptions must apply:

- The computational domain has a spherical shape
- The outer-perimeter boundary condition does not change with the position on the surface, that is, it does not vary with the space angles θ and φ
- At any given time for a time-dependent problem, the material properties depend only on the radial distance from the center, r, and not on the space angles θ and φ
- For a time-dependent problem, the initial condition depends only on the radial distance from the center, r, and not on the space angles θ and φ

Model Definition

This following example simulates the initial transient heating process of a pelletized piece of magnetite ore. This is the first step in the process of making hematite ore pellets, an important raw material for the steel industry.

During the initial heating of a magnetite pellet the temperature is in a range that allows you to disregard any phase change of moisture. Thus it is possible to use a transient heat-conduction equation with constant properties in spherical symmetry. You can also scale the equation for easy parameterization of the radius.

Figure 5-20 depicts some pellets together with a push pin as a scale reference.

Figure 5-20: Hematite pellets after drying and oxidation (end product).

The figure shows that these pellets are indeed not perfectly spherical. Nonetheless, this model takes advantage of the assumption of spherical symmetry.

DOMAIN EQUATIONS

Starting with the time-dependent heat conduction equation

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (-k\nabla T) = Q$$

and expanding it in spherical polar coordinates, the result is the equation

$$\rho c_p \frac{\partial T}{\partial t} - k\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 T}{\partial\varphi^2}\right] = Q$$

where ρ is the density (kg/m^3), c_p gives the heat capacity (J/(kg·K)), k denotes the thermal conductivity (W/(m·K)), and Q is an internal heat source (W/m^3). Further, r, θ, and φ are the space coordinates.

Assuming a perfect sphere of radius R_p and no change in temperature with differing space angles, or $\partial T/\partial\theta = \partial T/\partial\varphi = 0$, gives

$$\rho c_p \frac{\partial T}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(-kr^2\frac{\partial T}{\partial r}\right) = Q\,.$$

To avoid division by zero at $r = 0$, which causes numerical problems, multiply this equation by r^2

$$r^2 \rho c_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial r}\left(-k r^2 \frac{\partial T}{\partial r}\right) = r^2 Q \,. \tag{5-8}$$

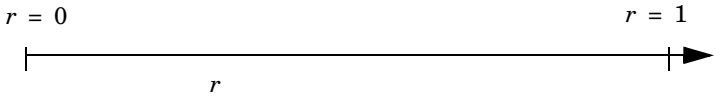
Using a dimensionless radial coordinate $\hat{r}$ by scaling the equation provides the option to quickly change the pellet's radius without changing or parameterizing the geometry size[4]. Introducing the dimensionless coordinate

$$\hat{r} = \frac{r}{R_p}, \quad \frac{\partial}{\partial r} = \frac{1}{R_p}\frac{\partial}{\partial \hat{r}}$$

and substituting in Equation 5-8 leads to

$$\hat{r}^2 \rho c_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial \hat{r}}\left(\frac{-k \hat{r}^2}{R_p^2}\frac{\partial T}{\partial \hat{r}}\right) = \hat{r}^2 Q \tag{5-9}$$

on the following domain:



In a similar manner, it is possible to derive equations similar to Equation 5-9 for porous media flow, diffusion-reaction problems, and so on.

The model uses the following material data:

SYMBOL	NAME	VALUE
ρ	Density	2000 kg/m^3
c_p	Heat capacity	300 J/(kg·K)
k	Conductivity	0.5 W/(m·K)
R_p	Pellet radius	0.005 m
Q	Heat source	0 W/m^3

4. Note that scaling the variables to get well-conditioned problems is not necessary in COMSOL Multiphysics because the solvers use automatic variable scaling.

BOUNDARY CONDITIONS AND INITIAL CONDITIONS

Because of symmetry about $r = 0$, there is zero flux through this point, meaning $\frac{\partial T}{\partial \hat{r}} = 0$.

At the surface, $\hat{r} = 1$, you use a convective heating expression with a heat transfer coefficient, h_s (W/(m^2·K), for the influx of heat (W/m^2):

$$q_{\text{in}} = h_s(T_{\text{ext}} - T) . \tag{5-10}$$

This expression describes a hot gas with a temperature T_{ext} flowing around the pellet. T_{ext} is chosen at 95 °C. The heat transfer coefficient is set to 1000 W/(m^2·K). The initial condition is set to 25 °C.

Results

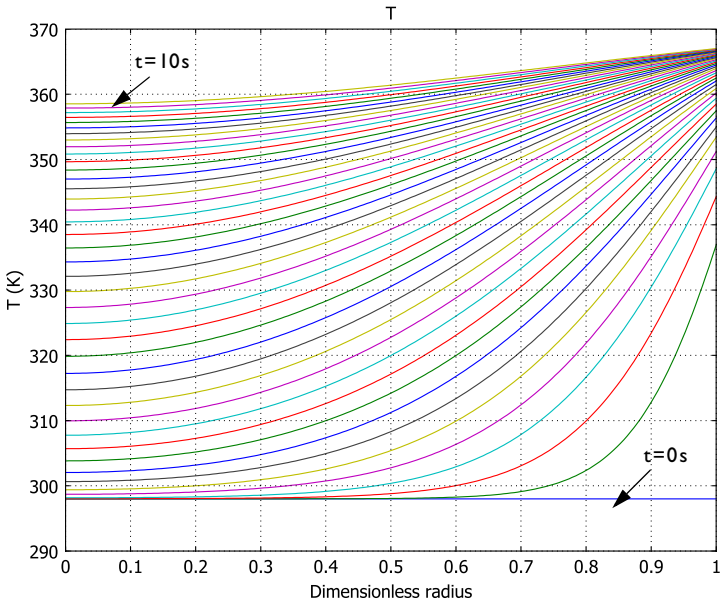


Figure 5-21: Temperature profiles from t = 0 to t = 10 s.

Figure 5-21 shows the temperature profiles from 0 to 10 seconds. Each line represents an increment of 0.5 s from the preceding line. From the topmost line it is clear that

the center of the pellet has not reached steady state at 10 s. You can also plot the time evolution of the temperature at the center of the pellet.

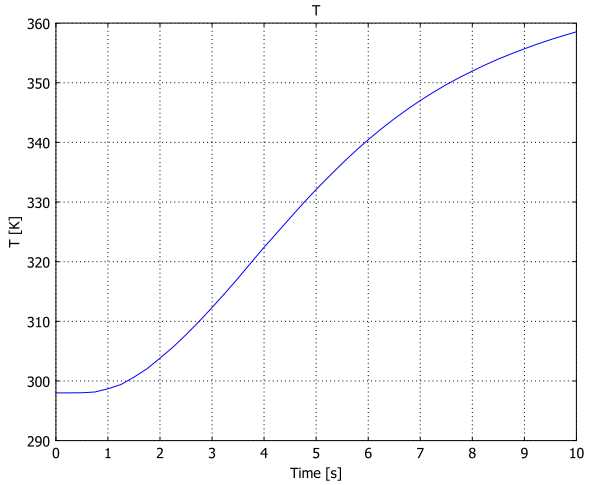


Figure 5-22: Time evolution of temperature in the center of a pellet with radius R_p = 5 mm

Figure 5-22 shows even more clearly how long the process must yet go before it reaches steady state. An interesting next step is to experiment with different particle radii, R_p, and different heating times.

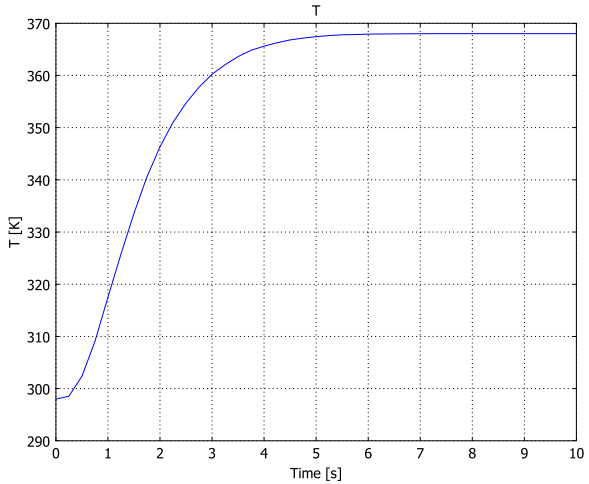


Figure 5-23: Time evolution in the center of a pellet with radius R_p = 2.5 mm.

Simply reducing the radius somewhat lets the model reach steady state within 7 s.

Modeling in COMSOL Multiphysics

To implement Equation 5-9 and the boundary conditions of this problem, use the 1D time-dependent version of the PDE, General Form application mode:

$$\begin{cases} e_a \dfrac{\partial^2 u}{\partial t^2} + d_a \dfrac{\partial u}{\partial t} + \nabla \cdot \Gamma = F & \text{in } \Omega \\ -\mathbf{n} \cdot \Gamma = G + \left(\dfrac{\partial R}{\partial u}\right)^T \mu & \text{on } \partial\Omega \\ 0 = R & \text{on } \partial\Omega \end{cases}$$

For more information about using this application mode, please refer to the section "The Scalar General Form Equation" on page 258 in the *COMSOL Multiphysics Modeling Guide*.

The space coordinate in the model is $\hat{r}$. For typographical reasons we use **rh** in this model for "*r*-hat." Identifying the general form with Equation 5-9, the following settings generate the correct equation:

COEFFICIENT	EXPRESSION
e_a	0
d_a	$\hat{r}^2 \rho c_p$
Γ (flux vector)	$\dfrac{-k\hat{r}^2}{R_p^2}\dfrac{\partial T}{\partial \hat{r}}$
F (source term)	0

You must take special care when setting the heat-influx boundary condition on the pellet surface. $h_s(T_{ext} - T) = k\partial T/\partial r$ on the surface, so you need to compensate G accordingly:

$$G = \frac{\hat{r}^2}{R_p} h_s (T_{ext} - T) .$$

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/spherical_symmetry_ore`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**. Click the **Multiphysics** button and click the **Add Geometry** button.

2 The **Add Geometry** dialog box appears. In the **Space dimension** list select **1D**, and in the **Independent variables** edit field enter `rh theta phi`. In the **Unit system** list select **None**. Click **OK**.

3 In the list of application modes, select **COMSOL Multiphysics>PDE Modes>PDE, General Form>Time-dependent analysis**. Do *not* click **OK** yet.

4 In the **Dependent variables** edit field type `T`.

5 In the **Application mode name** edit field type `ore_pellet`.

6 In the **Element** list verify that **Lagrange - Quadratic** is selected.

7 Click **Add**, then click **OK**.

OPTIONS AND SETTINGS

From the **Options** menu select **Constants**. Enter the following names, expressions, and (optionally) descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	2000	Density (kg/m^3)
cp	300	Heat capacity (J/(kg*K))
k	0.5	Conductivity (W/(m*K))
Rp	0.005	Pellet radius (m)
Qs	0	Heat source (W/m^3)
hs	1000	Heat transfer coefficient (W/(m^2*K))
Text	368	External temperature (K)
Tinit	298	Initial value (K)

GEOMETRY MODELING

1 Select the menu item **Draw>Specify Objects>Line**.

2 In the **rh** edit field enter `0 1`, then click **OK**.

3 Click the **Zoom Extents** button on the main toolbar.

PHYSICS SETTINGS

Subdomain Settings

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

2 Go to the **Subdomain selection** list and choose Subdomain 1. Enter the coefficients from the following table:

COEFFICIENT	VALUE/EXPRESSION
Γ	`-k*rh^2/Rp^2*Trh`
F	`rh^2*Qs`
e_a	0
d_a	`rh^2*rho*cp`

Note: Trh is COMSOL Multiphysics syntax for $\partial T/\partial(\mathrm{rh})$ if T and rh are defined variables.

3 Click the **Init** tab, and in the **T(t_0)** edit field enter `Tinit`.

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu choose **Boundary Settings**.

2 In the **Boundary Settings** dialog box enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 2
Boundary condition type	Neumann	Neumann
G	0	`rh^2/Rp*hs*(Text-T)`

Note: Clicking the **Neumann boundary condition** button disables the **R** edit field and sets it to 0. You can also manually type 0 in the **R** field to get a Neumann condition.

MESH GENERATION

1 Go to the **Mesh** menu and select **Free Mesh Parameters**.

2 Set the **Maximum element size scaling factor** to `0.4` and click **Remesh**.

3 Click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu choose **Solver Parameters**.

2 Find the **Times** edit field and enter the time steps as `range(0,0.25,10)`.

3 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

To create a line plot with all temperature profiles for the time steps in Figure 5-21 on page 162, follow these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters**.

2 On the **General** page, in the **Plot type** area click the **Line/Extrusion plot** option button.

3 Verify that all the entries in the **Solutions to use** list are selected (the default).

4 Go to the **Line/Extrusion** page, and select the **Line plot** button.

5 In the **y-axis data** area go to the **Predefined quantities** list and select **T**.

6 Click the **General** tab. Click the **Title/Axis** button and enter the **Title** `Temperature`, the **First axis label** `Dimensionless radius`, and the **Second axis label** `T (K)`. Click **OK**.

7 Click **OK** to close the **Domain Plot Parameters** dialog box and create the plot.

To create a line plot with time evolution of the temperature at the center as in Figure 5-22 on page 163, follow these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters**.

2 Go to the **General** page, then to the **Plot type** area, and then select the **Point plot** option button.

3 Verify that all the entries in the **Solutions to use** list are selected (the default).

4 Click the **Point** tab.

5 In the **y-axis data** area find the **Predefined quantities** list and select **T**.

6 In the **Boundary selection** list choose 1.

7 Click the **General** tab. Click the **Title/Axis** button and set all fields to **Auto**.

8 Click **OK**, then **OK** again.

Finally, if you want to make an animation, execute the following instructions:

1 Click the **Plot Parameters** button on the Main toolbar (or press F12).

2 On the **Animate** page click the **Start Animation** button to launch the **COMSOL Movie Player** window, then click **OK** to close the **Plot Parameters** dialog box.

The Telegraph Equation

Introduction

This model examines how telegraph wire transmits a pulse of voltage using the *telegraph equation*. The telegraph equation models mixtures between diffusion and wave propagation by introducing a term that accounts for effects of finite velocity to a standard heat or mass transport equation.

This example models a small section of a telegraph wire and contains a study of the pulse of voltage moving along it. A parametric analysis provides results showing the shape of the pulse with varying damping coefficients.

Model Definition

The model is simple to define. The geometry is a one-dimensional line of length 1. To model the pulse, the initial condition is a bell-shaped voltage distribution. The boundary conditions define the flux at both ends of the wire section, which allows the voltage to vary freely.

DOMAIN EQUATIONS

The telegraph equation is the following:

$$u_{tt} + (\alpha + \beta)u_t + \alpha\beta u = c^2 u_{xx}$$

where:

- α and β are positive constants.
- c is the transport velocity.
- u is the voltage (the dependent variable).

The model begins with the values $\alpha = \beta = 0.25$ and $c = 1$.

BOUNDARY CONDITIONS

The boundary conditions at both ends are homogeneous Neumann conditions:

$$u_x(t, 0) = 0$$
$$u_x(t, 1) = 0$$

INITIAL CONDITION

The following equations for the initial condition describe a bell-shaped pulse with the highest point at 0.2 and a base width of 0.4:

$$u(0,x) = e^{-3\left(\frac{x}{0.2}-1\right)^2}$$
$$u_t(0,x) = 0$$

Results

The figure below shows the results of the first simulation. It is clear that the pulse gets smoother as it propagates along the wire section. Figure 5-24 shows the shape of the pulse at $t = 0$, 0.5, and 1:

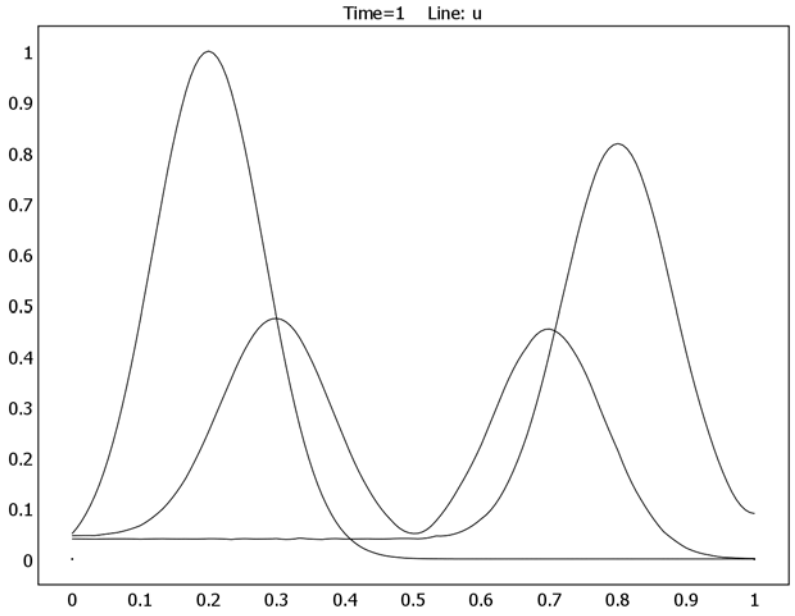


Figure 5-24: Shape of the pulse at t = 0, 0.5, and 1: $\alpha + \beta = 0.5$.

Small values of the term $\alpha\beta$ result in a smoother pulse compared to larger values, while the term $\alpha + \beta$ sets the amount of damping. The following plots shows the influence

of the term $\alpha+\beta$ on the damping. A value of $\alpha+\beta = 1$ yields the pulse in Figure 5-25 at $t = 0$, 0.5, and 1:

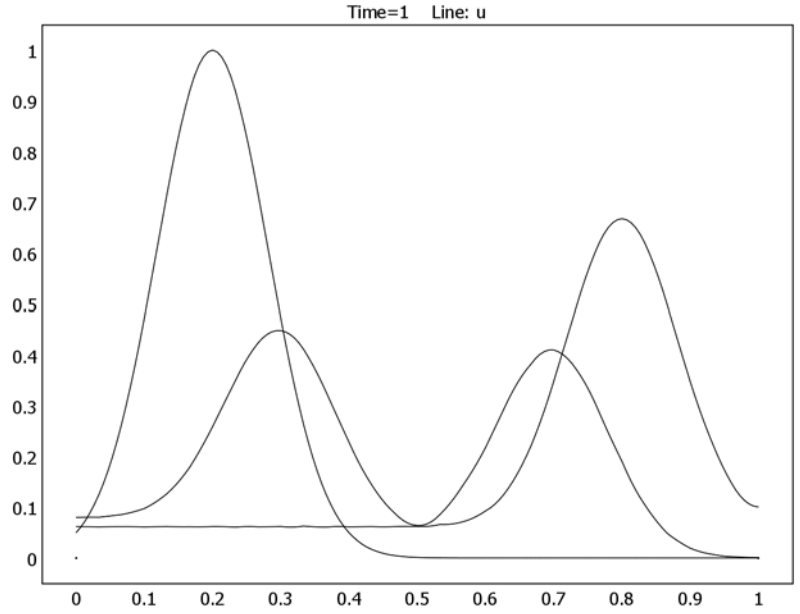


Figure 5-25: Shape of the pulse at t = 0, 0.5, and 1: $\alpha + \beta = 1$.

In the figure above the height of the pulse decreases only slightly from the initial value. In Figure 5-26, the decrease in height is more pronounced owing to a damping term that is four times as large as the one used for Figure 5-25.

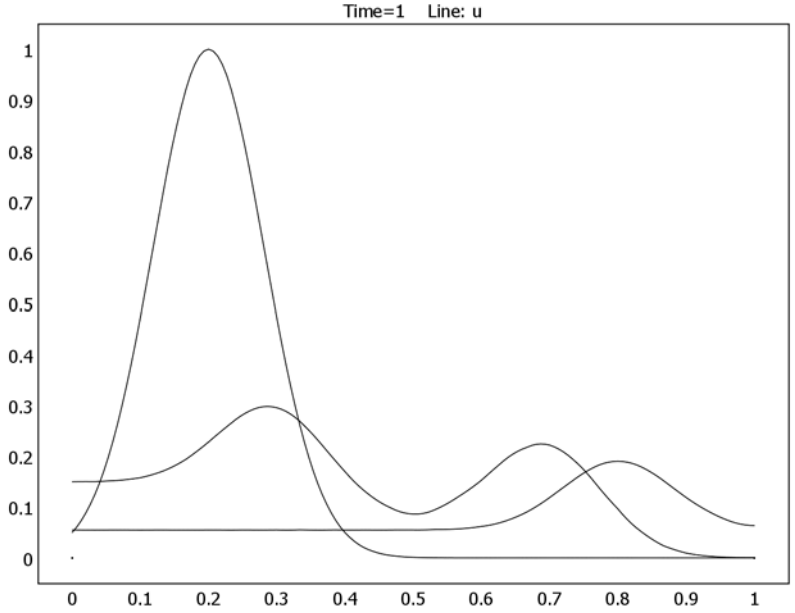


Figure 5-26: Shape of the pulse at t = 0, 0.5, and 1: $\alpha + \beta = 2$.

Applying the telegraph equation to 2D and 3D models follows the same protocol shown here but produces a more complex systems of equations.

Modeling in COMSOL Multiphysics

To set up the telegraph equation, use a Coefficient Form PDE application mode for time-dependent analysis.

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/telegraph_equation`

MODEL NAVIGATOR

1 Select **1D** in the **Space dimension** list.

2 In the list of application modes, browse to **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form**.

3 Select **Time-dependent analysis, wave type**. Make sure that **Lagrange - Quadratic** elements is selected in the **Element** list.

4 Click **OK**.

OPTIONS AND SETTINGS

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

2 Enter the following constants in the **Constants** dialog box:

NAME	EXPRESSION
c	1
alpha	0.25
beta	0.25

3 Click **OK**.

GEOMETRY MODELING

1 Click the **Line** button and draw a line of length 1 from 0 to 1 on the x-axis.

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

PHYSICS SETTINGS

Boundary Conditions

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

2 Select Boundaries 1 and 2. From the **Boundary condition** list select **Neumann**.

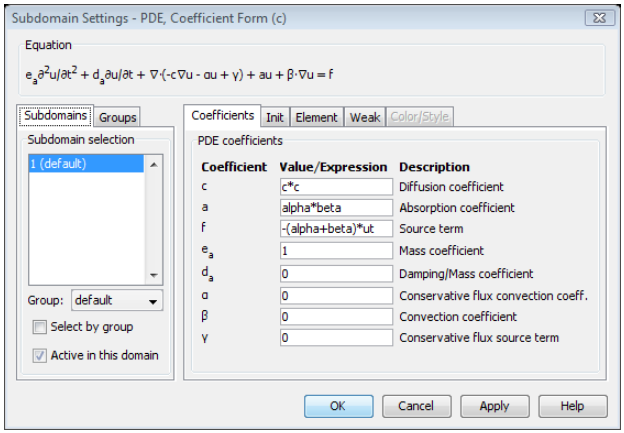
3 Click **OK**.

Subdomain Settings

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

2 On the **Coefficients** page in the **Subdomain Settings** dialog box, enter these PDE coefficients (the e_a and d_a coefficients are the default values):

PROPERTY	SUBDOMAIN 1
c	`c*c`
a	`alpha*beta`
f	`-(alpha+beta)*ut`
d_a	0
e_a	1



3 Click the **Init** tab and enter the following initial conditions:

PROPERTY	SUBDOMAIN 1
$u(t_0)$	`exp(-3*(x/0.2-1)^2)`
$ut(t_0)$	0

4 Click **OK**.

MESH GENERATION

Initialize the mesh and refine it once.

COMPUTING THE SOLUTION

1 From the **Solve** menu, choose **Solver Parameters**.

2 Click the **Time Stepping** tab.

3 Select the **Manual tuning of step size** check box. Type `0.002` in the **Maximum time step** edit field. To get a good solution to the telegraph equation with this mesh, a time step of around 0.002 is sufficient. It means that the solver takes about 500 steps.

4 Click **OK**.

5 Click the **Solve** button on the Main toolbar to run the analysis.

POSTPROCESSING AND VISUALIZATION

1 From the **Postprocessing** menu, choose **Plot Parameters**.

2 Select the **Keep current plot** check box and plot the solution at time 0, 0.5, and 1.

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

4 In the **Constants** dialog box, change `alpha` and `beta` to `0.5`.

5 Click **OK**.

6 Click the **Solve** button.

Continue to investigate the effect of the α and β coefficients by changing their values.

A Transport Problem

Introduction

This model features a pure stationary transport problems with a single convective term. It shows how to address oscillations and instabilities that arise from the numerical method. Here you stabilize a formulation with continuous Langrange elements by streamline diffusion and using a formulation with discontinuous elements with upwinding.

Model Definition

The following 1st-order equation models pure stationary transport in the direction of the constant vector β:

$$\begin{cases} \beta \cdot (\nabla u) = 0 & \Omega \\ u = u_0 & \Gamma \end{cases}$$

Here Γ is the inflow boundary, and the vector $\beta = (\beta_x, \beta_y)$ points into the domain Ω. The exact solution is constant on the characteristics

$$\begin{aligned} x &= x_0 + t\beta_x \\ y &= y_0 + t\beta_y \end{aligned}$$

where t is a real number. Thus, if a characteristic intersects Γ at the point (x, y), then the value of u is $u_0(x, y)$ along the entire characteristic.

In this example, the domain Ω is the unit square and $\beta = (1, 1)$. Thus Γ corresponds to the left and lower edges of the square. Use the expression $u_0 = y > x$ to define the boundary conditions $u = 1$ on the left boundary and $u = 0$ on the lower boundary. The exact solution then equals

$$u(x, y) = \begin{cases} 1 & y > x \\ 0 & y < x \end{cases}$$

Streamline Diffusion

Streamline diffusion stabilizes oscillations and instabilities that arise from the numerical method. Streamline diffusion is an example of a *Petrov-Galerkin* method where the test-function space differs from the solution space. The modified test functions give rise to additional terms in the weak formulation of the problem. The streamline-diffusion contribution to the transport equation is

$$-\frac{h}{\sqrt{2}}(\beta_x \hat{u}_x + \beta_y \hat{u}_y)(\beta_x u_x + \beta_y u_y)$$

where the "hat" symbol denotes the corresponding test functions.

The Convection and Diffusion, Convection and Conduction, and Incompressible Navier-Stokes application modes have built-in artificial diffusion of several types, including streamline diffusion. This model explicitly adds the streamline-diffusion contributions.

The section "Stabilization Techniques" on page 481 in the *COMSOL Multiphysics Modeling Guide* describes general techniques for introducing contributions from artificial diffusion.

Upwinding Using Discontinuous Basis Functions

When you use continuous basis functions, the usual Galerkin method must be numerically stabilized, for example using streamline diffusion. Another approach is to use ***discontinuous basis functions*** (also know as the ***discontinuous Galerkin method***).

The term $\beta \cdot (\nabla u)$ must be treated carefully because if u is discontinuous over an element boundary, this term is a δ-function on the boundary. Assume the vector field β is continuous within an element and has a continuous normal component across element boundaries (this is certainly true for the constant β used here). Define the *upstream* and *downstream* sides of an element boundary such that β points in the downstream direction, and define the normal vector n to be pointing in the opposite direction, from the *downside* to the *upside*. Also let the superscripts ^{u} and ^{d} indicate evaluation on the respective sides of a boundary.

It is then possible to assemble the contribution from the discontinuities as $\hat{u}^d(\beta \cdot n)(u^d - u^u)$ (note that if β happens to be parallel to the boundary, "up" and "down" are undefined, but this is no problem because the factor $\beta \cdot n$ is then zero anyway). Using the test function on the downwind side gives sufficient stabilization

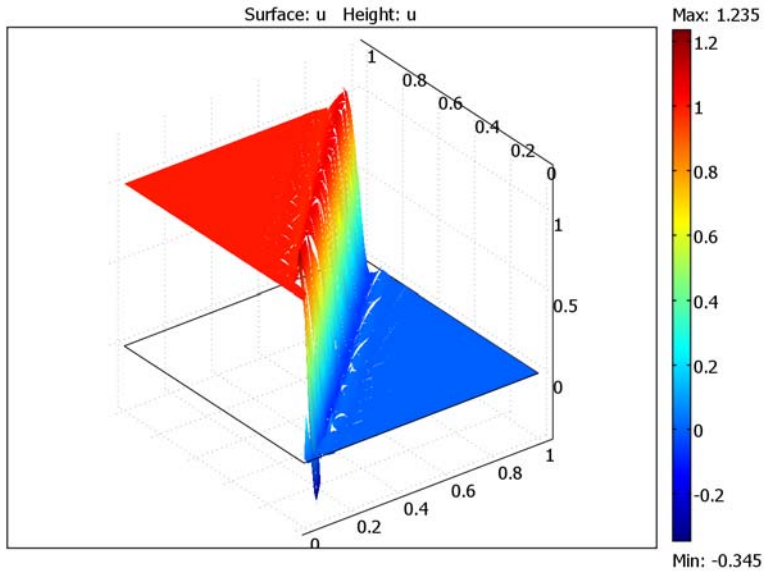
since it means that information is always taken from the upwind side and transported downwind (*upwinding stabilization*).

When using discontinuous elements, it does not make sense to impose a boundary condition on u by constraints because the value of u is not well defined on an element boundary. Instead use the same transport term, where you can imagine an element upstream of Γ with a value u_0. Thus assemble a contribution $\hat{u}^d(\beta \cdot n)(u^d - u_0)$ at element boundaries belonging to the inflow boundary Γ.

Note: This upwinding method is not suited for problems with diffusion terms.

Results

The PDE is stationary but has a discontinuity in the solution. The model shows how you can prevent instabilities from propagating into areas where the solution should be constant by using streamline diffusion or upwinding.



The plot shows the discontinuities between elements stabilized with upwinding.

Modeling in COMSOL Multiphysics

When setting up this model, think of the equation as a special case ($c = 0$) of a general convection-diffusion equation:

$$-\nabla \cdot (c\nabla u) + \beta \cdot \nabla u = f \quad \text{in } \Omega$$

Using the Convection-Diffusion application mode, this transport problem is easy to set up and solve. A second step adds explicit streamline diffusion.

Further steps change the model to use discontinuous elements and upwinding. In COMSOL Multiphysics all boundaries have an "up" and "down" side defined independent of the β direction. However, you can use the expression

```
(bx*dnx+by*dny<0)*(bx*dnx+by*dny)*test(down(u))*(down(u)-up(u))+
(bx*unx+by*uny<0)*(bx*unx+by*uny)*test(up(u))*(up(u)-down(u))
```

for the interior mesh boundaries using an *ultraweak term*, and use the expression

```
(bx*dnx+by*dny<0)*(bx*dnx+by*dny)*test(down(u))*(down(u)-u0)+
(bx*unx+by*uny<0)*(bx*unx+by*uny)*test(up(u))*(up(u)-u0)
```

for the inflow boundaries, which are independent of the definitions of "up" and "down."

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/transport_problem`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Open the Model Navigator, and select **2D** from the **Space dimension** list.
2. In the list of application modes select **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form**.
3. Make sure that **Lagrange - Quadratic** elements are selected in the **Element** list.
4. Click **OK**.

GEOMETRY MODELING

1 On the **Draw** menu point to **Specify Objects**, select **Square**, then click **OK**.

   Because you do not change any settings in the **Square** dialog box, you create the default square with its corner at (0, 0) and with a side length of 1.

2 Press the **Zoom Extent** button on the Main toolbar.

OPTIONS AND SETTINGS

Constants and Expressions

1 From the **Options** menu select **Expressions>Global Expressions**.

2 Enter the following names and expressions; when done, click **OK**.

NAME	EXPRESSION
bx	1
by	1
u0	y>x

PHYSICS SETTINGS

Boundary Conditions

1 From the **Physics** menu choose **Boundary Settings**.

2 Enter the following settings in the **Boundary Settings** dialog box; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 2	BOUNDARIES 3, 4
Type	Dirichlet	Neumann
r	u0	-

Subdomain Settings

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

2 Select Subdomain 1.

3 Change these PDE coefficients in the **Subdomain Settings** dialog box:

PROPERTY	SUBDOMAIN 1
c	0
f	0
d_a	0
β	bx by

4 Click the **Weak** tab.

5 Type `-h*(bx*ux_test+bx*uy_test)/sqrt(2)*(bx*ux+bx*uy)` in the **weak** edit field.

6 Click **OK**.

To add streamline diffusion automatically, instead use the Convection and Diffusion application mode. When in that mode open the **Subdomain Settings** dialog box, click the **Artificial Diffusion** button and select the **Streamline diffusion** check box to add stabilization by streamline diffusion.

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

Click the **3D Surface Plot** button on the Plot toolbar to visualize the solution.

Investigate the effect of streamline diffusion stabilization by turning it off and then setting the weak contribution to `0`. You can increase the accuracy by refining the mesh.

Continue with the same model using discontinuous elements and upwinding instead of Lagrange elements and streamline diffusions.

PHYSICS SETTINGS

Boundary Conditions

1 From the **Physics** menu choose **Boundary Settings**.

2 Select all the boundaries and click the **Neumann boundary conditions** button.

3 Click the **Weak** tab.

4 Enter the following settings in the **Boundary Settings** dialog box; when done, click **OK**.

TERM	ALL
weak	`(bx*dnx+by*dny<0)*(bx*dnx+by*dny)*test(down(u))*(down(u)-u0)+ (bx*unx+by*uny<0)*(bx*unx+by*uny)*test(up(u))*(up(u)-u0)`
dweak	0
constr	0

Subdomain Settings

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

2 Select Subdomain 1, click the **Weak** tab, and enter these terms:

TERM	ALL
weak	0
dweak	0
constr	0
bnd.weak	`(bx*dnx+by*dny<0)*(bx*dnx+by*dny)*test(down(u))*(down(u)-up(u))+ (bx*unx+by*uny<0)*(bx*unx+by*uny)*test(up(u))*(up(u)-down(u))`

3 Click the **Element** tab.

4 Type `shdisc(2,2,'u')` in the **shape** edit field. This is the syntax to specify a second-order 2D discontinuous element shape function with one dependent variable, u.

5 Click **OK**.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

1 From the **Postprocessing** menu choose **Plot Parameters**.

2 On the **Surface** page clear the **Smooth** check box.

3 Click **OK**.

Discontinuities between elements are clearly visible in the plot.

The Two-Term Boltzmann Equation[5]

Introduction

Fluid models of plasma dynamics require a full and consistent set of electron transport and rate coefficients. In the drift-diffusion approximation for the electron density, n, and the mean electron energy, $\bar{\varepsilon}$, the electron mobility, μ_e, electron diffusivity, D_e, and energy mobility, μ_ε, energy diffusivity, D_ε are required inputs, and are functions of background neutral particle number density, N, and mean electron energy. The rate coefficients, k_j, for the inelastic collisions occurring in a plasma are strong functions of the electron energy distribution function (EEDF). In general, the EEDF cannot be assumed to be Maxwellian; a better approximation is obtained by solving a two-term truncation of a spherical-harmonic expansion in velocity space of the Boltzmann equation (Ref. 1). The rate coefficients and transport properties are then computed as appropriate integrals over the EEDF. The inputs are the gas temperature, neutral particle number density, electric field, and a set of electron-impact cross sections. Each electron-impact cross section is a table of collision cross section versus energy.

Figure 5-27: Plasma discharge in an oxygen-filled glass sphere. Image courtesy of Technorama, Switzerland.

In this example, you solve the two-term Boltzmann equation for an oxygen plasma to obtain the EEDF. The electron-oxygen collisions occurring in an oxygen plasma are listed in Table 5-2 and the corresponding cross sections are plotted in Figure 5-28.

5. This model is courtesy of Daniel Smith of MKS Instruments, Wilmington, Mass., USA.

(The model neglects electron-electron collisions, although their inclusion would be relatively straightforward; for further details on this issue, see Ref. 1.)

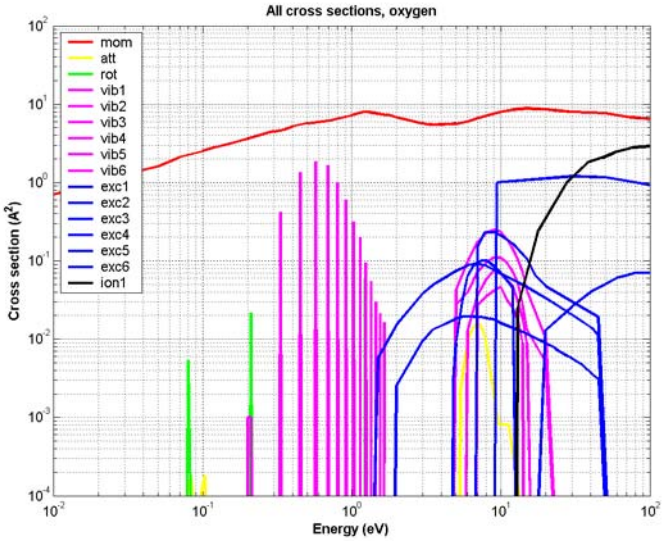


Figure 5-28: Electron-impact cross sections for molecular oxygen.

TABLE 5-2: ELECTRON-OXYGEN COLLISIONS IN AN OXYGEN PLASMA.

INDEX	LEGEND	REACTION	TYPE	$\Delta\varepsilon$ (eV)
1	mom	$O_2 + e \rightarrow O_2 + e$	Momentum	0
2	att	$O_2 + e \rightarrow O + O^-$	Attachment	0
3	rot	$O_2 + e \rightarrow O_2(rot) + e$	Excitation	0.02
4	vib1	$O_2 + e \rightarrow O_2(v=1) + e$	Excitation	0.19
5	vib2	$O_2 + e \rightarrow O_2(v=1) + e$	Excitation	0.19
6	vib3	$O_2 + e \rightarrow O_2(v=2) + e$	Excitation	0.38
7	vib4	$O_2 + e \rightarrow O_2(v=2) + e$	Excitation	0.38
8	vib5	$O_2 + e \rightarrow O_2(v=3) + e$	Excitation	0.75
9	vib6	$O_2 + e \rightarrow O_2(v=3) + e$	Excitation	0.75
10	exc1	$O_2 + e \rightarrow O_2(a^1\Delta) + e$	Excitation	0.977
11	exc2	$O_2 + e \rightarrow O_2(b^1\Sigma) + e$	Excitation	1.627
12	exc3	$O_2 + e \rightarrow O + O + e$	Dissociation	4.5
13	exc4	$O_2 + e \rightarrow O + O + e$	Dissociation	6.0

TABLE 5-2: ELECTRON-OXYGEN COLLISIONS IN AN OXYGEN PLASMA.

INDEX	LEGEND	REACTION	TYPE	$\Delta\varepsilon$ (eV)
14	exc5	$O_2 + e \rightarrow O + O + e$	Dissociation	8.4
15	exc6	$O_2 + e \rightarrow O + O + e$	Dissociation	9.97
16	ion1	$O_2 + e \rightarrow O_2^+ + 2e$	Ionization	12.06

Model Definition

The assumption of a Maxwellian EEDF can lead to substantial errors in the rate coefficients. This is particularly true in electronegative gases with a low ionization threshold where attachment removes the low-energy electrons and strong ionization "chops off" the tail of the EEDF. The two-term Boltzmann equation accounts for these effects. Here, a truncation of the velocity-space spherical-harmonic expansion

$$f(\mathbf{v}) = f_0(v) + f_1(v)\cos\theta + \ldots, \quad \cos\theta \equiv \mathbf{v}\cdot\mathbf{E}/(vE)$$

inserted in the full Boltzmann equation results in a system of two PDEs: one for the isotropic part, f_0, and one for the first anisotropic perturbation, f_1, of the EEDF. These two first-order PDEs can be combined into a single second-order PDE for f_0:

$$\frac{\partial}{\partial\varepsilon}\left(\frac{\varepsilon}{3\sigma_m}\frac{\partial f_0}{\partial\varepsilon}\left(\frac{E}{N}\right)^2 + \sigma_\varepsilon\varepsilon^2\left(f_0 + \frac{k_B T}{e}\frac{\partial f_0}{\partial\varepsilon}\right)\right) = S, \qquad f_1 = \frac{E}{N}\frac{1}{\sigma_m}\frac{\partial f_0}{\partial\varepsilon}$$

$$\sigma_\varepsilon = \sum_{k\,\in\,\{\text{elastic}\}} 2\frac{m_e}{M}\sigma_k \qquad S = \sum_{k\,\notin\,\{\text{elastic}\}} C_k \tag{5-11}$$

$$C_{k\,\in\,\{\text{attachment}\}} = -\varepsilon\sigma_k(\varepsilon)f_0(\varepsilon)$$

$$C_{k\,\in\,\{\text{exc., dissoc.}\}} = -[\varepsilon\sigma_k(\varepsilon)f_0(\varepsilon) - (\varepsilon + \Delta\varepsilon_k)\sigma_k(\varepsilon + \Delta\varepsilon_k)f_0(\varepsilon + \Delta\varepsilon_k)]$$

$$C_{k\,\in\,\{\text{ionization}\}} = -[\varepsilon\sigma_k(\varepsilon)f_0(\varepsilon) - 2(2\varepsilon + \Delta\varepsilon_k)\sigma_k(2\varepsilon + \Delta\varepsilon_k)f_0(2\varepsilon + \Delta\varepsilon_k)]$$

Here f_0 and f_1 are functions of $\varepsilon = m_e v^2/(2e)$, the electron energy in electronvolts; σ_m is the effective momentum-transfer cross section (m^2); m_e is the electron mass (kg); M is the mass of an oxygen molecule (kg); T is the neutral gas temperature (K); k_B is Boltzmann's constant, e is the elementary charge, E is the external electric field (V/m); N is the number density of molecular oxygen; and each σ_k (m^2) is a cross section corresponding to collision k. Notice that the source term, S, for the inelastic collisions is nonlocal in energy space. The interpretation of this is that electrons with energy above the activation threshold, $\Delta\varepsilon$, inelastically collide with neutral O_2 molecules, which results in the electrons being reinserted into the EEDF at a lower energy. In the case of ionization ($k = 16$), two equally energetic electrons are reinserted into the

EEDF (the two electrons having equal energy is a simplifying assumption whose validity is best for low energies; see Ref. 1). For attachment, electrons are simply removed from the EEDF. Further, f_0 is subject to the integral constraint

$$\lambda \equiv \int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon - 1 = 0 \tag{5-12}$$

and the boundary conditions

$$\begin{aligned} f_0 &= 0 \qquad \text{at } \varepsilon = \infty \\ \frac{\partial f_0}{\partial \varepsilon} &= 0 \qquad \text{at } \varepsilon = 0 \end{aligned} \tag{5-13}$$

Having solved for $f_0(\varepsilon)$, you compute the mobility and the diffusion coefficient as

$$\begin{aligned} \mu_e N(\bar{\varepsilon}) &= -\frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{\sigma_m}\frac{\partial f_0}{\partial \varepsilon} d\varepsilon \\ D_e N(\bar{\varepsilon}) &= \frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{\sigma_m} f_0 d\varepsilon \end{aligned} \tag{5-14}$$

where $\gamma \equiv (2e/m_e)^{1/2}$ and $\bar{\varepsilon}$ is the mean electron energy in electronvolts:

$$\bar{\varepsilon} = \int_0^\infty \varepsilon^{3/2} f_0(\varepsilon) d\varepsilon \tag{5-15}$$

In the energy equation, the energy mobility and the energy-diffusion coefficient are

$$\begin{aligned} \mu_\varepsilon N(\bar{\varepsilon}) &= -\frac{\gamma}{3\bar{\varepsilon}}\int_0^\infty \frac{\varepsilon^2}{\sigma_m}\frac{\partial f_0}{\partial \varepsilon} d\varepsilon \\ D_\varepsilon N(\bar{\varepsilon}) &= \frac{\gamma}{3\bar{\varepsilon}}\int_0^\infty \frac{\varepsilon^2}{\sigma_m} f_0 d\varepsilon \end{aligned} \tag{5-16}$$

The all-important rate coefficients are computed from the following integrals:

$$k_j = \gamma \int_0^\infty \sigma_j(\varepsilon)\varepsilon f_0(\varepsilon)d\varepsilon \qquad (5\text{-}17)$$

For comparative purposes, you can plot the computed rate coefficients against the ones calculated by assuming a Maxwellian EEDF

$$f_0 = \frac{2}{\sqrt{\pi}}\tau_e^{-3/2}\exp\left(-\frac{\varepsilon}{\tau_e}\right)$$

where the electron "temperature," τ_e (eV), is related to the mean electron energy by $\tau_e = 2\bar{\varepsilon}/3$.

Results and Discussion

Figure 5-29 compares the Maxwellian EEDF to the EEDF computed from the two-term Boltzmann equation. The strong ionization at high electron energies tends to "chop off" the high energy tail in the EEDF. In the case of oxygen, attachment is also strong and it tends to "mop up" the low-energy electrons.

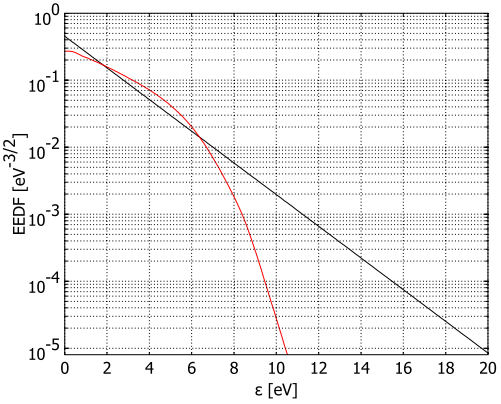


Figure 5-29: EEDF for an oxygen plasma calculated using the Maxwellian approximation (black) and the two-term Boltzmann equation (red).

Figure 5-30 similarly compares the ionization rate coefficient, k_{16}, calculated with the EEDF from the two-term Boltzmann approximation with the corresponding Maxwellian result. As the figure shows, the Maxwellian EEDF overpredicts the rate coefficient for ionization—at a mean electron energy of 2 eV by nearly 10 orders of magnitude.

Furthermore, the calculated rate coefficients for all 16 electron-impact reactions are plotted in Figure 5-31, and Figure 5-32 displays the corresponding transport properties ($\mu_e N$, $D_e N$, $\mu_\varepsilon N$, and $D_\varepsilon N$) as functions of $\bar{\varepsilon}$.

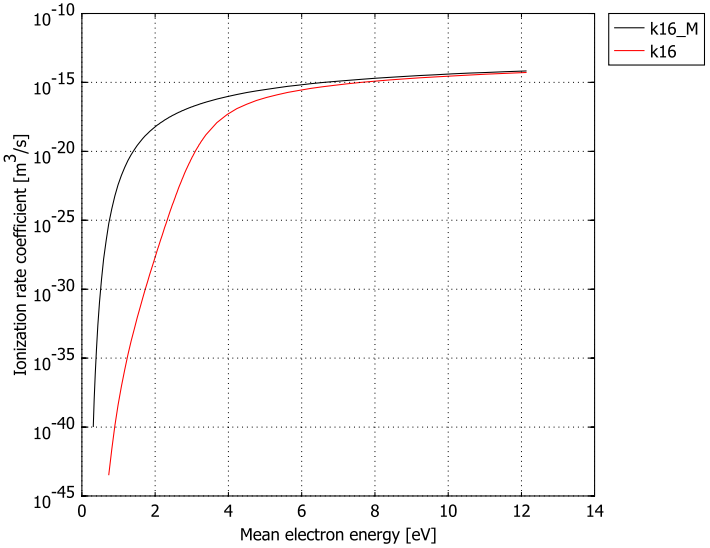


Figure 5-30: Ionization rate coefficient calculated for Maxwellian (black) and non-Maxwellian (red) EEDF.

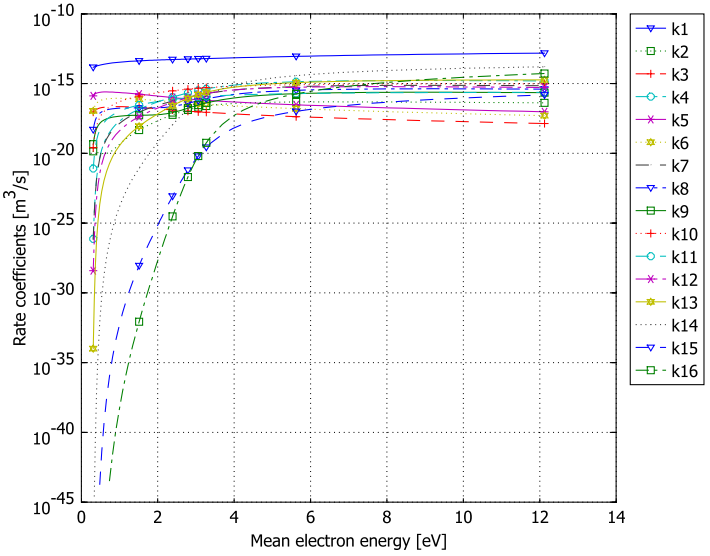


Figure 5-31: Rate coefficients calculated using the two-term Boltzmann equation.

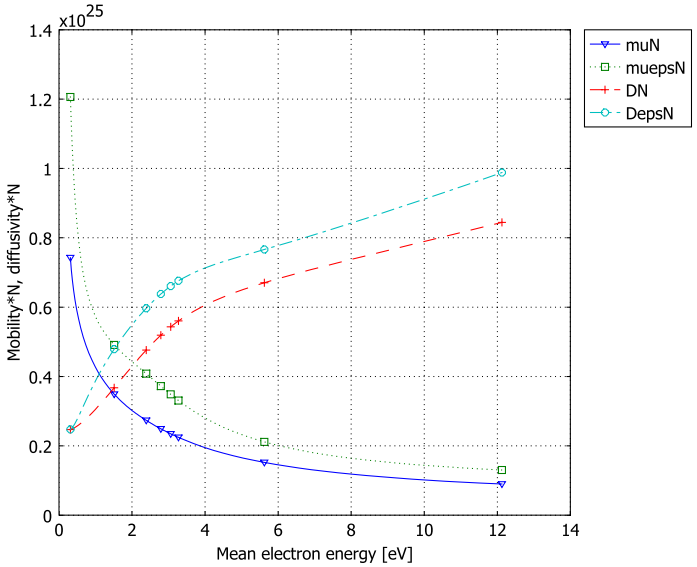


Figure 5-32: Transport properties calculated using the two-term Boltzmann equation.

These computed rate coefficients and transport properties can be fed into a full fluid model for the electron density and energy, either as a look up table or by approximating the rate coefficients with a curve fit.

Finally, using MATLAB, you can visualize the effect of the inelastic collisions on the Jacobian matrix using the `spy` command. The sparsity-pattern plot in Figure 5-33 shows that the Jacobian matrix is different from the traditional banded matrix formed with a regular 1D convection-diffusion equation. Because the inelastic collisions dominate the system, it is essential that they contribute to the Jacobian matrix.

Modeling in COMSOL Multiphysics

To solve Equation 5-11, use a PDE, General Form application mode in 1D, letting the x-coordinate represent the electron energy expressed in electronvolts. An additional auxiliary 2D geometry allows you to handle the nonlocal couplings in the source term, S, using extrusion coupling variables (see the section "Extrusion Coupling Variables" on page 275 of the *COMSOL Multiphysics User's Guide* for further details). To implement the integral constraint Equation 5-12, use an integration coupling variable and COMSOL Multiphysics' interface for solving ODEs; for descriptions of these features, see the sections "Integration Coupling Variables" on page 269 of the

COMSOL Multiphysics User's Guide and "Solving ODEs and Global Equations" on page 340 of the *COMSOL Multiphysics Modeling Guide*, respectively. The collision cross-section data, obtained from Ref. 2, is included in a set of text files that comes with your COMSOL Multiphysics installation.

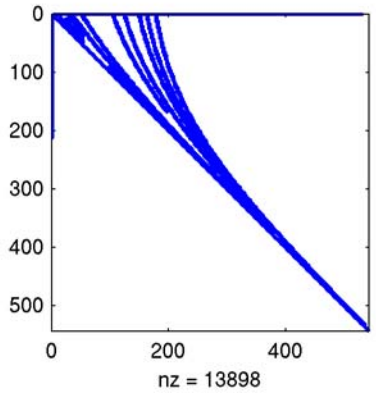


Figure 5-33: Sparsity-pattern plot of the assembled Jacobian matrix. The far off-diagonal elements are a result of the nonlocal couplings.

References

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models," *Plasma Sources Sci. Technol.*, vol. 14, pp. 722–733, 2005.

2. The Siglo Database, CPAT and Kinema Software, http://www.siglo-kinema.com/database/index.htm

Model Library path: `COMSOL_Multiphysics/Equation-Based_Models/two_term_boltzmann`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

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

3 From the **Application Modes** list, choose **COMSOL Multiphysics>PDE Modes>PDE, General Form**.

4 In the **Dependent variables** edit field, change the name to `f`.

5 Click **Multiphysics**, then click **Add**.

6 Click **Add Geometry**. From the **Space dimension** list, select **2D**. Click **OK**.

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

GEOMETRY MODELING

1 Click the **Geom1** tab.

2 Shift-click the **Line** button on the Draw toolbar. In the **Coordinates** area, enter `0 500` in the **x** edit field to draw a line between $x = 0$ and $x = 500$. Click **OK**.

3 In the same manner, draw a second line between $x = 500$ and $x = 550$.

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

5 Click the **Geom2** tab.

6 Using the **Rectangle** dialog box, which you open by shift-clicking the **Rectangle/Square** button on the Draw toolbar, draw two rectangles, R1 and R2, with the properties in the table below. Click **OK** after specifying each rectangle.

PROPERTY	R1	R2
Width	250	250
Height	50	50
Base	Corner	Corner
x	0	250
y	0	0

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

OPTIONS AND SETTINGS

Model Settings

Because this x-coordinate in this model signifies energy, and the energy is expressed in the nonstandard unit electronvolt, disable COMSOL Multiphysics' unit support:

1 From the **Physics** menu, open the **Model Settings** dialog box.

2 On the **Geom2** page, select **None** from the **Base unit system** list.

3 Click the **Geom1** tab, and do the same for this geometry.

4 Click **OK** to close the dialog box.

Constants

1 From the **Options** menu, open the **Constants** dialog box.

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

NAME	EXPRESSION	DESCRIPTION
e	1.602e-19	The elementary charge (C)
m_e	9.109e-31	Electron mass (kg)
gam	sqrt(2*e/m_e)	Energy-velocity conversion factor
k_B	1.381e-23	Boltzmann's constant (J/K)
N_A	6.022e23	Avogadro's constant (1/mol)
T_g	300	Gas temperature (K)
tau_g	k_B*T_g/e	Gas temperature (eV)
tau_ei	0.025	Initial electron temperature (eV)
M_O2	0.032/N_A	O2 molecule mass (kg)
EoN	32	Reduced electric field (Td)
dH3	0.02	Threshold energy, reaction 3 (eV)
dH4	0.19	Threshold energy, reaction 4 (eV)
dH5	0.19	Threshold energy, reaction 5 (eV)
dH6	0.38	Threshold energy, reaction 6 (eV)
dH7	0.38	Threshold energy, reaction 7 (eV)
dH8	0.57	Threshold energy, reaction 8 (eV)
dH9	0.75	Threshold energy, reaction 9 (eV)
dH10	0.977	Threshold energy, reaction 10 (eV)
dH11	1.627	Threshold energy, reaction 11 (eV)
dH12	4.5	Threshold energy, reaction 12 (eV)
dH13	6.0	Threshold energy, reaction 13 (eV)
dH14	8.4	Threshold energy, reaction 14 (eV)
dH15	09.97	Threshold energy, reaction 15 (eV)
dH16	12.06	Threshold energy, reaction 16 (eV)

Here, `EoN` is the value of the *reduced electric field*—that is, the ratio between the electric field and the neutral particle number density—expressed in *townsend* (1 Td $= 10^{-21}$ V·m^2). When computing the solution, you use `EoN` as the solver parameter.

Functions

Next define functions `sig1`, …, `sig16` that encode the electron-impact cross sections σ_1, …, σ_{16} for the collisions listed in Table 5-2 using data provided in text files.

1 From the **Options** menu, open the **Functions** dialog box.

2 Click **New**. In the **Function name** edit field, type `sig1`.

3 Click the **Interpolation** option button.

4 In the **Use data from** list, select **File**. Browse to the folder `models/Equation-Based_Models` in your COMSOL Multiphysics installation directory. Select the file `two_term_boltzmann_cs1.txt`, then click **OK**.

5 From the **Interpolation method** list, select **Linear**. From the **Extrapolation method** list, select **Specific number**, then set the **Value outside range** to `0`.

6 Repeat Steps 2–5 to define the functions `sig2`, …, `sig16` by loading, in turn, the text files `two_term_boltzmann_cs2.txt`, …, `two_term_boltzmann_cs16.txt`.

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

Global Expressions

1 Choose **Options>Expressions>Global Expressions**.

2 Define the expressions listed in the following table (the descriptions are optional).

NAME	EXPRESSION	DESCRIPTION
sigma_eps	2*(m_e/M_O2)*sig1(x)	Elastic-collision cross section
sigma_m	sig1(x)	Effective momentum-transfer cross section
W_es	-sigma_eps*x^2	PDE energy-space flow-velocity coefficient
D_es	(1/3)*(x/sigma_m)*(EoN*1e-21)^2+ sigma_eps*tau_g*x^2	PDE energy-space diffusion coefficient
tau_e	(2/3)*eps_mean	Electron temperature (eV)
f_M	(2/sqrt(pi))*tau_e^(-3/2)*exp(-x/tau_e)	Maxwellian EEDF
f_init	(2/sqrt(pi))*tau_ei^(-3/2)*exp(-x/tau_ei)	Initial EEDF
C2	-x*sig2(x)*f	Inelastic source/sink
C3	(x+dH3)*sig3(x+dH3)*f3-x*sig3(x)*f	Inelastic source/sink
C4	(x+dH4)*sig4(x+dH4)*f4-x*sig4(x)*f	Inelastic source/sink
C5	(x+dH5)*sig5(x+dH5)*f5-x*sig5(x)*f	Inelastic source/sink
C6	(x+dH6)*sig6(x+dH6)*f6-x*sig6(x)*f	Inelastic source/sink
C7	(x+dH7)*sig7(x+dH7)*f7-x*sig7(x)*f	Inelastic source/sink
C8	(x+dH8)*sig8(x+dH8)*f8-x*sig8(x)*f	Inelastic source/sink
C9	(x+dH9)*sig9(x+dH9)*f9-x*sig9(x)*f	Inelastic source/sink
C10	(x+dH10)*sig10(x+dH10)*f10-x*sig10(x)*f	Inelastic source/sink

NAME	EXPRESSION	DESCRIPTION
C11	(x+dH11)*sig11(x+dH11)*f11-x*sig11(x)*f	Inelastic source/sink
C12	(x+dH12)*sig12(x+dH12)*f12-x*sig12(x)*f	Inelastic source/sink
C13	(x+dH13)*sig13(x+dH13)*f13-x*sig13(x)*f	Inelastic source/sink
C14	(x+dH14)*sig14(x+dH14)*f14-x*sig14(x)*f	Inelastic source/sink
C15	(x+dH15)*sig15(x+dH15)*f15-x*sig15(x)*f	Inelastic source/sink
C16	2*(2*x+dH16)*sig16(2*x+dH16)*f16 -x*sig16(x)*f	Inelastic source/sink
S	C2+C3+C4+C5+C6+C7+C8+C9+C10+ C11+C12+C13+C14+C15+C16	Inelastic collision source
R_norm	-nojac(k16-k2)*sqrt(x)*f	Growth-renormalization term

Here, f3, …, f16 represent the nonlocal factor $f(\varepsilon + \Delta\varepsilon_k)$ or (in the case of f16) $f(\varepsilon + 2\Delta\varepsilon_k)$ in Equation 5-11; later, you define these as extrusion coupling variables using the auxiliary geometry **Geom2**.

To preserve the normalization of f_0 in the presence of collision processes that do not conserve the electron number, the growth-renormalization term, R_norm, must be added to the right-hand side of the PDE multiplied by the constraint λ defined by Equation 5-12; see Ref. 1 for a discussion. For this model, the electron-number changing processes are the attachment and ionization reactions (no. 2 and 16 in Table 5-2). The nojac operator in the expression for R_norm instructs COMSOL Multiphysics not to include the argument, k16-k2, in the Jacobian computation; see "The nojac Operator" on page 164 of the *COMSOL Multiphysics User's Guide* for additional information on this operator.

3 Click **OK** to close the **Global Expressions** dialog box.

Integration Coupling Variables

Compute the integrals appearing in Equations 5-12–5-17 and make them globally available in the model by defining corresponding integration coupling variables.

1 With **Geom1** active, choose **Options>Integration Coupling Variables>Subdomain Variables**.

2 Select Subdomain 1, then define integration coupling variables according to the table below. In all cases, use the default settings for **Integration order** (4) and **Global destination** (selected).

NAME	EXPRESSION
f_norm	sqrt(x)*f
eps_mean	x^(3/2)*f

NAME	EXPRESSION
mu_N	-(1/3)*gam*fx*x/sigma_m
D_N	(1/3)*gam*f*x/sigma_m
mu_epsN	-(1/(3*eps_mean))*gam*fx*x^2/sigma_m
D_epsN	(1/(3*eps_mean))*gam*f*x^2/sigma_m
k1	gam*sig1(x)*x*f
k2	gam*sig2(x)*x*f
k3	gam*sig3(x)*x*f
k4	gam*sig4(x)*x*f
k5	gam*sig5(x)*x*f
k6	gam*sig6(x)*x*f
k7	gam*sig7(x)*x*f
k8	gam*sig8(x)*x*f
k9	gam*sig9(x)*x*f
k10	gam*sig10(x)*x*f
k11	gam*sig11(x)*x*f
k12	gam*sig12(x)*x*f
k13	gam*sig13(x)*x*f
k14	gam*sig14(x)*x*f
k15	gam*sig15(x)*x*f
k16	gam*sig16(x)*x*f
k1_M	gam*sig1(x)*x*f_M
k2_M	gam*sig2(x)*x*f_M
k3_M	gam*sig3(x)*x*f_M
k4_M	gam*sig4(x)*x*f_M
k5_M	gam*sig5(x)*x*f_M
k6_M	gam*sig6(x)*x*f_M
k7_M	gam*sig7(x)*x*f_M
k8_M	gam*sig8(x)*x*f_M
k9_M	gam*sig9(x)*x*f_M
k10_M	gam*sig10(x)*x*f_M
k11_M	gam*sig11(x)*x*f_M
k12_M	gam*sig12(x)*x*f_M
k13_M	gam*sig13(x)*x*f_M
k14_M	gam*sig14(x)*x*f_M

NAME	EXPRESSION
k15_M	gam*sig15(x)*x*f_M
k16_M	gam*sig16(x)*x*f_M

3 Click **OK**.

Extrusion Coupling Variables

To implement the nonlocal collision source terms, use extrusion coupling variables.

1 With **Geom1** still selected, choose **Options>Extrusion Coupling Variables>Subdomain Variables**.

2 On the **Source** page, select both subdomains, then enter the following data:

NAME	EXPRESSION	TRANSFORMATION TYPE	SOURCE TRANSFORMATION
f_extr	f	General transformation	x
f_extr_ion	f	General transformation	x

3 Click the **Destination** tab.

4 From the **Geometry** list, select **Geom2**, and from the **Level** list, select **Subdomain**.

5 From the **Variable** list, select **f_extr**. Select Subdomains 1 and 2, then select the **Use selected subdomains as destination** check box.

6 Set the **Destination transformation** to x+y.

7 From the **Variable** list, select **f_extr_ion**. Select Subdomain 1 only, then select the **Use selected subdomains as destination** check box.

8 Set the **Destination transformation** to 2*x+y, then click **OK**.

9 Now with **Geom2** selected, choose **Options>Extrusion Coupling Variables>Subdomain Variables**.

10 On the **Source** page, select both subdomains, then enter the following data:

NAME	EXPRESSION	TRANSFORMATION TYPE	SOURCE TRANSFORMATION			
f3	f_extr	General transformation	x	x	y	y

11 Define the variables f4, …, f15 using the same data as for f3 in the previous step.

12 Select only Subdomain 1, then enter the following data:

NAME	EXPRESSION	TRANSFORMATION TYPE	SOURCE TRANSFORMATION			
f16	f_extr_ion	General transformation	x	2*x	y	y

13 Click the **Destination** tab.

14 From the **Geometry** list, select **Geom1**, and from the **Level** list, select **Subdomain**.

15 Select Subdomain 1.

16 From the **Variable** list, select **f3**. Select the **Use selected subdomains as destination** check box, and set the **Destination transformation** for **x** to `x` and that for **y** to `dH3`.

17 Repeat the previous step for each of the variables **f4**, …, **f16**, using as the **Destination transformation** for **y** `dH4`, …, `dH16`, respectively.

18 Click **OK** to close the **Subdomain Extrusion Variables** dialog box.

PHYSICS MODELING

Global Equations

To implement the normalization constraint in Equation 5-12, first define a state for λ:

1 From the **Physics** menu, open the **Global Equations** dialog box.

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

NAME	EQUATION	INIT	INITT	DESCRIPTION
`lam`	`f_norm-1`	`1e-5`	`0`	`Normalization constraint`

3 From the **Base unit system** list, select **None**, then click **OK**.

Subdomain Settings

1 Click the **Geom1** tab.

2 From the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Specify the following PDE coefficients:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
Γ	`W_es*f-D_es*fx`	`0`
F	`S+lam*R_norm`	`-f`
e_a	`0`	`0`
d_a	`0`	`0`

Note, in particular, the addition to the source term for Subdomain 1 of the growth-renormalization term multiplied by the integral constraint, λ. On Subdomain 2, which is introduced solely to allow consistent definitions for the extrusion coupling variables, you simply set f_0 to zero.

4 Click the **Init** tab. Select Subdomain 1, then type `f_init` in the **f(t_0)** edit field.

5 Click **OK**.

Boundary Conditions

Implement the boundary conditions in Equation 5-13, substituting $x = 500$ for infinity.

1. From the **Physics** menu, open the **Boundary Settings** dialog box.
2. Select the **Interior boundaries** check box.
3. Specify boundary conditions as in the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3
Type	Neumann	Dirichlet
G	0	0
R		`-f`

MESH GENERATION

1. From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.
2. On the **Global** page, type `1.02` in the **Element growth rate** edit field.
3. On the **Subdomain** page, select Subdomain 1. Set the **Maximum element size** to `20`.
4. On the **Boundary** page, select Boundary 1. Set the **Maximum element size** to `0.05`.
5. Click **Remesh**, then click **OK**.
6. Select **Geom2**.
7. From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.
8. Click the **Custom mesh size** option button, then set the **Maximum element size** to `10`.
9. Click the **Boundary** tab. Select Boundaries 1, 2, and 5, then set the **Maximum element size** to `1.5`.
10. Click the **Point** tab. Select Point 1, then set the **Maximum element size** to `0.05`.
11. Click **Remesh**, then 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 names** edit field, type `EoN`, and in the **Parameter values** edit field, type `range(1.953,(49-1.953)/99,49) range(50,(414-50)/24,414)`.
4. Click **OK**.
5. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

First, verify the normalization constraint Equation 5-12 for the solution.

1. Click the **Geom1** tab.
2. From the **Postprocessing** menu, choose **Subdomain Integration**.
3. Select Subdomain 1. In the **Expression** edit field, type `sqrt(x)*f`.
4. In the **Solution to use** area, select an arbitrary solution from the **Parameter value** list, then click **Apply**.

   The result, which should be 1 (or very close to 1), appears in the message log below the drawing area.
5. Try a few other solutions. When done, click **OK**.

Reproduce the EEDF plots in Figure 5-29 on page 187 with the following steps:

1. From the **Postprocessing** menu, choose **Domain Plot Parameters**.
2. On the **General** page, select **26.664556** from the **Solutions to use** list. Select the **Keep current plot** check box.
3. Click the **Line/Extrusion** tab.
4. In the **Expression** edit field, type `f_M`.
5. Click the **Line Settings** button. From the **Line color** list, select **Color**, then click the **Color** button. Select the black swatch, then click **OK**.
6. Click **OK** to close the **Line Settings** dialog box.
7. In the **Domain Plot Parameters** dialog box, click **Apply**.
8. In the **Expression** edit field, type `f`.
9. Click the **Line Settings** button. From the **Line color** list, select **Color**, then click the **Color** button. Select a red swatch, then click **OK**.
10. On the **General** page, click the **Title/Axis** button.
11. Click the option button next to the **Title** edit field; leave the edit field empty.
12. Click the option button next to the **First axis label** edit field, then enter the label `Electron energy [eV]`.
13. Click the option button next to the **Second axis label** edit field, then enter the label `EEDF [eV<sup>-3/2</sup>]`. Select the associated **Log scale** check box.
14. Click **OK** to close the **Title/Axis** dialog box.
15. In the **Domain Plot Parameters** dialog box, click **OK**.

16 In the figure window, click the **Zoom Window** button, then select the area $0 < x < 20$ and $10^{-5} < y < 10^{0}$ in the upper left corner to finish the plot.

Proceed to generate the plots of the ionization-rate coefficients in Figure 5-30:

1 From the **Postprocessing** menu, choose **Global Variables Plot**.

2 In the **Expression** edit field, type `k16_M`, then click the **Add Entered Expression** button.

3 In the **x-axis data** area, click the lower option button, then click the **Expression** button. In the **Expression** edit field, type `eps_mean`, then click **OK** to close the **X-Axis Data** dialog box.

4 Click the **Line Settings** button. From the **Line color** list, select **Color**, then click the **Color** button. Select black, then click **OK**.

5 Select the **Legend** check box, then click **OK** to close the **Line Settings** dialog box.

6 Click the **Title/Axis** button.

7 Click the option button next to the **Title** edit field; leave the edit field empty.

8 Click the option button next to the **First axis label** edit field, then enter the label `Mean electron energy [eV]`.

9 Click the option button next to the **Second axis label** edit field, then enter the label `Ionization rate coefficient [m<sup>3</sup>/s]`. Select the associated **Log scale** check box.

10 Click **OK** to close the **Title/Axis** dialog box.

11 Click **Apply** to generate the first graph.

12 Select the **Keep current plot** check box.

13 In the **Quantities to plot** list, select **k16_M**, then click the **Remove Selected Quantities to Plot** button.

14 In the **Expression** edit field, type `k16`, then click the **Add Entered Expression** button.

15 Click the **Line Settings** button.Click the **Color** button. Select red, then click **OK** twice.

16 Click **Apply** to generate the second graph and finish the plot.

Next, reproduce Figure 5-31:

1 In the **Quantities to plot** list, select **k16**, then click the **Remove Selected Quantities to Plot** button.

2 In the **Expression** edit field, type `k1`, then click the **Add Entered Expression** button.

3 Repeat the previous step 15 times for, in turn, `k2`, …, `k16`.

4 Click the **Line Settings** button. Select **Cycle** from the **Line color**, **Line style**, and **Line marker** lists, then click **OK**.

5 Click the **Title/Axis** button. Change the **Second axis label** to `Rate coefficients [m<sup>3</sup>/s]`, then click **OK**.

6 From the **Plot in** list, select **New figure**, then click **Apply** to generate the plot.

To reproduce the plot of the transport properties in Figure 5-32, do as follows:

1 Click in the **Quantities to plot** list, then press Ctrl+A to select all entries. Click the **Remove Selected Quantities to Plot** button.

2 In the **Expression** edit field, type `mu_N`, then click the **Add Entered Expression** button.

3 Repeat the previous step for `mu_epsN`, `D_N`, and `D_epsN`.

4 Click the **Title/Axis** button. Change the **Second axis label** to `Mobility*N, diffusivity*N`. Clear the associated **Log scale** check box, then click **OK**.

5 From the **Plot in** list, select **New figure**, then click **OK** to generate the plot and close the **Global Variables Plot** dialog box.

Finally, if you have access to MATLAB, you can reproduce the sparsity-pattern plot of the assembled Jacobian matrix in Figure 5-33 in the following way:

1 Press Ctrl+F or choose **File>Export>FEM Structure as 'fem'**.

2 In the MATLAB command window, enter the following commands:

```
[KC,LC] = femlin(fem);
spy(KC)
```

The sparsity-pattern plot appears in the last opened figure window.

6

Fluid Dynamics Models

This chapter includes examples of fluid dynamics modeling using the incompressible Navier-Stokes equations for stationary and time-dependent fluid flow and the Euler equations for compressible flow in gas dynamics.

Backstep with Argyris Element

Introduction

This model shows the use of stream functions to model incompressible fluid flow in a divergence-free approach. Instead of conventional p2-p1 Lagrange elements, the model uses C^1-continuous Argyris elements to discretize the incompressible Navier-Stokes equations. Formulating the flow equations in terms of a stream function eliminates the continuity equation altogether.

Model Definition

The stream function Ψ is introduced through the following definition:

$$(u, v) = \nabla \times \Psi = \left(\frac{\partial \Psi}{\partial y}, -\frac{\partial \Psi}{\partial x}\right).$$

That is, the velocity field is the curl of the stream function. Therefore the divergence of the velocity field is identically zero wherever the stream function is smooth enough.

Introducing the stream function is in itself motivated by the requirement that the divergence of the velocity field should vanish: you can write any divergence-free field as the curl of some vector field, known as a vector potential. The velocity field determines the stream function Ψ only up to the gradient of some function, which means that the stream function corresponding to a given velocity field is not unique.

The Argyris elements belong to the C^1-class of functions, implying that they have continuous first derivatives and function values. Therefore the continuity equation is satisfied weakly everywhere in the domain. Also, pressure has been eliminated from the equations, but you can determine the pressure field afterwards by solving a Poisson-type equation. To get this equation you essentially take the divergence of the momentum equations.

Argyris Element Properties

The advantage of using Argyris elements in the discretization is that the continuity equation is always satisfied. Convergence toward a solution is not inhibited by poor fulfillment of the incompressibility criterion. There are, however, some disadvantages. When using the Argyris elements, 21 degrees of freedom are associated with any

triangle compared to 15 for the standard p2-p1 Lagrange elements. Due to different node usage, the total number of degrees of freedom in the model is roughly the same in the two cases, but the Argyris elements are more tightly connected to one another, which leads to increased memory usage. Further, the Argyris elements are in all respects more complex, thus it takes more time to prepare the problem for the solvers.

Results

Fifth-order Argyris elements provide very high accuracy for smooth solutions. This model has a discontinuity in the gradient of the velocity field at the backstep corner. The Argyris element has degrees of freedoms representing this quantity in its corners. This causes some convergence and accuracy problems, which mean that you must use the parametric solver. The results, however, are of similar accuracy as in the introductory backstep model, "Example—Steady Incompressible Flow" on page 154 in the *COMSOL Multiphysics Modeling Guide*, on a mesh of half the size in number of elements.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/backstep_argyris`

Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** from the **Space dimension** list.
2. In the list of application modes, select **COMSOL Multiphysics>PDE Modes>PDE, General Form>Stationary analysis**.
3. In the **Dependent variables** edit field, type `u v`.
4. Click **OK**.

You set the element type to Argyris later on.

OPTIONS AND SETTINGS

Model Settings

Because the PDE application modes do not support units, change the base unit system as follows:

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

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

3 Click **OK**.

Constants

1 From the **Options** menu, choose **Constants** to set the values needed to parameterize the model.

2 In the **Constants** dialog box, enter the following constants representing fluid properties and the velocity (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho0	1.23	Fluid density (kg/m^3)
eta0	1.79e-5	Dynamic viscosity (kg/(m*s))
V_mean	0.1	Average inlet velocity (m/s)

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar to specify a rectangle.

2 In the **Rectangle** dialog box, type `0.08` in the **Width** edit field and `0.0101` in the **Height** edit field.

3 Click **OK**.

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

5 Shift-click the **Rectangle/Square** button on the Draw toolbar to specify another rectangle.

6 In the **Rectangle** dialog box, type `0.02` in the **Width** edit field and `0.0049` in the **Height** edit field.

7 Click **OK**.

8 Press Ctrl+A to select both rectangles.

9 Click the **Difference** button on the Draw toolbar.

PHYSICS SETTINGS

Point Settings

Because the equations contain only derivatives of the real dependent variable—the stream function Ψ—you must set a reference level somewhere to remove the ambiguity in the solution.

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

2 Select Point 1 and enter the following constraint:

SETTINGS	POINT 1
constr	-psi 0

Boundary Conditions

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

2 Select Boundary 1, then click the **R** tab.

3 Enter the following boundary coefficients:

SETTINGS	BOUNDARY 1	BOUNDARIES 2–5	BOUNDARY 6
R(1)	V_mean*6*s*(1-s)-u	-u	0
R(2)	-v	-v	0

The equation for the boundary condition is $R = 0$, so these values make sure that u and v are equal to zero, except on the inlet boundary (Boundary 1), where u, the velocity in the x-direction, is a parabolic velocity profile that represents a fully developed laminar flow. The parameter `s` is an curve length parameter that runs from 0 to 1 along the direction of the boundary.

4 Click **OK**.

Subdomain Settings

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

2 On the Γ and **F** tabs, respectively, enter the PDE coefficients from the following table:

SETTINGS	SUBDOMAIN 1
Γ(1,1)	2*eta0*ux
Γ(1,2)	eta0*(uy+vx)
Γ(2,1)	eta0*(uy+vx)
Γ(2,2)	2*eta0*vy
F(1)	rho0*(u*ux+v*uy)
F(2)	rho0*(u*vx+v*vy)

These settings implement the equations for the fluid flow.

3 Click the **Element** tab.

4 In the **Shape** edit field, type `sharg_2_5('psi')`.

5 In the **gporder** edit field, type `8 8`.

6 In the **cporder** edit field, type `5 5`.

7 Click **OK**.

The standard integration order for the Argyris element is 10 (and the standard constraint order is half of that value, 5). In this case only derivatives of `psi` appear in equations and boundary conditions. Therefore an integration order of 8 is sufficient. Reducing the order reduces assembly time.

Expression Variables

1 From the **Options** menu, select **Expressions>Subdomain Expressions**.

2 In the **Subdomain Expressions** dialog box, define the following variables.

VARIABLE NAME	LEVEL	DOMAIN	EXPRESSION
u	Subdomain	1	psiy
ux	Subdomain	1	psiyx
uy	Subdomain	1	psiyy
v	Subdomain	1	-psix
vx	Subdomain	1	-psixx
vy	Subdomain	1	-psixy

3 Click **OK**.

4 From the **Options** menu, select **Expressions>Boundary Expressions**.

5 In the **Boundary Expressions** dialog box define the following variables.

VARIABLE NAME	LEVEL	DOMAINS	EXPRESSION
u	Boundary	1–6	psiy
v	Boundary	1–6	-psix

6 Click **OK**.

MESH GENERATION

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

2 In the **Free Mesh Parameters** dialog box, click the **Custom mesh size** button, then type `2e-3` in the **Maximum element size** edit field.

3 Click the **Point** tab.

4 Select Point 4 and in the **Maximum element size** edit field type `4e-4`.

5 Click the **Remesh** button, then click **OK**.

COMPUTING THE SOLUTION

It is possible to use the parametric solver to increase the velocity—and thereby the Reynolds number—step by step. Either give an explicit list of parameter values or let the solver automatically decide an optimum step length. The last option is usually the proper choice when using the parametric solver for difficult problems such as those with medium to high Reynolds number flows.

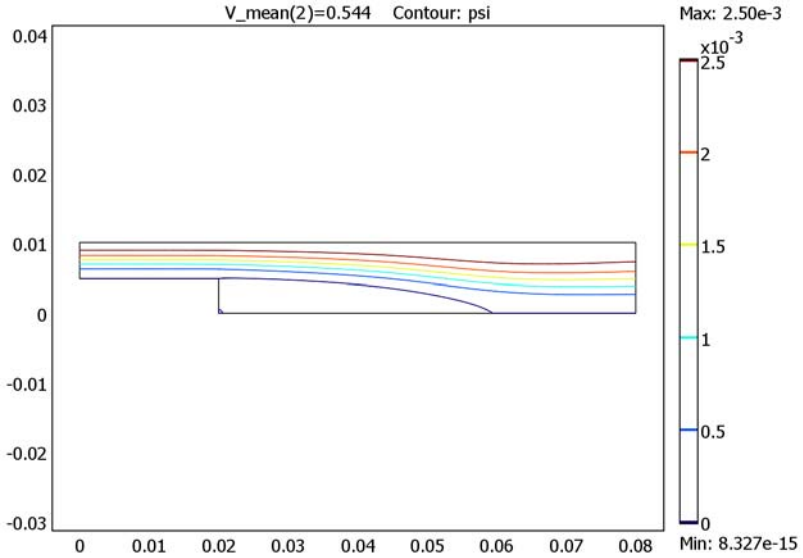
1. From the **Solve** menu, choose **Solver Parameters**.
2. In the **Solver** list, select **Parametric**.
3. Go to the **Parameter** area. In the **Parameter names** edit field, type `V_mean`. Then, in the **Parameter values** edit field, type `0.1 0.544`.
4. Click the **Advanced** tab.
5. In the **Null-space function** list, select **Orthonormal**.
6. From the **Solution form** list, select **General**. This is because the weak form gives expressions that include u, which is not a dependent variable when you use Argyris elements.
7. Click **OK**, then click the **Solve** button on the Main toolbar to start the simulation.

POSTPROCESSING AND VISUALIZATION

The software displays the solution for the last parameter value. The value of the stream function itself is hardly interesting, but you can take advantage of the fact that contour lines of the stream function are the same as streamlines of the velocity field. The zero-level contour is of particular interest because it immediately shows the extent of the recirculation region and the location of the stagnation point.

1. From the **Postprocessing** menu, open the **Plot Parameters** dialog box.
2. In the **Plot type** area, clear the **Surface** check box. Then, select the **Contour** check box.
3. Change the value in the **Element refinement** edit field to `10`. Before you can enter the number, you must clear the **Auto** check box.
4. Click the **Contour** tab.
5. Type `psi` in the **Expression** edit field.
6. In the **Contour levels** area, click the button under **Vector with isolevels,** and then type `range(0,0.0005,0.003)` in the edit field.

7 Click **OK** to close the dialog box and generate the following plot.



Flow Past a Cylinder

Introduction

The flow of fluid behind a blunt body such as an automobile is difficult to compute due to the unsteady flows. The wake behind such a body consists of unordered eddies of all sizes that create large drag on the body. In contrast, the turbulence in the thin boundary layers next to the streamlined bodies of aircraft and fish create only weak disturbances of flow.

An exception to this occurs when you place a slender body at right angles to a slow flow because the eddies organize. A von Karman vortex street appears with a predictable frequency and involves the shedding of eddies from alternating sides. Everyday examples of this phenomenon include singing telephone wires and an automobile radio antenna vibrating in an air stream.

From an engineering standpoint, it is important to predict the frequency of vibrations at various fluid speeds and thereby avoid undesirable resonances between the vibrations of the solid structures and the vortex shedding. To help reduce such effects, plant engineers put a spiral on the upper part of high smokestacks; the resulting variation in shape prohibits the constructive interference of the vortex elements that the structure sheds from different positions.

Model Definition

To illustrate how you can study such effects, the following model examines unsteady, incompressible flow past a long cylinder placed in a channel at right angle to the oncoming fluid. The cylinder is offset somewhat from the center of the flow to destabilize what otherwise would be steady-state symmetrical flow. The simulation time necessary for a periodic flow pattern to appear is difficult to predict. A key predictor is the Reynolds number, which is based on cylinder diameter. For low values (below 100) the flow is steady. In this simulation, the Reynolds number equals 100, which gives a developed Karman vortex street, but the flow still is not fully turbulent.

The frequency and amplitude of oscillations are stable features, but flow details are extremely sensitive to perturbations. To gain an appreciation for this sensitivity, you can compare flow images taken at the same time but with such minor differences as are created by different tolerances for the time stepping. It is important to note that this sensitivity is a physical reality and not simply a numerical artifact.

Before calculating the time-varying forces on the cylinder, you can validate the method of computation at a lower Reynolds number using the direct nonlinear solver. This saves time because you can find and correct simple errors and mistakes before the final time-dependent simulation, which requires considerable time.

The viscous forces on the cylinder are proportional to the gradient of the velocity field at the cylinder surface. Evaluating the velocity gradient on the boundary by directly differentiating the FEM solution is possible but not very accurate. The differentiation produces 1st-order polynomials when 2nd-order elements are used for the velocity field. A far better approach is to use a pair of reaction force operators to compute the integrals of the viscous forces, comparable to 2nd-order accurate integrals of the viscous forces. An alternative approach would be to use a pair of weak-constraint variables to enforce the no-slip condition. Preferably use the reaction force operator instead of weak constrains when computing integrals of reaction forces or fluxes in postprocessing.

The drag and lift forces themselves are not as interesting as the dimensionless drag and lift coefficients. These depend only on the Reynolds number and an object's shape, not its size. The coefficients are defined as

$$C_D = \frac{2F_D}{\rho U_{\text{mean}}^2 D}$$

$$C_L = \frac{2F_L}{\rho U_{\text{mean}}^2 D}$$

using the following parameters:

- F_D and F_L are the drag and lift forces
- ρ is the fluid's density
- U_{mean} is the mean velocity
- D is the characteristic length, in this case the cylinder's diameter

Results

Figure 6-1 shows the flow pattern resulting from the geometry.

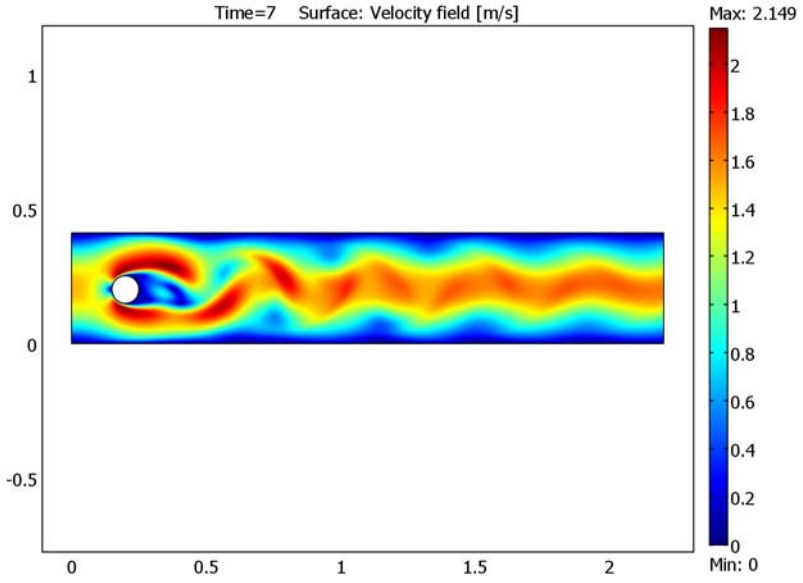


Figure 6-1: A plot of the last time step clearly shows the von Karman path.

The flow around a cylinder is a common benchmark test for CFD algorithms. Various research teams have tried their strengths on this problem using different techniques. Results from some of these experiments have been collected by Schäfer and Turek (Ref. 1), who also used them to compute a probable value for the "real" answer.

Reference

1. M. Schäfer and S. Turek, "Benchmark computations of laminar flow around cylinder", E.H. Hirschel (editor), *Flow Simulation with High-Performance Computers II, Volume 52 of Notes on Numerical Fluid Mechanics*, Vieweg, 1996, pp. 547–566.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow`

MODEL NAVIGATOR

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

2 In the list of application modes, select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Steady-state analysis**. Accept the default entry in the **Element** list, **Lagrange - P_2 P_1** elements.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Axes/Grid Settings** dialog box, specify the following settings. To enter the grid spacing, first click the **Grid** tab and then clear the **Auto** check box.

AXIS		GRID	
x min	-0.3	x spacing	0.2
x max	2.5	Extra x	
y min	-0.3	y spacing	0.05
y max	0.7	Extra y	0.41

3 Click **OK**.

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

5 Enter the following names, expressions, and descriptions (optional):

NAME	EXPRESSION	DESCRIPTION
rho0	1[kg/m^3]	Density
eta0	1e-3[Pa*s]	Dynamic viscosity
Umax	0.3[m/s]	Maximum inlet velocity

6 Click **OK**.

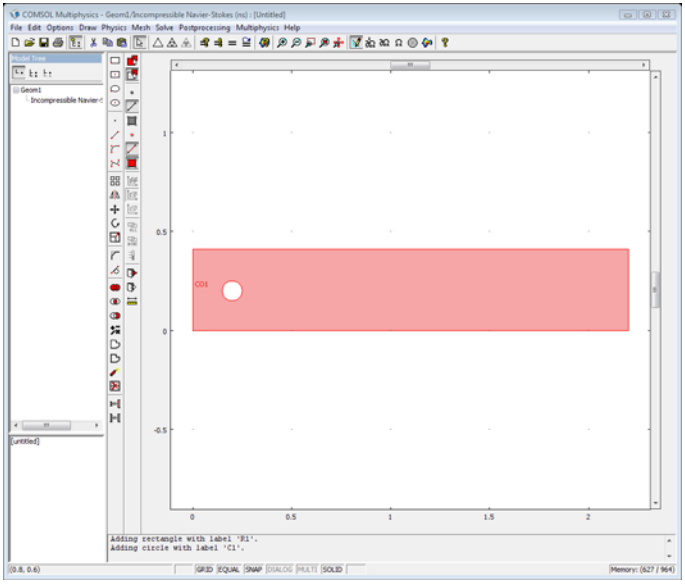
These values together with the cylinder having a diameter of 0.1 m lead to a Reynolds number of 20.

GEOMETRY MODELING

1 From the Draw menu, select the **Rectangle/Square** button. With the mouse, create a rectangle R1 from (0, 0) to (2.2, 0.41).

2 From the Draw menu, select the **Ellipse/Circle (Centered)** button. Using the mouse, create a circle C1 with center at (0.2, 0.2) and a radius of 0.05. Use the right mouse button to ensure that you are creating a circle and use the tick mark at $y = 0.15$ to obtain the correct radius.

3 Create the composite object. From the Draw toolbar, click the **Create Composite Object** button. In the **Set formula** edit field enter `R1-C1`. Click **OK**.



PHYSICS SETTINGS

Boundary Conditions

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

2 In the **Boundary Settings** dialog box, enter the following:

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3, 5–8	BOUNDARY 4
Boundary type	Inlet	Wall	Outlet
Boundary condition	Velocity	No slip	Pressure, no viscous stress
u_0	`4*Umax*s*(1-s)`		
v_0	0		
p_0			0

3 Click **OK**.

Subdomain Settings

Define the properties of the fluid:

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

2 In the **Subdomain Settings** dialog box, enter the following material properties:

SETTINGS	SUBDOMAIN 1
ρ	rho0
η	eta0

3 Click **OK**.

MESH GENERATION

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

2 Click the **Custom mesh size** button, enter `0.03` in the **Maximum element size** edit field, enter `1.2` in the **Element growth rate** edit field, and enter `0.1` in the **Mesh curvature factor** edit field.

3 Click **OK**.

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

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to solve the model.

POSTPROCESSING AND VISUALIZATION

The quantities in the benchmark study are the drag and lift coefficients. These you can calculate easily by integrating reaction force operators (which are really Lagrange multipliers corresponding to the viscous forces) and the pressure over the surface of the cylinder. First calculate the drag coefficient:

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

2 Select Boundaries 5 to 8, corresponding to the cylinder surface. Enter the drag force expression `-reacf(u)*2/(rho0*(2*Umax/3)^2*0.1)` in the **Expression** edit field.

3 Click **Apply**.

The result, 5.579373, appears in the message log and agrees well with the interval [5.57, 5.59] given in Ref. 1. Now calculate the lift coefficient.

4 Change the integrand in the **Expression** edit field to `-reacf(v)*2/(rho0*(2*Umax/3)^2*0.1)`.

5 Click **OK**.

Also this value, 0.010683, is in perfect agreement with Schäfer and Turek (Ref. 1), who give the interval [0.0104, 0.0110] for acceptable solutions.

Time-Dependent Simulation

Now that you know that the machinery works for low Reynolds numbers and steady flow, you can do a time-dependent simulation at Re = 100.

OPTIONS AND SETTINGS

In the **Constants** dialog box change the maximum inflow velocity `Umax` to `1.5[m/s]`, corresponding to a Reynolds number of 100.

PHYSICS SETTINGS

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

2 In the **Boundary Settings** dialog box, select Boundary 1.

3 In the **u0** edit field, type `4*Umax*s*(1-s)*flc1hs(t[1/s]-0.1,0.1)`.

4 Click **OK**.

The `flc1hs` function guarantees that the inlet velocity is smoothly ramped up from zero to its maximum value.

COMPUTING THE SOLUTION

During the first few seconds of the simulation, before the system reaches a state of steady periodic motion, the output is not really interesting. Therefore you can save memory by saving only the value five times per second up to 3.5 seconds, and then fifty times per second for another second and a half. Perform the following steps for the time-dependent simulation of drag and lift:

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

2 Select **Transient** from the **Analysis type** list. Click **OK**.

1 From the **Solve** menu, select **Solver Parameters**.

2 In the **Solver** list, select **Time dependent**.

3 In the **Times** edit field type `range(0,0.2,3.5) range(3.52,0.02,7)`.

4 In the **Absolute tolerance** edit field type `1e-4`. Click **OK**.

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

The difference from the former case can be seen immediately. Downstream of the cylinder, the Karman path is clearly visible (see Figure 6-1 earlier in this discussion).

To see the evolution of the vortex trail from zero velocity until the flow is fully developed, click the **Animation** button on the Plot toolbar on the left-hand side of the user interface. Notice that the time scale of the movie changes after 3.5 seconds.

You can also investigate the forces on the tube as a function of time using the reaction force operator and the **Boundary Integration** dialog box:

1. From the **Postprocessing** menu, select **Boundary Integration**. Make sure the **Expression** edit field still contains `-reacf(v)*2/(rho0*(2*Umax/3)^2*0.1)`. Select Boundaries 5–8 and click **Plot**; then click **OK**. Click the **Edit Plot** button in the figure window and change the title and *y*-axis label to `Lift`. Click **OK**.

The plot clearly shows the oscillations in the lift force.

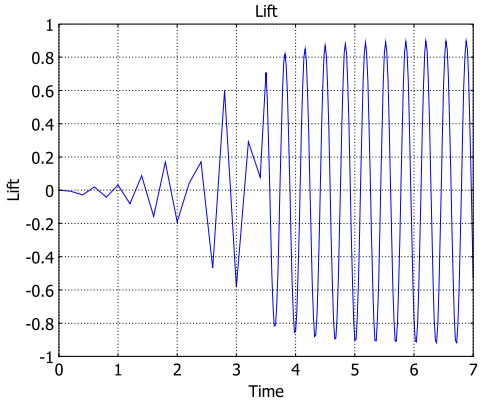


Figure 6-2: Time evolution of the total lift force on the cylinder.

Finally, you can investigate how suspended particles behave in the flow stream. Consider, for example, small water droplets entering with the air flow.

1. In the **Plot Parameters** dialog box, go to the **Particle Tracing** page.
2. Select the **Particle tracing plot** check box. In the **Plot type** list, select **Points**.
3. In the **Predefined forces** list, select the **Khan and Richardson force (ns)**.
4. On the **Start Points** page, enter `0` in the **x** edit field and then enter `range(0.1,0.05,0.3)` in the **y** edit field.

5 Go to the **Initial Values** page. Clear the **Auto** check box and enter `3.6` in the **Start time** edit field to study the particles only for fully developed flow.

6 In the **Initial velocity** edit fields, type `u` and `v` to give the particles the same initial velocity as the inflow.

7 Go to the **Point Settings** page, find the **When particles leaves domain** list, and select **Disappear**.

8 On the **Release** page, select **Time between releases** and specify the time as `0.4`.

9 Click the **Advanced** button.

10 Select the **Manual tuning of step size** check box and enter `0.02` in the **Initial time step** edit field and `0.01` for **Maximum time step**.

11 Click **OK** to close the **Advanced Parameters** window.

12 Go to the **Animate** page and click **Start Animation**. Remember that the time scale of the movie changes after 3.5 seconds.

Terminal Falling Velocity of a Sand Grain

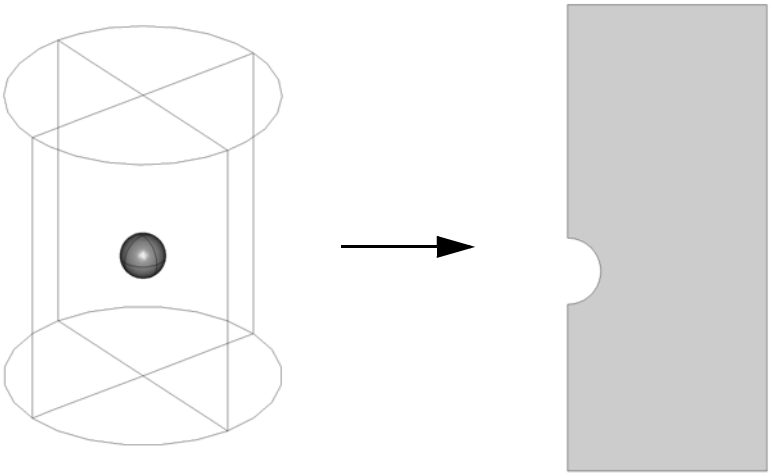
Introduction

The first stop for polluted water entering a water work is normally a large tank, where large particles are left to settle. More generally, gravity settling is an economical method of separating particles. If the fluid in the tank is moving at a controlled low velocity, the particles can be sorted in separate containers according to the time it takes for them to reach the bottom.

This model simulates a spherical sand grain falling in water. The grain accelerates from standstill and rapidly reaches its terminal velocity. The results agree very well with experimental studies. The model is an axially symmetric fluid-flow simulation in a moving coordinate system, coupled to an ordinary differential equation (ODE) describing the grain's motion.

Model Definition

The model couples the flow simulation in cylindrical coordinates with an ODE for the force balance of the particle. Due to axial symmetry, you can model the flow in 2D instead of 3D. The figure below shows the modeling domain.



DOMAIN EQUATIONS

The fluid flow is described by the Navier-Stokes equations

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

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

where ρ denotes the density (kg/m^3), $\mathbf{u}$ the velocity (m/s), η the viscosity (Ns/m^2), and p the pressure (Pa). The fluid is water with a viscosity of $1.51 \cdot 10^{-3}$ Ns/m^2 and a density of 1000 kg/m^3. The model uses the accelerating reference system of the sand grain. This means that the volume force density $\mathbf{F}$ is given by:

$$F_r = 0, \qquad F_z = -\rho(a + g)$$

where a (m/s^2) is the acceleration of the grain and $g = 9.81$ m/s^2 is the acceleration due to gravity. The ODE that describes the force balance is:

$$m\ddot{x} = F_g + F_z$$

where m (kg) denotes the mass of the particle, x (m) the position of the particle, F_g (N) the gravitational force, and F_z the z-component of the force that the water exerts on the sand grain. The gravitational force is given by:

$$F_g = -\rho_{\text{grain}} V_{\text{grain}} g$$

where V_{grain} (m^3) is the volume of the sand grain and ρ_{grain} (kg/m^3) its density. The force that the water exerts on the grain is calculated by integrating the normal component of the stress tensor over the surface of the particle. Because the model is axially symmetric, only the force's z-component is nonzero:

$$F_z = 2\pi \int_S r\mathbf{n} \cdot [-pI + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)]dS$$

where r (m) is the radial coordinate and $\mathbf{n}$ is the normal vector on the surface of the grain.

The initial values for position and velocities are $u_0 = v_0 = x_0 = \dot{x}_0 = 0$.

BOUNDARY CONDITIONS

At the surface of the sphere, the velocity relative the sphere is zero. Therefore, the model uses a *no-slip* condition, $\mathbf{u} = \mathbf{0}$. At the inlet of the fluid domain the velocity equals the falling velocity: $\mathbf{u} = (0, \dot{x})$. Symmetry, $\mathbf{n} \cdot \mathbf{u} = 0$, applies at the outer

boundary of the water domain, and a *neutral* condition, $\mathbf{n} \cdot [-pI + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] = 0$, describes the outlet. An axial symmetry condition models the symmetry axis at $r = 0$.

Results

Figure 6-3 shows the velocity field at the final simulation time, $t = 1$ s, when the particle has reached steady state.

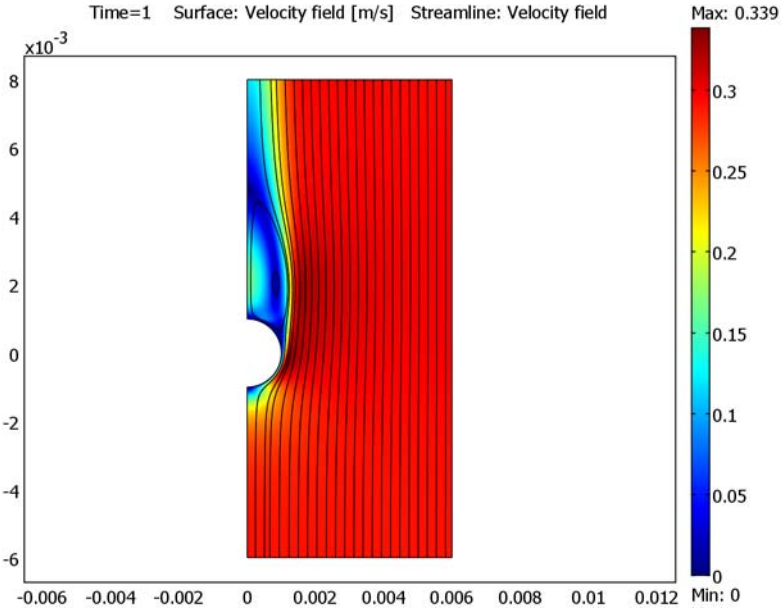


Figure 6-3: The velocity field at steady state. Note that the velocities are plotted in the reference system of the sand grain.

The following series of snapshots display velocity field from a moment just after the sand grain is released until it is approaching steady state. Notice the recirculation forming above the grain.

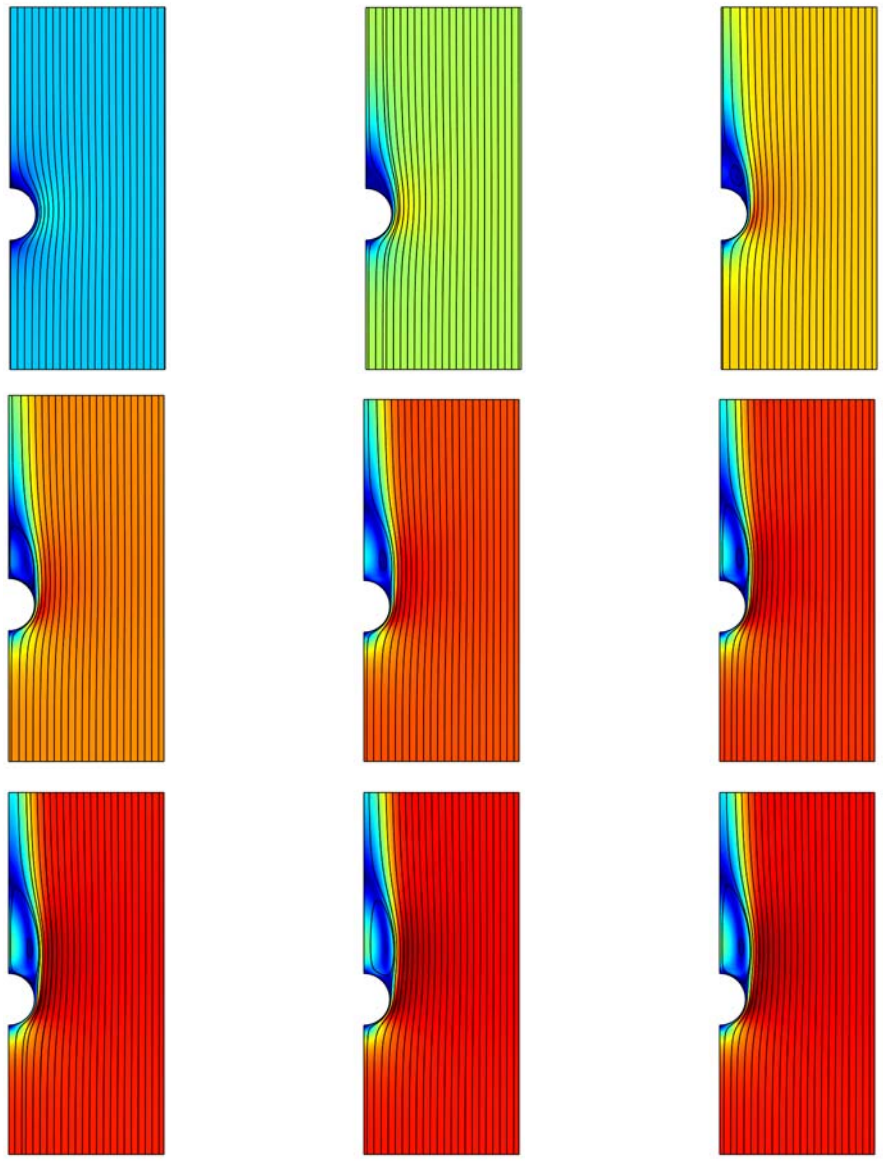


Figure 6-4: The velocity field around the sand grain at a series of times (t = 0.025 s, 0.05 s, 0.075 s, 0.1 s, 0.15 s, 0.2 s, 0.3 s, 0.5 s, and 0.75 s). For a color legend, see Figure 6-3.

Figure 6-5 shows the falling velocity of the grain as a function of time.

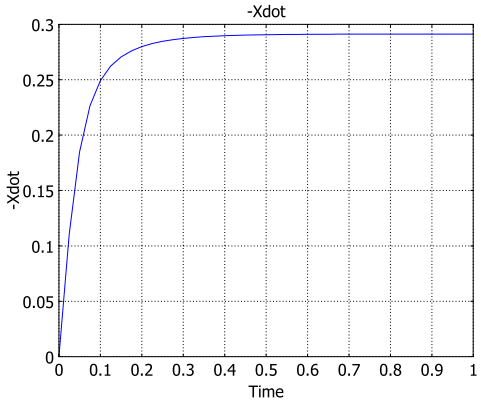


Figure 6-5: Falling velocity (m/s) of the grain versus time. After the solution time of 1 s, the velocity approaches the terminal velocity.

The terminal velocity equals 0.291 m/s. When this state is reached, the gravity and the forces from the water cancel out. Figure 6-6 shows the forces on the sand grain.

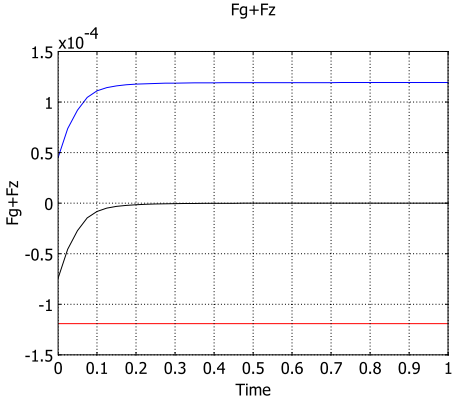


Figure 6-6: The forces on the sand grain. The force that the water exerts on the sphere (upper line) increases as the grain gains speed. The gravity force (lower line) remains the same, and the total force (middle line) tends toward zero as the solution approaches steady state.

Several approximate equations have been proposed for the terminal velocity of a sphere falling in a fluid. Ref. 1 cites the following expression for the total force that the fluid exerts on the sphere, as a function of the velocity:

$$F = \frac{\pi}{4} d^2 \rho v^2 (1.84\mathrm{Re}^{-0.31} + 0.293\mathrm{Re}^{0.06})^{3.45}$$

where d (m) is the diameter of the sphere, ρ (kg/m^3) the fluid density, v (m/s) the velocity, and $\mathrm{Re} = (\rho v d)/\mu$ is the Reynolds number, with μ (Ns/m^2) being the viscosity of the fluid. The gravity force is given analytically as $F_g = \pi d^3(\rho - \rho_s)g/6$, where ρ_s (kg/m^3) is the density of the sphere. Equating the two forces and introducing the values used in the simulation gives an approximate terminal velocity of 0.284 m/s.

The same reference discusses correction factors for non-spherical particles. You can easily adapt the model to hold for a general axially symmetric object (by redrawing the geometry) or even an arbitrarily shaped object (by modeling in 3D).

Reference

1. J.M. Coulson and J.F. Richardson, *Chemical Engineering vol. 2*, 4th ed., 1993.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/falling_sand`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list.
2. In the list of application modes, select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis**.
3. Click **Multiphysics**, and then **Add**.
4. Click the **Application Mode Properties** button and set **Weak constraints** to **On** and **Constraint type** to **Non-ideal**. Click **OK**.
5. Click **OK** to close the dialog box.

OPTIONS AND SETTINGS

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

2 Enter the following constant names, expressions, and (optionally) descriptions:

NAME	EXPRESSION	DESCRIPTION
rho_water	1000[kg/m^3]	Density, water
eta_water	1.51e-3[Pa*s]	Dynamic viscosity, water
r_grain	1[mm]	Radius, grain
V_grain	4/3*pi*r_grain^3	Volume, grain
rho_grain	2900[kg/m^3]	Density, grain
m_grain	V_grain*rho_grain	Mass, grain
g	9.81[m/s^2]	Acceleration due to gravity
Fg	-m_grain*g	Gravitational force on grain

3 Click **OK** to close the **Constants** dialog box.

GEOMETRY MODELING

1 Go to **Draw>Specify Objects** and specify a rectangle with the following properties:

PROPERTY	EXPRESSION
Width	6e-3
Height	14e-3
Position: Base	Corner
Position: r	0
Position: z	-6e-3

2 Click the **Zoom Extents** button to see the rectangle you just created.

3 Specify a circle centered at (0, 0) with the radius 10^{-3}.

4 Select both objects, then click the **Difference** button.

PHYSICS SETTINGS

Global Equations

1 From the **Physics** menu, choose **Global Equations**.

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

NAME	EQUATION	INIT (U)	INIT (UT)
X	Xt-Xdot	0	0
Xdot	Xdott-(Fz+Fg)/m_grain	0	0

Boundary Conditions

1 In the **Boundary Settings** dialog box, enter boundary coefficients as indicated in the table below; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 3	BOUNDARY 2	BOUNDARY 4	BOUNDARY 5	BOUNDARIES 6, 7
Boundary type	Symmetry boundary	Inlet	Open boundary	Symmetry boundary	Wall
Boundary condition	Axial symmetry	Velocity	Normal stress	Symmetry	No slip
U_0		`-Xdot`			
f_0			0		

The warning for inconsistent unit in the setting for the normal inflow velocity is caused because the variable `Xdot` from the ODE for the particle's position does not have a unit. You can ignore this warning.

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

3 On the **Source** tab, select Boundaries 6 and 7. Specify a boundary integration coupling variable with the **Name** `Fz` and the **Expression** `-2*pi*lm2`. Leave the **Integration order** at the default value `4` and the **Global destination** set to on. The Lagrange multiplier lm2 is equal to the z component of the total stress tensor times the r coordinate. Using the expression `-T_z_ns*2*pi*r` gives a similar solution but with a worse accuracy and a slightly higher memory consumption.

4 Click **OK** to close the dialog box.

Subdomain Settings

In the **Subdomain Settings** dialog box, enter the subdomain settings indicated in the table below.

PROPERTY	VALUE
ρ	`rho_water`
η	`eta_water`
F_r	`0`
F_z	`-rho_water*(Xdott+g)`

MESH GENERATION

1 Open the **Free Mesh Parameters** dialog box

2 Select **Fine** among the **Predefined mesh sizes**.

3 Click the **Custom mesh size** button and Set the **Element growth rate** to `1.1`.

4 On the **Boundary** page, set the **Maximum element size** for Boundary 3 to `2e-4`, and for Boundaries 6 and 7 to `1e-4`.

5 Click the **Remesh** button.

6 Click **OK** to close the dialog box.

COMPUTING THE SOLUTION

1 Open the **Solver Manager**.

2 On the **Output** page, select the **Include time derivatives** check box.

3 Click **OK** to close the dialog box.

1 Open the **Solver Parameters** dialog box.

2 On the **General** tab, enter `range(0,0.025,1)` in the **Times** edit field.

3 In the **Absolute tolerance** edit field, enter `1e-5`.

4 Click **OK** to close the dialog box.

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the velocity field in the reference system of the grain.

1 Open the **Plot Parameters** dialog box.

2 On the **Surface** page, click the **Surface Data** tab and then click the **Range** button.

3 In the **Color Range** dialog box, clear the **Auto** check box and enter `0.0` and `0.338` in the **Min** and **Max** edit fields, respectively. Click **OK**.

4 On the **Streamline** page, select the **Streamline plot** check box.

5 From the **Streamline plot type** list, select **Magnitude controlled**.

6 On the **Line Color** page, click the **Color** button. In the **Streamline Color** dialog box, select a black color. Click **OK**.

7 Click **OK** to see the combined surface and streamline plot in Figure 6-3.

You can also visualize the velocity as a function of time:

8 Choose **Postprocessing>Domain Plot Parameters**.

9 On the **Point** page, select Point 1 and type `-Xdot` in the **Expression** edit field.

10 Click **Apply** to reproduce the plot in Figure 6-5.

To view all the forces in the same figure, follow these instructions:

11 On the **Point** page, select an arbitrary point and enter `Fz` in the **Expression** edit field.

12 Click **Apply** to plot the viscous and pressure contributions to the force against time.

13 On the **General** page, select the **Keep current plot** check box.

14 On the **Point** page, click the **Line Settings** button. Select a red color, then click **OK**.

15 In the **Expression** edit field, enter `Fg`. Click **Apply**.

16 Click the **Line settings** button again and select a black color.

17 In the **Expression** edit field, enter `Fg+Fz`.

18 Click **OK** to reproduce the plot in Figure 6-6 and close the dialog box.

Fluid Valve

Introduction

Many different applications such as printers involve the periodic opening and closing of fluid-flow channels. This is generally a difficult problem to model as it implies a moving boundary condition for the part of the geometry that acts as an obstacle for the flow.

An alternative is to use a material property (viscosity), which is easy to vary over time. In this case, specify a very large viscosity (ideally it should be an infinite viscosity) that in effect stops the flow in regions where this large viscosity is present. To simulate the movement of this region of large viscosity, the model includes a logical expression in the subdomain settings.

The model describes a valve where it is possible to direct the flow into one of the two channels. Flow of varying degrees can also occur in both channels during the opening and closing stages.

Model Definition

Figure 6-7 shows the model domain.

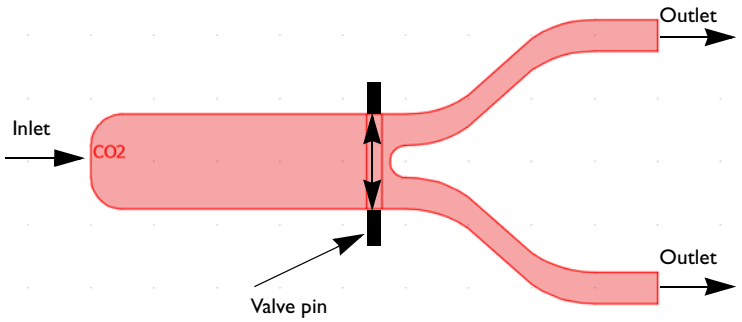


Figure 6-7: Depiction of the geometry and the operation of the fluid valve. Flow enters from one inlet at the left, but can leave the valve through two outlets at the right. The choice of outlet depends upon the position of the valve pin. In this model, two valve pins oscillate between the following positions: in front of one outlet channel to in front of the other. Sometimes flow is possible through both outlets, depending on the position of the pins.

In this model, the valve pin moves according to a sinusoidal function of time. The inlet velocity is constant.

DOMAIN EQUATIONS

The fluid flow is described by the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = 0$$
$$\nabla \cdot \mathbf{u} = 0 \tag{6-1}$$

where ρ denotes the density (kg/m^3), $\mathbf{u}$ the velocity vector (m/s), η the viscosity (Ns/m^2), and p the pressure (Pa). The modeled fluid is air with viscosity 10^{-5} Ns/m^2 and density 1 kg/m^3.

The movement of the valve is described with an analytic expression pin, which returns the value of one in the area corresponding to the valve pin and zero elsewhere. The viscosity is then expressed by

$$\eta = \eta_0 + \mathrm{pin} \cdot \eta_\infty \tag{6-2}$$

where η_0 is the fluid viscosity, η_∞ is a very large viscosity (ideally infinite), and pin is described by

$$\mathrm{pin} = x_{\mathrm{pin}} y_{\mathrm{pin}} \tag{6-3}$$

where

$$x_{\mathrm{pin}} = (x > x_0)(x < x_1) \tag{6-4}$$

$$y_{\mathrm{pin}} = 1 - (y > y_1) + (y > y_2) \tag{6-5}$$

y_1 and y_2 depend on time, t, according to:

$$y_1 = -y_0 + y_{\max}\sin(2\pi t)$$
$$y_2 = y_0 + y_{\max}\sin(2\pi t) \tag{6-6}$$

and where y_0, x_0, x_1, and $y_{\max}$ are fixed in time and describe the size of the valve pin and the amplitude with which the pin moves.

BOUNDARY CONDITIONS

At the inlet, the model uses a fully developed laminar flow. The velocity is set to a parabolic velocity profile with maximum velocity $v_{\max}$ equal to 0.25 m/s. At the outlets, a neutral boundary condition states that the normal component of the stress tensor is zero:

$$\mathbf{n} \cdot [-pI + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] = 0 \quad (6\text{-}7)$$

All other boundaries have a no-slip condition

$$\mathbf{u} = 0 \quad (6\text{-}8)$$

Results

Figure 6-8 shows the velocity field (modulus of the velocity vector) when the valve is completely open. Firstly, the plot shows that the inlet is smaller than the compartment that it enters, so that some distance is required before the flow reaches another parabolic profile for the main body of the inlet chamber. If you investigate the velocity, some recirculation occurring at the corners of the chamber beside the inlet is visible.

Secondly, the structure of the outlet channels leads to a slight thinning toward the middle of the channels. This provides a slight acceleration, and subsequently greater velocity magnitude, in these regions.

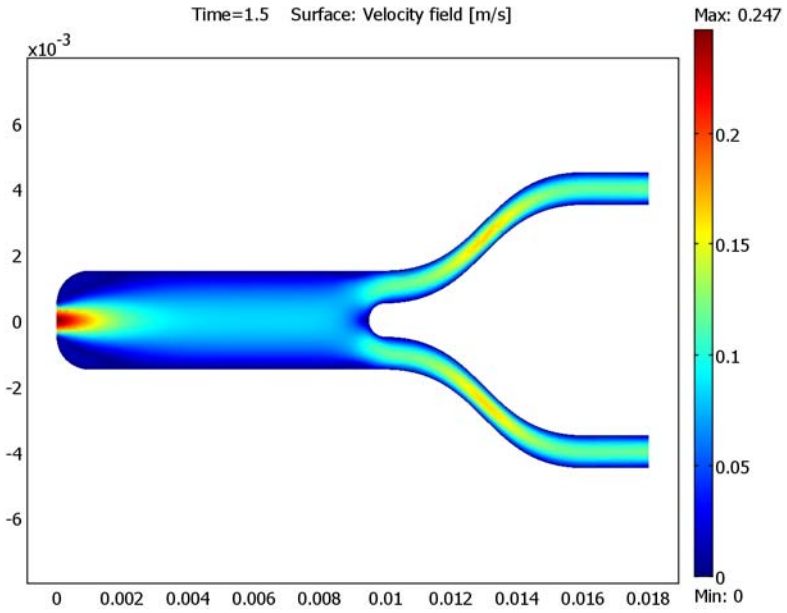


Figure 6-8: Velocity field when the valve is completely open.

Figure 6-9 shows the velocity field when the valve is halfway closed from above and fully closed from below. The use of a very large viscosity not only simulates the solidity

of the valve pin but also does a good job of providing a no-slip boundary condition at the edge of the valve pin.

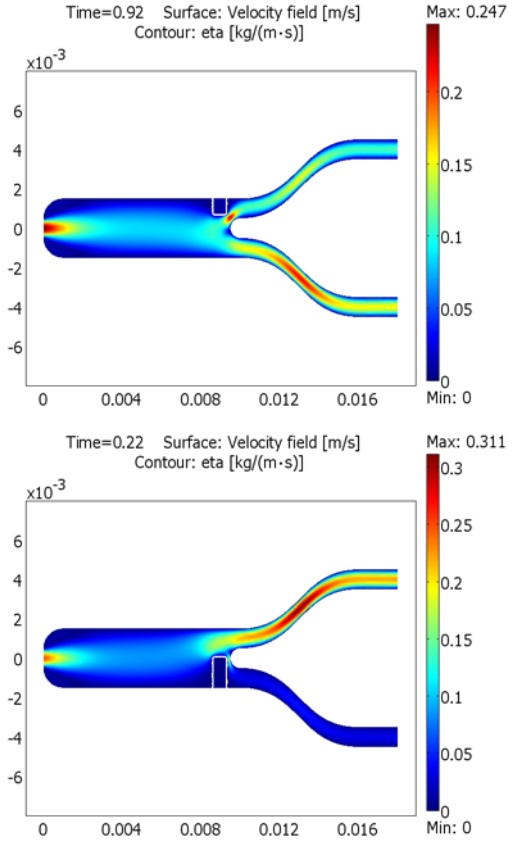


Figure 6-9: Velocity field when the valve is half way closed from above (top) and fully closed from below (bottom).

Figure 6-10 shows a plot of the flow rates (integral of the velocity vector over the outlets) in the upper and lower channels as well as the total flow rate. The figure illustrates the periodic flow due to the periodic motion of the valve pin.

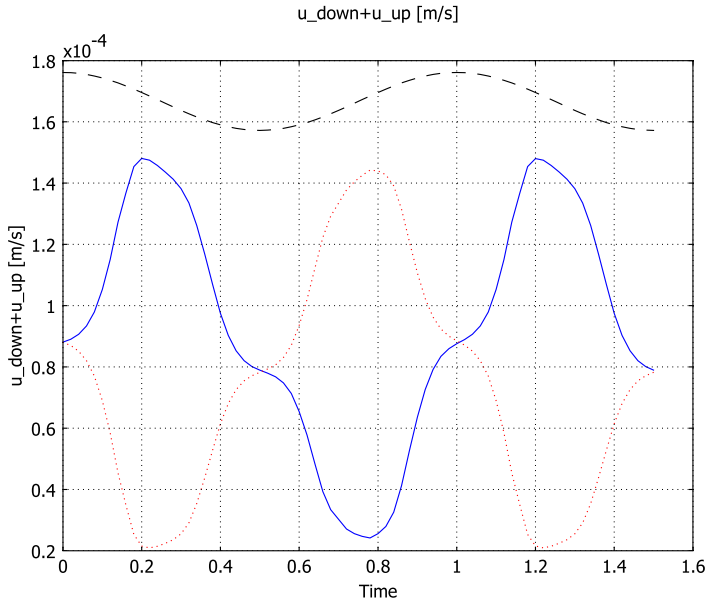


Figure 6-10: The blue line (solid) shows flow rate in the upper branch as a function of time, while the dotted line shows the flow rate in the lower branch. The dashed line shows the sum of the flow in the two branches.

Modeling in COMSOL Multiphysics

The inequalities used to describe the pin motion are, in the COMSOL Multiphysics implementation, replaced by smooth step functions. The smooth step function in this model is `flc2hs`, which returns a C^2-continuous step with a given step width.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/fluid_valve`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

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

3 From the list of application modes, select **COMSOL Multiphysics> Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis**.

4 Click **OK**.

GEOMETRY MODELING

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

2 Specify the rectangle settings according to the following table; when done, click **OK**.

PROPERTY	EXPRESSION
Width	0.01
Height	3e-3
Position: Base	Corner
Position: x	0
Position: y	-1.5e-3

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

4 Draw another rectangle according to:

PROPERTY	EXPRESSION
Width	5e-4
Height	3e-3
Position: Base	Center
Position: x	9e-3
Position: y	0

5 Open the **Axes/Grid Settings** dialog box from the **Options** menu.

6 Enter the following axis settings:

PROPERTY	EXPRESSION
x min	0.009
x max	0.019
y min	0
y max	5e-3

7 Click the **Grid** page, clear the **Auto** check box and set **y spacing** to 5e-4.

8 Click **OK**.

9 Click the **3rd Degree Bézier Curve** button in the Draw toolbar.

10 Click in the points (0.01, 0.0015), (0.013, 0.0015), (0.013, 0.0045), and (0.016, 0.0045).

11 Switch to the **Line** tool by clicking the **Line** button in the Draw toolbar.

12 Click the points (0.018, 0.0045), (0.018, 0.0035), and (0.016, 0.0035).

13 Switch back to the **3rd Degree Bézier Curve** and click the points (0.013, 0.0035), $(0.013, 5{\cdot}10^{-4})$, and $(0.01, 5{\cdot}10^{-4})$.

14 Close the geometry object by right-clicking anywhere in the drawing area.

15 To make the lower branch, use the mirror tool. Make sure that the upper branch geometry object is selected and click the **Mirror** button in the Draw toolbar.

16 Let the **Point on line** settings remain at the default settings. Change the **Normal vector** from (1, 0) to (0, 1).

17 Click **OK**.

18 Draw a circle with radius $5{\cdot}10^{-4}$ centred in the point (0.01, 0).

19 Click the **Zoom Extents** button.

20 Click the **Create Composite Object** button in the Draw toolbar to open the **Create Composite Object** dialog box.

21 Clear the **Keep interior boundaries** check box, type `R1+C01+C02-C1` in the **Set formula** edit field, and click **Apply**.

22 Select the **Keep interior boundaries** check box, type `R2+C03` in the **Set formula** edit field, and click **OK**.

23 The last step of the geometry modeling is to fillet the left corners. Click the **Fillet/Chamfer** button in the Draw toolbar.

24 Select Points 1 and 2, enter `1e-3` in the **Radius** edit field and click **OK**.

OPTIONS AND SETTINGS

1 Open the **Constants** dialog box from the **Options** menu and enter constants according to the following table. When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
x0	8.7[mm]	Valve left end point
x1	9.2[mm]	Valve right end point
scale	1e-4	Step function scaling
y_max	1.5[mm]	Valve pin amplitude
eta_0	1e-5[Pa*s]	Fluid viscosity

NAME	EXPRESSION	DESCRIPTION
eta_inf	1[Pa*s]	Large viscosity
rho	1[kg/m^3]	Fluid density
v_max	0.25[m/s]	Maximum inlet velocity

2 From the **Options** menu, choose **Expressions>Scalar Expressions**.

3 Enter scalar expressions according to the following table. When done, click **OK**.

NAME	EXPRESSION
x_range	flc2hs((x-x0)[1/m],scale)*(1-flc2hs((x-x1)[1/m],scale))
y_range	1-flc2hs((y-y1)[1/m],scale)+flc2hs((y-y2)[1/m],scale)
y1	-1.5[mm]+y_max*sin(2*pi*t[1/s])
y2	1.5[mm]+y_max*sin(2*pi*t[1/s])
pin	y_range*x_range
eta	eta_0+eta_inf*pin
pin_vel	y_max*pi*2[1/s]*cos(2*pi*t[1/s])

The reason for the `[1/m]` entries for the input arguments to `flc2hs` is to make them dimensionless. Likewise, the input argument to the `sin` and `cos` functions must be dimensionless; appending `[1/s]` to the variable `t` for time accomplishes this.

4 Select **Integration Coupling Variables>Boundary Variables** from the **Options** menu.

5 Select Boundary 15 from the **Boundary selection** list. Type `u_up` in the **Name** edit field and `u` in the **Expression** edit field. Leave the **Integration order** at 4 and **Global destination** active.

6 Select Boundary 14 from the **Boundary selection** list. On the second row, type `u_down` in the **Name** edit field and `u` in the **Expression** edit field. Leave the **Integration order** at 4 and **Global destination** active.

7 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

Define the properties of the fluid:

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

2 Select all subdomains.

3 Set the **Density** to `rho` and the **Dynamic viscosity** to `eta`.

4 Click **OK**.

Boundary Conditions

Open the **Boundary Settings** dialog box from the **Physics** menu and enter boundary conditions according to the following table. When done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 5, 6	BOUNDARIES 14, 15	ALL OTHERS
Boundary type	Inlet	Inlet	Open boundary	Wall
Boundary condition	Velocity	Velocity	Normal stress	No slip
U_0	`4*v_max*s*(1-s)`	`pin_vel`	-	-
f_0	-	-	0	-

MESH GENERATION

1. Open the **Free Mesh Parameters** dialog box from the **Mesh** menu.
2. On the **Global** page, click the **Custom mesh size** button, and then set **Maximum element size** to `0.0004` and **Element growth rate** to `1.5`.
3. Click the **Subdomain** tab.
4. Select Subdomain 2 from the **Subdomain selection** list. Set **Maximum element size** to `0.0001`.
5. Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1. Open the **Solver Parameters** dialog box from the **Solve** menu.
2. In the **Time stepping** area, set **Times** to `range(0,0.02,1.5)`, **Relative tolerance** to `0.001`, and **Absolute tolerance** to `0.0001`.
3. On the **Time Stepping** page, select **Free** from the **Time steps taken by solver** list. The default CFL number-based time step uses a viscous time scale as a lower limit. This limit is not suitable when using the viscosity to model a solid.
4. Click **OK**.
5. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create the image in Figure 6-8, do the following steps.

1. Open the **Plot Parameters** dialog box from the **Postprocessing** menu.
2. On the **General** page, clear the **Geometry edges** check box and make sure that the **Surface** check box is selected.

3 On the **Surface** page, select **Velocity field** from the **Predefined quantities** list on the **Surface Data** tab and click **Apply**.

To create the images in Figure 6-9 do the following steps:

4 On the **General** page, select the time step at **0.22** from the **Solution at time** list.

5 Select the **Contour** plot type.

6 On the **Contour** page, type `eta` in the **Expression** edit field.

7 In the **Contour levels** frame, select the **Vector with isolevels** and type `range(1e-3,1e-5,1.1e-3)`.

8 In the **Contour color** area, select **Uniform color**, click the **Color** button, and select white. Click **OK** to close the **Contour Color** dialog box. Clear the **Color legend** check box.

9 Click **Apply** in the **Plot Parameters** dialog box.

To create the top image, repeat the above steps but for time step 0.92.

Use the following steps to create Figure 6-10:

1 Open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

2 On the **General** page, select the **Keep current plot** check box.

3 Click the **Point** tab and select Point 1 from the **Point selection** list.

4 Type `u_up` in the **Expression** edit field.

5 Click the **Line Settings** button and set **Line color** to a blue color by first selecting **Color** from the **Line color** list and then clicking the **Color** button. Select **Solid line** from the **Line style** list. Click **OK**.

6 Click **Apply**.

7 Type `u_down` in the **Expression** edit field.

8 Click the **Line Settings** button and set **Line color** to a red color and **Line style** to **Dotted line**. Click **OK**.

9 Click **Apply**.

10 Repeat for the expression `u_down+u_up` with a dashed, black line.

Micromixer

Introduction

This example studies a laminar static mixer with two parallel sets of split-reshape-recombine mixing elements. Figure 6-11 shows the geometry of a single mixing element.

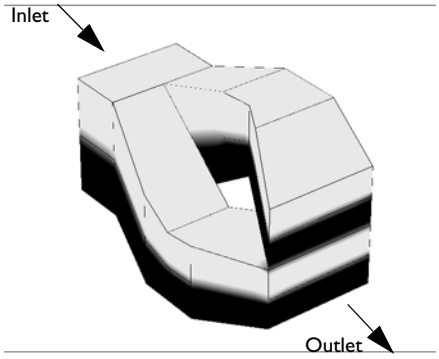


Figure 6-11: The micromixer splits the incoming fluid in the direction perpendicular to the interface separating the two fluid layers. After recombining them, the mixer stacks the two flows on top of each other, resulting in four fluid layers.

Each mixing element doubles the number of fluid layers, resulting in a fast mixing process. This technique is suited for laminar flow mixing and has small pressure losses. In this model, the mixing structure consists of two parallel sets of mixing elements, where each set is two elements long. You measure the mixing quality with the relative variance of the concentration profile, S, calculated as

$$S = \frac{s_x}{s_{\text{inlet}}}$$

$$s_x = \int_{K_x} (c - \bar{c})^2 dA$$

where K_x is the yz-plane intersecting the mixing structure at coordinate x, and c is the mean concentration.

DOMAIN EQUATIONS

The fluid flow is described by the Navier-Stokes equations

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

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

where ρ denotes the density (kg/m^3), $\mathbf{u}$ the velocity (m/s), η denotes the viscosity (N·s/m^2), and p represents the pressure (Pa). The modeled fluid is water with a viscosity of $1 \cdot 10^{-3}$ N·s/m^2 and a density of 1000 kg/m^3.

The mass flux is given by diffusion and convection, and the resulting mass balance is

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

where D denotes the diffusion coefficient (m^2/s) and c gives the concentration (mol/m^3). The modeled species is bicarbonate ions with a diffusion coefficient of $1.49 \cdot 10^{-9}$ m^2/s.

BOUNDARY CONDITIONS

At the inlet the model assumes fully developed laminar flow. It sets the velocity to a parabolic profile with a mean velocity of 0.01 m/s. At the outlet, the model sets the pressure to zero. All other boundaries have a no-slip condition

$$\mathbf{u} = 0.$$

The inlet concentration has a discontinuous profile where the upper half has a concentration of 27 mol/m^3 and the lower half is pure water. The boundary condition is defined such that

$$c|_{\text{inlet}} = \begin{cases} c_0 & z > 0 \\ 0 & z \le 0. \end{cases}$$

Results

Figure 6-12 shows the final concentration profile. The concentration values in some points of the solution are slightly negative; this is due to the numerical method.

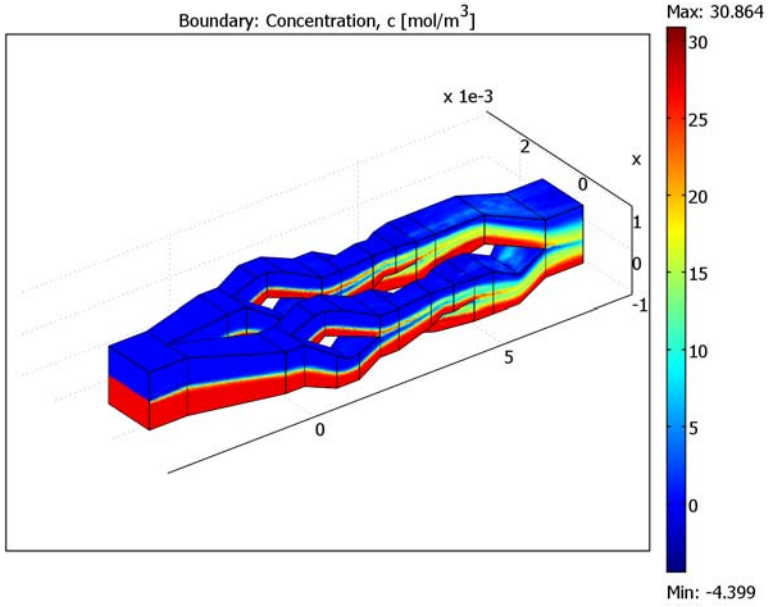


Figure 6-12: Following three split-reshape-recombine cycles, the outflow has eight fluid layers.

Using boundary integration to calculate the relative variance of the concentration at the inlet and outlet, this setup reaches a mixing quality of 0.31 (for perfect mixing this value would be 0, and a value of 1 means no mixing at all). To improve this quality, add mixing elements.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/micromixer`

MODEL NAVIGATOR

1 Open the **Model Navigator,** go to the **Space dimension** list and select **3D**. Click the **Multiphysics** button.

2 Select the application mode **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Steady-state analysis**, then click the **Add** button.

3 Select **COMSOL Multiphysics>Convection and Diffusion>Convection and Diffusion**. Click the **Add** button once again.

4 Click **OK**.

OPTIONS AND SETTINGS

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

2 Define the following names, expressions, and (optionally) descriptions:

NAME	EXPRESSION	DESCRIPTION
rho	1e3[kg/m^3]	Density
eta	1e-3[Pa*s]	Dynamic viscosity
U_mean	0.01[m/s]	Mean inlet velocity
c0	27[mol/m^3]	Inlet concentration
D	1.49e-9[m^2/s]	Diffusion coefficient

3 Click **OK**.

GEOMETRY MODELING

This section describes how to build the model geometry step by step. Because it is a rather lengthy procedure, we have included the finished geometry as a CAD file to give you the option of skipping this modeling stage. Thus, if you prefer to use the finished geometry, you can skip directly to "Importing the Geometry from a CAD File" on page 248.

The geometry consists of a rectangular channel that is split and recombines several times. Start by defining a work plane.

1 From the **Draw** menu select **Work-Plane Settings**. Click **OK** to select the default **x-y** work plane at $z = 0$.

2 Select the menu item **Options>Axes/Grid Settings**.

3 Verify that you are on the **Axis** page. Enter the following settings:

PROPERTY	EXPRESSION
x min	-1e-3
x max	3e-3
y min	-1e-3
y max	1e-3

4 Go to the **Grid** page. Clear the **Auto** check box, then in both the **x spacing** and **y spacing** edit fields enter 1e-4.

5 Click **OK**.

Constructing a Single Mixing Element

1 Go to the Draw toolbar on the left side of the user interface and click the **Line** button. Draw a seven-sided polygon in the drawing area by clicking, in order, the coordinates (0, 0), (0, $0.5\cdot10^{-3}$), ($0.7\cdot10^{-3}$, $0.7\cdot10^{-3}$), ($1.3\cdot10^{-3}$, $0.7\cdot10^{-3}$), ($2\cdot10^{-3}$, $0.5\cdot10^{-3}$), ($2\cdot10^{-3}$, $-0.5\cdot10^{-3}$), ($1\cdot10^{-3}$, $0.1\cdot10^{-3}$), and (0, 0). Finally, click the right mouse button to create the solid object. (Soon you will learn about an alternative method for creating polygons.)

2 From the **Draw** menu choose **Extrude**. In the **Distance** edit field enter 2e-3, then click **OK**.

3 Click the **Move** button on the Draw toolbar. Set the **Displacement: z** to -1e-3, then click **OK**.

4 Press Ctrl+C and then Ctrl+V to make a copy of the extruded object and paste it. In the **Paste** dialog box that opens, leave all **Displacement** components at 0. Click **OK**.

5 On the Draw toolbar click the **Rotate** button. Set the **Rotation angle** to 90, then set the **Rotation axis direction vector** to **x**, **y**, and **z** values of 1, 0, and 0, respectively. Click **OK**.

6 Return to the Draw toolbar and again click the **Rotate** button. Set the **Rotation angle** to 180. This time go to the **Point on rotation axis** area, and in the **x**, **y**, and **z** edit fields enter 1e-3, 0, and 0, respectively. Click **OK**.

7 Press Ctrl+A to select both objects, then click the **Intersection** button on the Draw toolbar.

8 Make a copy of the object by pressing Ctrl+C, then Ctrl+V, and choosing **OK**.

9 Go to the Draw toolbar and click the **Rotate** button. Set the **Rotation angle** to 180, then set the **Rotation axis direction vector** to **x**, **y**, and **z** values of 1, 0, and 0, respectively. Click **OK**.

Connecting a Second Mixing Element in the Series

1. Press Ctrl+A to select both objects.
2. Go to the Draw toolbar and click the **Mirror** button and in the **Normal vector** row enter values for **x**, **y**, and **z** of `0`, `1`, and `0`, respectively. Click **OK**.
3. Click the **Move** button on the Draw toolbar. Set the **Displacement: x** to `2.5e-3`. Click **OK**.

Making Square Channel Connections Between the Mixing Elements

1. From the **Draw** menu select the **Geom2** work plane.
2. From the Draw menu select the **Rectangle/Square** button and note that the cursor changes to a crosshair (alternatively, select **Draw>Draw Objects>Rectangle/Square**). Using the mouse, drag the cursor to create a rectangle with its base corner at $(-0.5\cdot10^{-3}, -0.5\cdot10^{-3})$, a width of $0.5\cdot10^{-3}$, and a height of $1\cdot10^{-3}$.
3. Select the menu item **Draw>Extrude**. In the **Distance** edit field enter `1e-3`, then click **OK**.
4. On the Draw toolbar click the **Move** button. Set the **Displacement: z** to `-0.5e-3`.
5. On the Draw toolbar click the **Array** button. Change the **Displacement: x** to `2.5e-3` and the **Array size: x** to `3`. Click **OK** to create the array.

Getting Two Mixing Channels in Parallel

1. Press Ctrl+A to select all the objects.
2. From the Draw toolbar select **Move**. Set the **Displacement: y** to `1e-3`. Click **OK**.
3. Press Ctrl+C and Ctrl+V to copy and paste the objects. Set the **Displacement: y** to `-2e-3`, then click **OK**.

Connecting the Two Parallel Channels to a Single Channel at Both Ends

1. From the **Draw** menu select the **Geom2** work plane.
2. On the Draw toolbar, Shift-click the **Rectangle/Square** button. In the **Rectangle** dialog box create a rectangle with its base corner at $(-3.5\cdot10^{-3}, -0.7\cdot10^{-3})$, a width of 10^{-3}, and a height of $1.4\cdot10^{-3}$.
3. From the **Draw** menu choose **Extrude**. Set the **Distance** to `1.4e-3`, then click **OK**.
4. Go to the Draw toolbar and click the **Move** button. Set the **Displacement: z** to `-0.7e-3`, then click **OK**.
5. Press Ctrl+C and Ctrl+V to copy and paste the objects; set the **Displacement: x** to `10.5e-3`, then click **OK**.

6 Click on the tab at the top of the drawing area to return to the Geom2 work plane. On the Visualization/Selection toolbar on the left side of the user interface choose **Projection of All 3D Geometries**.

7 Draw a four-sided polygon with corners at the points $(-2.5\cdot10^{-3}, 0)$, $(-0.5\cdot10^{-3}, 0.5\cdot10^{-3})$, $(-0.5\cdot10^{-3}, 1.5\cdot10^{-3})$, and $(-2.5\cdot10^{-3}, 0.7\cdot10^{-3})$. To do so, select the menu item **Draw>Specify Objects>Line** (or Shift-click the **Line** button in the Draw toolbar). In the resulting dialog box find the **Style** list and select **Closed polyline (solid)**. In the **x** edit field enter the sequence of x-coordinates from the coordinate pairs just given, then do the same for the y-coordinates in the **y** edit field. Click **OK**.

8 Next, extrude the polygon: select the menu item **Draw>Extrude**, then in the **Distance** edit field type `2e-3`. Click **OK**.

9 Move the extruded polygon. From the Draw toolbar select the **Move** tool. You default to the **Displacement** area, and in the **z** edit field enter `-1e-3`.

Setting Up a Second Work Plane

1 From the **Draw** menu select **Work-Plane Settings**, then click **Add**. A new work plane, **Geom3**, appears. Select the **z-x** plane and click **OK**.

2 On the Visualization/Selection toolbar choose **Projection of All 3D Geometries**.

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

4 From the **Options** menu open the **Axes/Grid Settings** dialog box. On the **Grid** page clear the **Auto** check box. In both the **x spacing** and **y spacing** edit fields enter `1e-4`.

5 Using the **Closed polyline (solid)** technique already described, draw a four-sided polygon with corners at the points $(-0.7\cdot10^{-3}, -2.5\cdot10^{-3})$, $(0.7\cdot10^{-3}, -2.5\cdot10^{-3})$, $(0.5\cdot10^{-3}, -0.5\cdot10^{-3})$, and $(-0.5\cdot10^{-3}, -0.5\cdot10^{-3})$.

6 Select **Draw>Extrude**, then in the **Distance** edit field type `2e-3`. Click **OK**.

7 Select the two extruded geometries (EXT9 and EXT10). Go to the Draw toolbar and click the **Intersection** button.

8 Go back to the Draw toolbar and click the **Mirror** button. Set the **x**, **y**, and **z** values of the **Normal vector** to `0`, `1`, and `0`, respectively. Click **OK**.

Doubling the Number of Fluid Layers

When building the outflow connections, notice that you can double the fluid layers one more time by guiding the channels properly.

1 Click the appropriate tab at the top of the drawing area to return to the Geom2 work plane.

2 Using the **Closed polyline (solid)** technique already described, draw a five-sided polygon with corners at the points $(5\cdot10^{-3}, 0.5\cdot10^{-3})$, $(6\cdot10^{-3}, 0.1\cdot10^{-3})$, $(7\cdot10^{-3}, -0.7\cdot10^{-3})$, $(7\cdot10^{-3}, 0.7\cdot10^{-3})$, and $(5\cdot10^{-3}, 1.5\cdot10^{-3})$.

3 Select **Draw>Extrude**, then in the **Distance** edit field type `2e-3`. Click **OK**.

4 Move the extruded polygon. From the Draw toolbar select the **Move** tool. You default to the **Displacement** area, and in the **z** edit field enter `-1e-3`. Click **OK**.

5 Go to the **Geom3** work plane.

6 Using the **Closed polyline (solid)** technique already described, draw a six-sided polygon with corners at the points $(0.5\cdot10^{-3}, 5\cdot10^{-3})$, $(0.8\cdot10^{-3}, 6\cdot10^{-3})$, $(0.7\cdot10^{-3}, 7\cdot10^{-3})$, $(0, 7\cdot10^{-3})$, $(0.1\cdot10^{-3}, 6\cdot10^{-3})$, and $(-0.5\cdot10^{-3}, 5\cdot10^{-3})$.

7 Select **Draw>Extrude**, then in the **Distance** edit field type `3e-3`. Click **OK**.

8 From the Draw toolbar select the **Move** tool. You default to the **Displacement** area, and in the **y** edit field enter `-1e-3`. Click **OK**.

9 Select the EXT9 and EXT10 geometries; on the Draw toolbar click the **Intersection** button.

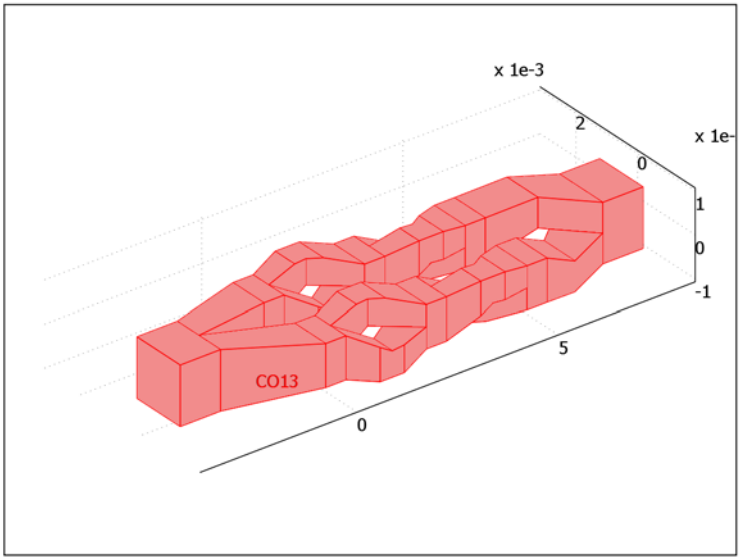
10 Press Ctrl+C and Ctrl+V to make a copy of the new object. In the **Paste** dialog box, leave all **Displacement** components at `0`. Click **OK**.

11 Go to the Draw toolbar and click the **Rotate** button. Set the **Rotation angle** to `180`, then set the **Rotation axis direction vector** to **x**, **y**, and **z** values of `1`, `0`, and `0`, respectively. Click **OK**.

12 Press Ctrl+A to select all the geometry objects.

13 From the Draw toolbar choose **Create Composite Object**. Clear the **Keep interior boundaries** check box, then click **OK**.

This completes the geometry-modeling stage. The resulting geometry should look like that in the figure below.



Model geometry.

Importing the Geometry from a CAD File

If you followed the step-by-step instructions for how to generate the geometry, skip this section and proceed to "Physics Settings—Incompressible Navier-Stokes" below.

To import the model geometry CAD file follow these steps:

1. From the **File** menu select **Import>CAD Data From File**.
2. In the **Import CAD Data From File** dialog box, browse to the folder `models/COMSOL_Multiphysics/Fluid_Dynamics` in the COMSOL installation directory.
3. Select the file `micromixer.mphbin`, then click **Import**.

PHYSICS SETTINGS—INCOMPRESSIBLE NAVIER-STOKES

Boundary Conditions

1. From the **Multiphysics** menu select **1 Incompressible Navier-Stokes (ns)**.

2 From the **Physics** menu open the **Boundary Settings** dialog box. Enter settings from the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 136	ALL OTHERS
Boundary type	Inlet	Outlet	Wall
Boundary condition	Velocity	Pressure, no viscous stress	No slip
u_0	`(9/4)*U_mean*16*s1*(1-s1)*s2*(1-s2)`	-	-
v_0	0	-	-
w_0	0	-	-
P_0	-	0	-

Subdomain Settings

1 Select the menu item **Physics>Subdomain Settings**.

2 Select Subdomain 1. Set the **Density** to `rho` and the **Dynamic viscosity** to `eta`.

3 Click the **Init** tab and then select Subdomain 1. Set the following initial conditions; when finished, click **OK**.

VARIABLE	VALUE
$u(t_0)$	`U_mean`
$v(t_0)$	0
$w(t_0)$	0
$p(t_0)$	0

PHYSICS SETTINGS—CONVECTION AND DIFFUSION

Boundary Conditions

1 From the **Multiphysics** menu select **2 Convection and Diffusion (cd)**.

2 Select the menu item **Physics>Boundary Settings**. Enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 136	ALL OTHERS
Type	Concentration	Convective flux	Insulation/Symmetry
c_0	`c0*(z<0)`		

Subdomain Settings

1 From the **Physics** menu open the **Subdomain Settings** dialog box.

2 Select all the subdomains, then enter coefficients from the following table:

NAME	EXPRESSION
D (isotropic)	D
R	0
u	u
v	v
w	w

3 Click the **Artificial Diffusion** button. In the resulting dialog box, select the **Streamline diffusion** check box. Click **OK**.

4 Click the **Init** tab. In the **$c(t_0)$** edit field enter `c0`.

5 Click **OK**.

MESH GENERATION

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

2 Click the **Custom mesh size** button and enter `3e-4` in the **Maximum element size** edit field.

3 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Because the fluid's properties do not change with concentration, this example solves the Navier-Stokes equations independently.

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

2 Go to the **Solve For** page. Select **Incompressible Navier-Stokes (ns)**, then click **OK**.

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

4 On the **General** page, select **Geometric multigrid** from the **Linear system solver** list and then click **OK**. This also sets up the Vanka smoother with pressure as the Vanka variable.

5 Click the **Solve** button on the Main toolbar to calculate the flow field.

Solving the Mass Balance

With the flow field computed, it is time to turn to the mass balance equation. The example solves the mass balance on a finer mesh so it can resolve the high gradients in the interface between the fluid layers.

1 From the **Mesh** menu open the **Free Mesh Parameters** dialog box.

2 Click the **Custom mesh size** button and in the **Maximum element size** edit field enter `1.25e-4`.

3 Click **Remesh**, then click **OK**.

Adjust the solver settings to solve for the mass balance:

1 From the **Solve** menu open the **Solver Manager** dialog box.

2 Click the **Solve For** tab. Select **Convection and Diffusion (cd)**.

3 Click the **Initial Value** tab, then click the **Store Solution** button.

4 In the **Initial value** area, click the **Stored solution** option button. Click **OK**.

5 From the **Solve** menu open the **Solver Parameters** dialog box.

6 From the **Linear system solver** list, choose **BiCGStab**. Click **OK**. The BiCGStab solver is slightly more memory-efficient than GMRES, which is an alternative solver for large linear systems.

7 Compute the final solution by clicking the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Follow these instructions to reproduce the plot in Figure 6-12:

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

2 On the **General** page, locate the **Element refinement** label, clear the **Auto** check box, then in the associated edit field enter `2`.

3 In the **Plot type** area clear the **Slice** check box and select the **Boundary** check box.

4 Go to the **Boundary** page. In the **Predefined quantities** list select **Convection and Diffusion (cd)>Concentration, c**.

5 Click **OK**.

Finally calculate the mixing quality:

1 From the **Postprocessing** menu open the **Boundary Integration** dialog box.

2 Select Boundary 1 (the inlet), then in the **Expression** edit field enter `(c-c0/2)^2`.

3 Click **Apply** to perform the integration. The result appears in the report log at the bottom of the user interface.

4 Select Boundary 136 (the outlet). Click **OK** to perform the integration and close the dialog box.

5 Dividing the outlet value by the inlet value gives a measure of the mixing quality.

Shock Tube

Introduction

Shock waves arise from sudden jumps in gas properties such as temperature or pressure. We generally associate shock waves with violent processes such as supersonic flight or explosion blasts. However, even the slow movement of a piston in a tube can create flows that eventually turn into shock waves due to the inherent dynamics of the conservation of mass, momentum, and energy.

Discontinuities in flows were the topic of debate in the late 19th century, and even Lord Rayleigh at some point concluded they could not exist. What finally settled the issue was photographic evidence from a shock-tube experiment such as the one described here.

A shock tube is a device for studying shock waves. Prior to starting an experiment, a diaphragm inside the tube blocks any flow. You then increase the pressure on one side, for example, by using a compressor, and start the flow by rupturing the diaphragm. The gas then expands down the other half of the tube. Through optical means you can observe the flow and model the action of shocks. A pressurized tube of this type can store substantial amounts of energy, allowing for the study of quite violent flows—albeit for only very short periods.

Model Definition

The effects of viscosity and heat conduction are small for the time scales of interest here. Therefore the Euler equations of gas dynamics define the flow as movement of a compressible inviscid gas in the tube according to

$$\rho_t + u\rho_x + u_x\rho = 0$$

$$u_t + uu_x + \frac{p_x}{\rho} = 0$$

$$p_t + up_x + a^2\rho u_x = 0$$

where u is the velocity, ρ is the density, and p is the pressure.

The speed of sound a in a polytropic gas is given by:

$$a^2 = \gamma \frac{p}{\rho}$$

Here γ gives the ratio of specific heats at constant pressure to constant volume; for a diatomic gas such as air, γ is $7/5$. Thus you can write the equations as

$$0 = -(\rho_t + u\rho_x + u_x\rho)$$

$$0 = -\left(u_t + uu_x + \frac{p_x}{\rho}\right)$$

$$0 = -(p_t + up_x + \gamma p u_x)$$

Modeling in COMSOL Multiphysics

A clever way to conserve on model development time and computational cost is to solve this problem in a 2D geometry, using the y-coordinate as time. To do so, set up a rectangular domain in the ranges $-1.5 < x < 1.5$ and $0 < y < 1$. As initial conditions, use the following values:

$$\begin{cases} u = 0 \\ \rho = \begin{cases} 2 & x < 0 \\ 1 & x > 0 \end{cases} \\ p = \begin{cases} 2 & x < 0 \\ 1 & x > 0 \end{cases} \end{cases}$$

As these equations are numerically difficult to solve, stabilization with streamline diffusion facilitates convergence of the numerical scheme.

To derive the streamline-diffusion contributions, create a test function by taking each of the original equations and replacing the first-order derivatives with the corresponding test functions. Multiply the results by δh and the original equations to obtain equations for the streamline-diffusion contributions

$$-\delta h(\hat{\rho}_t + u\hat{\rho}_x + \hat{u}_x\rho)(\rho_t + u\rho_x + u_x\rho)$$

$$-\delta h\left(\hat{u}_t + u\hat{u}_x + \frac{\hat{p}_x}{\rho}\right)\left(u_t + uu_x + \frac{p_x}{\rho}\right)$$

$$-\delta h(\hat{p}_t + u\hat{p}_x + \gamma p\hat{u}_x)(p_t + up_x + \gamma p u_x)$$

The above equations denote test functions using the "hat" symbol. This streamline diffusion is of the Petrov-Galerkin type, which is one of the predefined types of artificial diffusion that you find, for example, in the Incompressible Navier-Stokes application mode.

In the model, you enter the Euler equations using a general form PDE with three dependent variables for pressure, density, and velocity. Use a weak term to add the streamline diffusion.

To resolve the shock wave, use the adaptive mesh generation in COMSOL Multiphysics.

Results

The plots below show distance across the tube's diaphragm on the horizontal axis and time along the vertical axis, where temperature and pressure are color coded. At $t = 0$ you can see constant states on both sides of the membrane, which is centered at $x = 0$. Specifically, in Figure 6-13, pressure is high to the left and low to the right; in Figure 6-14, temperature is uniform throughout the tube.

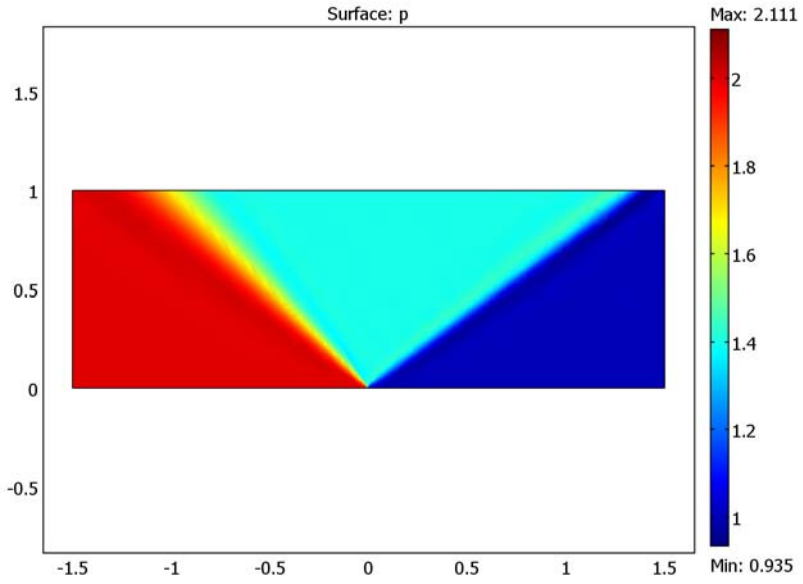


Figure 6-13: The pressure distribution in the shock tube. The y-axis represents time.

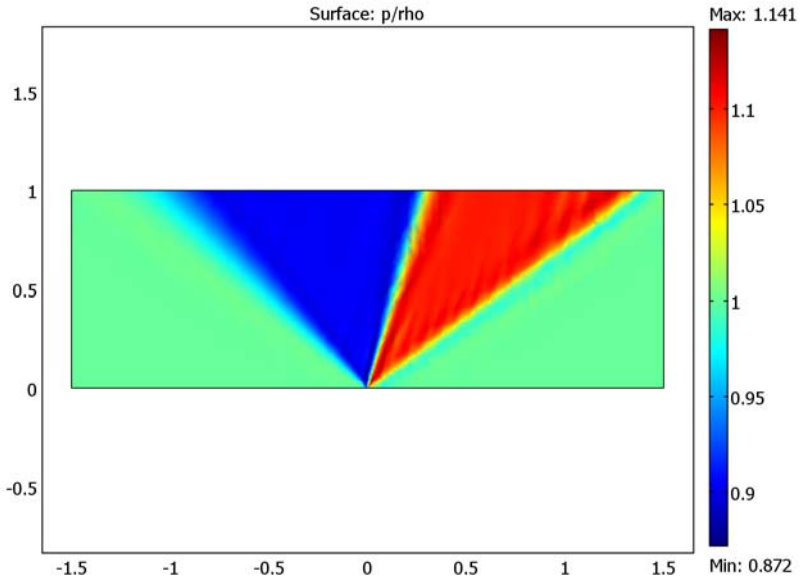


Figure 6-14: The nondimensional temperature distribution. The y-axis represents time.

The plots show the typical flow features of shock-tube problems. There are two possible types of jump solutions. At the time of a shock, all variables have jump discontinuities, and the second type of jump solution is a *contact surface* where pressure is continuous.

This case shows a shock traveling right, a contact surface moving more slowly to the right, and finally an expansion fan receding to the left into the denser, undisturbed gas.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/shock_tube`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 Click the **Multiphysics** button.

3 Click the **Add Geometry** button.

4 Keep **2D** in the **Space dimension** list and type `x time z` in the **Independent variables** edit field.

5 Click **OK**.

6 In the **COMSOL Multiphysics>PDE Modes** folder, select **PDE, General Form**.

7 Type `rho u p` in the **Dependent variables** edit field.

8 Click **Add** and then click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, define the following constants with names and expressions:

NAME	EXPRESSION
gamma	1.4
delta	1

3 Click **OK**.

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

5 Enter axis settings:

AXIS	
x min	-1.5
x max	1.5
time min	-0.5
time max	1.5

6 Click **OK**.

GEOMETRY MODELING

1 Click the **Rectangle/Square** button in the Draw toolbar.

2 Draw a rectangle with opposite corners in the points(–1.5, 0) and (1.5, 1).

PHYSICS SETTINGS

Expression Variables

1 On the **Options** menu, point to **Expressions** and then click **Subdomain Expressions**.

2 Select Subdomain 1 and enter the following expression variables:

PROPERTY	VALUE
F1	`-(rhotime+u*rhox+rho*ux)`
F2	`-(utime+u*ux+px/rho)`
F3	`-(ptime+u*px+gamma*p*ux)`

3 Click **OK**.

Boundary Conditions

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

2 In the **Boundary Settings** dialog box, enter the following settings:

SETTINGS	BOUNDARIES 1, 4	BOUNDARY 2	BOUNDARY 3
G(1)	0	0	0
G(2)	0	0	0
G(3)	0	0	0
R(1)	0	`(x<0)+1-rho`	0
R(2)	`-u`	`-u`	0
R(3)	0	`(x<0)+1-p`	0

3 Click **OK**.

Subdomain Settings

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

2 In the **Subdomain Settings** dialog box, enter the following settings:

PROPERTY	VALUE
Γ(1)	0 0
Γ(2)	0 0
Γ(3)	0 0
F(1)	F1
F(2)	F2
F(3)	F3

3 Click the **Init** tab and set the following initial conditions:

PROPERTY	VALUE
$rho(t_0)$	1
$u(t_0)$	0
$p(t_0)$	1

4 Click the **Weak** tab.

5 In the **weak** edit field, type the following streamline diffusion contributions as one single line, separating each contribution with a space:

```
delta*h*(rhotime_test+u*rhox_test+rho*ux_test)*F1
delta*h*(utime_test+u*ux_test+px_test/rho)*F2
delta*h*(ptime_test+u*px_test+gamma*p*ux_test)*F3
```

6 Click **OK**.

MESH GENERATION

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

COMPUTING THE SOLUTION

1 From the **Solve** menu, choose **Solver Parameters**.

2 Select the **Adaptive mesh refinement** check box.

3 Click the **Advanced** tab.

4 In the **Scaling of variables** area, select **None** in the **Type of scaling** list.

5 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

1 Open the **Plot Parameters** dialog box.

2 On the **Surface** page, visualize the pressure by selecting **PDE, General Form (g)>p** from the **Predefined quantities** list on the **Surface Data** page.

3 Click **Apply**.

This generates the plot in Figure 6-13.

4 Similarly, to visualize the nondimensional temperature, type `p/rho` in the **Expression** edit field on the **Surface Data** page.

5 Click **OK**.

This closes the **Plot Parameters** dialog box and generates the plot in Figure 6-14.

Sloshing Tank

Introduction

This 2D model demonstrates the ability of COMSOL Multiphysics to simulate dynamic free surface flow with the help of a moving mesh. The study models fluid motion with the incompressible Navier-Stokes equations. The fluid is initially at rest in a rectangular tank. The motion is driven by the gravity vector swinging back and forth, pointing up to 4 degrees away from the downward y direction at its extremes.

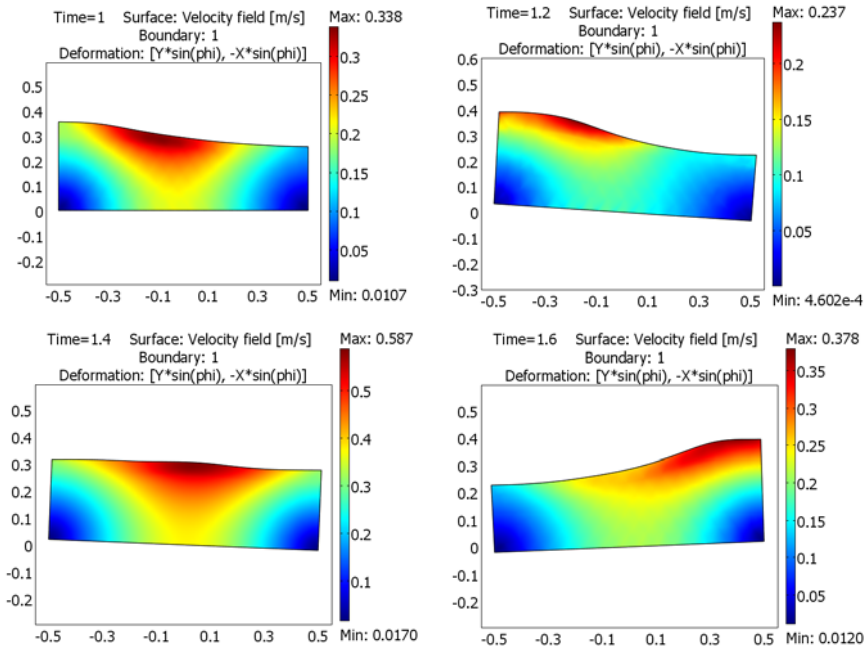


Figure 6-15: Snapshots of the velocity field at t = 1 s, t = 1.2 s, t = 1.4 s, and t = 1.6 s. The inclination of the gravity vector is indicated by the leaning of the tank.

Because the surface of the fluid is free to move, this model is a nonstandard computational task. The ALE (arbitrary Lagrangian-Eulerian) technique is, however, well suited for addressing such problems. Not only is it easy to set up using the Moving Mesh (ALE) application mode in COMSOL Multiphysics, but it also has the advantage that it represents the free surface boundary with a domain boundary on the moving mesh. This allows for the accurate evaluation of surface properties such as

curvature, making surface tension analysis possible. Note, however, that this example model neglects surface tension effects.

Model Definition

DOMAIN EQUATIONS

This model describes the fluid dynamics with the incompressible Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} - \nabla\cdot(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) = \mathbf{F}$$

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

where ρ is the density, $\mathbf{u} = (u, v)$ is the fluid velocity, p is the pressure, $\mathbf{I}$ is the unit diagonal matrix, η is the viscosity, and $\mathbf{F}$ is the volume force. In this example model, the material properties are for glycerol: $\eta = 1.49$ Pa·s, and $\rho = 1.27\cdot10^3$ kg/m^3. The gravity vector enters the force term as

$$F_x = \rho g\sin(\phi_{\max}\sin(2\pi ft))$$

$$F_y = -\rho g\cos(\phi_{\max}\sin(2\pi ft))$$

where $g = 9.81$ m/s^2, $\phi_{\max} = 4\pi/180$, and $f = 1$ Hz.

With the help of the Moving Mesh (ALE) application mode, you can solve these equations on a freely moving deformed mesh, which constitutes the fluid domain. The deformation of this mesh relative to the initial shape of the domain is computed using Winslow smoothing. For more information, please refer to "The Moving Mesh Application Mode" on page 455 in the *COMSOL Multiphysics Modeling Guide*. COMSOL Multiphysics takes care of the transformation of the Navier-Stokes equations to the formulation on the moving mesh.

BOUNDARY CONDITIONS FOR THE FLUID

There are two types of boundaries in the model domain. Three solid walls, that are modeled with slip conditions, and one free boundary (the top boundary). The slip boundary condition for the Navier-Stokes equations is

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

where $\mathbf{n} = (n_x, n_y)^T$ is the boundary normal. To enforce this boundary condition, select the Symmetry boundary type in the Incompressible Navier-Stokes application

mode. Because the normal vector depends on the degrees of freedom for the moving mesh, a constraint force would act not only on the fluid equations but also on the moving mesh equations. This effect would not be correct, and one remedy is to use non-ideal weak constraints. Ideal weak constraints (the other type of weak constraints) do not remove this effect of the constraint force. For more information about weak constraints, see "Using Weak Constraints" on page 350 in the *COMSOL Multiphysics Modeling Guide*. The Incompressible Navier-Stokes application mode does not make use of weak constraints by default, so you need to activate the non-ideal weak constraints.

The following weak expression, which you add to the model, enforces the slip boundary condition without a constraint force acting on the moving mesh equations:

$$\hat{\lambda}(\mathbf{u} \cdot \mathbf{n}) - \lambda(\hat{\mathbf{u}} \cdot \mathbf{n}) \tag{6-9}$$

for some Lagrange multiplier variable λ. Here λ and $\mathbf{u}$ denote test functions. See the step-by-step instructions later in this model documentation for details.

The fluid is free to move on the top boundary. The stress in the surrounding environment is neglected. Therefore the stress continuity condition on the free boundary reads

$$(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) \cdot \mathbf{n} = -p_0\mathbf{n}$$

where p_0 is the surrounding (constant) pressure and η the viscosity of the fluid. Without loss of generality, $p_0 = 0$ for this model.

BOUNDARY CONDITIONS FOR THE MESH

In order to follow the motion of the fluid with the moving mesh, it is necessary to (at least) couple the mesh motion to the fluid motion normal to the surface. It turns out that for this type of free surface motion, it is important to not couple the mesh motion to the fluid motion in the tangential direction. If you would do so, the mesh soon becomes so deformed that the solution no longer converges. The boundary condition for the mesh equations on the free surface is therefore

$$(x_t, y_t)^T \cdot \mathbf{n} = \mathbf{u} \cdot \mathbf{n}$$

where $\mathbf{n}$ is the boundary normal and $(x_t, y_t)^T$ the velocity of mesh (see "Mathematical Description of the Mesh Movement" on page 446 in the *COMSOL Multiphysics Modeling Guide*). In the Moving Mesh (ALE) application mode, you specify this boundary condition by selecting the tangent and normal coordinate system in the

deformed mesh and by specifying a mesh velocity in the normal direction, where you enter the right-hand side expression from above as `u*nx+v*ny`. The Moving Mesh (ALE) application mode uses non-ideal weak constraints by default, and for this boundary condition it adds the weak expression

$$\hat{\lambda}(((x_t, y_t)^T - \mathbf{u}) \cdot \mathbf{n}) - \lambda((\hat{x}, \hat{y})^T \cdot \mathbf{n})$$

to ensure that there are no constraint forces acting on the fluid equations. Here again, λ denotes some Lagrange multiplier variable (not the same as before) and λ, x, and y denote test functions. There is no need to modify this expression. Choose **Physics>Equation System>Boundary Settings** and select the free boundary (boundary 3) to see how to enter this expression in COMSOL Multiphysics. The expression implies that there is a flux (or force) on the free boundary for the moving mesh coordinate equations $\nabla x \cdot \mathbf{n} = \lambda n_x$ and $\nabla y \cdot \mathbf{n} = \lambda n_y$, respectively. Furthermore, to be able to follow the fluid motion with the mesh motion, the moving mesh must not be constrained in the tangential direction on the side walls. In the Moving Mesh (ALE) application mode, you specify this boundary condition by using the global coordinate system and setting the mesh displacement to zero in the x direction. At the bottom of the tank the mesh is fixed, which you obtain in a similar way by setting the mesh displacements to zero in both the x and y directions.

Results

Figure 6-16 below and Figure 6-15 on page 259 show the tank at a few different points in time. The colors represent the velocity field. Whereas you set up the model using a fixed tank and a swinging gravity vector, deformation plots enable you to give the tank an inclination at the postprocessing stage. The inclination angle of the tank is exactly the same as the angle of the gravity vector from its initial vertical position.

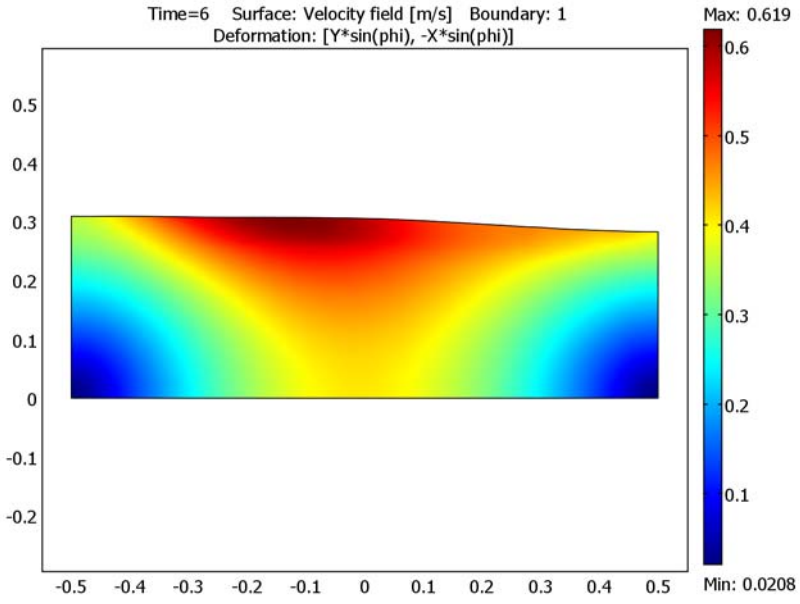


Figure 6-16: Velocity field inside the tank at $t = 6$ s.

To illustrate the dynamics in the tank, you can plot the wave height versus time at one of the vertical walls, as in the following plot.

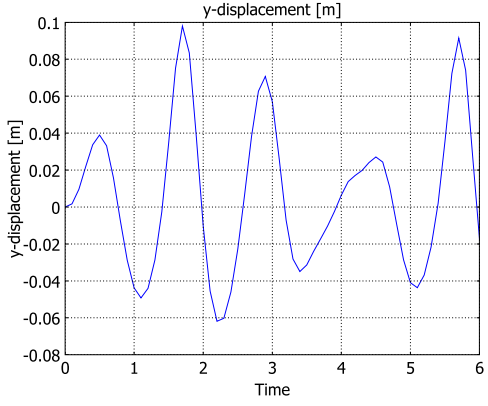


Figure 6-17: Wave height at $X = 0.5$ m for $t \in [0, 6$ s$]$.

Model Library path: `COMSOL_Multiphysics/Fluid_Dynamics/sloshing_tank`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, click the **Multiphysics** button.

3 Select **2D** from the **Space dimension** list.

4 Select **COMSOL Multiphysics>Deformed Mesh>Moving Mesh (ALE)>Transient analysis** and click **Add**.

5 Click the **Application Mode Properties** button.

6 Select **Winslow** from the **Smoothing method** list. Click **OK**.

7 Select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis** and click **Add**.

8 Click **OK**.

GEOMETRY MODELING

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

2 Specify the rectangle settings according to the table below.

PROPERTY	EXPRESSION
Width	1
Height	0.3
Position: Base	Corner
Position: X	-0.5
Position: Y	0

3 Click **OK** to close the **Rectangle** dialog box.

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

OPTIONS AND SETTINGS

1 Open the **Constants** dialog box from the **Options** menu and enter the following constants. The descriptions are optional. When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1270[kg/m^3]	Glycerol density
nu	1.49[Pa*s]	Glycerol viscosity
phi_max	(4*pi/180)[rad]	Maximum angle of inclination
freq	1[Hz]	Frequency
g	9.81[m/s^2]	Acceleration due to gravity

2 From the **Options** menu, choose **Expressions>Scalar Expressions**.

3 Enter the following scalar variables with names, expressions, and descriptions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
phi	phi_max*sin(2*pi*freq*t)	Angle of inclination
grav_x	g*sin(phi)	Gravity vector x component
grav_y	-g*cos(phi)	Gravity vector y component

PHYSICS SETTINGS

Properties

1 In the Incompressible Navier-Stokes application mode, choose **Properties** from the **Physics** menu.

2 In the **Application Mode Properties** dialog box, select **On** from the **Weak constraints** list and **Non-ideal** from the **Constraint type** list; then click **OK**.

Subdomain Settings

Open the **Subdomain Settings** dialog box and apply the settings in the table below.

SETTINGS	SUBDOMAIN 1
ρ	rho
η	nu
F_x	grav_x*rho
F_y	grav_y*rho

Boundary Conditions

1 Open the **Boundary Settings** dialog box from the **Physics** menu and enter boundary conditions according to the table below. When done, click **OK**.

SETTINGS	BOUNDARIES 1, 2, 4	BOUNDARY 3
Boundary type	Wall	Open boundary
Boundary condition	Slip	Normal stress
f_0		0

2 Go to the **Multiphysics** menu and select **Moving Mesh (ALE) (ale)**.

3 In the **Boundary Settings** dialog box, apply the following boundary conditions for the mesh displacements (only tangential movements on the sides and a fixed mesh at the bottom):

SETTINGS	BOUNDARIES 1, 4	BOUNDARY 2
dx	0	0
dy		0

4 On Boundary 3, select **Tangent and normal coord. sys. in deformed mesh** in the **Coordinate system** list. Then click the **Mesh velocity** button and type `u*nx+v*ny` in the **vn** edit field to specify the normal mesh velocity as $\mathbf{u}\cdot\mathbf{n}$.

5 On the **Weak Constr.** tab of the **Boundary Settings** dialog box, clear the **Use weak constraints** check box on Boundaries 1, 2, and 4. The strong constraints that you specified in the previous step are sufficient on these boundaries. Leave the **Use weak constraints** check box selected on Boundary 3.

6 Click **OK** to close the dialog box.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar to initialize the mesh.

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box from the **Solve** menu.

2 Enter `range(0,0.1,6)` in the **Times** edit field on the **General** page.

3 Type `0.001` in the **Relative tolerance** edit field. This provides a 0.1% relative tolerance, which is one order of magnitude less than the default value.

4 Click the **Time Stepping** tab.

5 Select **Exclude algebraic** from the **Error estimation strategy** list. This excludes the pressure and the moving mesh variables from the error estimation. The equations

for those variables do not include time derivatives and become algebraic when solving the equation system using the method of lines.

6 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the x-component of the moving mesh deformation, in the spatial frame.

1 To plot the velocity field of the glycerol instead, go to the **Surface** tab in the **Plot Parameters** dialog box and select **Incompressible Navier-Stokes (ns)>Velocity field** from the list of expressions.

2 On the **General** page, clear the **Geometry edges** check box. Click **Apply** to see the plot and use the **Solution at time** list on the **General** tab to browse through the output times.

You can visualize the tank's inclination by clever use of the deformation plot feature:

3 On the **Deform** page, select the **Deformed shape plot** check box and set the **Scale factor** to 1. Enter `Y*sin(phi)` in the **X component** edit field and `-X*sin(phi)` in the **Y component** edit field on the **Subdomain Data** tab.

4 Still on the **Deform** page, click the **Boundary Data** tab. Once again, enter `Y*sin(phi)` in the **X component** edit field and `-X*sin(phi)` in the **Y component** edit field.

5 On the **Boundary** tab, select the **Boundary plot** check box. Enter 1 in the **Expression** edit field. Select to use a **Uniform color** and pick a black color using the **Color** button.

6 To get a more liquid-looking plot, you may want to go to the **Surface** page and set the **Color table** to **GrayScale**.

7 Click **Apply** to see the plot.

8 To see the waves in action, go to the **Animate** page, click **Start Animation**, and then click **OK**.

To get a more comprehensive overview of the sloshing, you can plot the y-displacement from equilibrium in a point:

1 Open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

2 On the **Point** tab, select Point 4 from the **Point selection** list.

3 Enter `dy_ale` in the **Expression** edit field, then click **OK** to see the plot.

7

Geophysics Models

This chapter presents models of geophysics applications such as groundwater flow, contaminant transport, and the flow of fluids in rock fractures. You will find many more models and specialized application modes in the *Earth Science Module*.

Groundwater Flow and Solute Transport

Introduction

This model demonstrates the application of COMSOL Multiphysics to a benchmark case of steady-state subsurface fluid flow and transient solute transport along a vertical cross section in an unconfined aquifer. Because of profound geologic heterogeneity, the model must estimate solute transport subject to highly irregular flow conditions with strong anisotropic dispersion. Van der Heijde (Ref. 1) classifies this case as "Level 2," with enough potentially difficult parameter combinations to test a code's ability to tackle realistic hydrologic situations. Sudicky (Ref. 2) developed this problem to demonstrate a Laplace transform Galerkin code. This problem subsequently has been used to evaluate other flow and transport models, including MT3DMS by Zheng and Wang (Ref. 3).

This model makes use of several useful COMSOL Multiphysics features:

- Multiphysics coupling between fluid flow and solute transport
- Freely defined equations using the PDE, Coefficient Form application mode
- Upper boundary is water table with time-dependent solute source
- Incorporation of subsurface geological heterogeneity
- Customized expressions used to create anisotropic dispersion tensor

Model Definition

The hydrologic setting for this problem is described in Figure 7-1 (a) (see Ref. 2), for groundwater flow at steady state. The aquifer is composed largely of fine-grained silty sand of hydraulic conductivity $K_1 = 5 \cdot 10^{-4}$ cm/s, equivalent to $K_1 = 5 \cdot 10^{-6}$ m/s, with lenses of relatively course material of hydraulic conductivity $K_2 = 1 \cdot 10^{-2}$ cm/s, equivalent to $K_2 = 1 \cdot 10^{-4}$ m/s. Generally, groundwater moves from the upper surface of the saturated zone, the water table, to the outlet at $x = 250$ m. The water table is a free surface, that is, fluid pressure equals zero, across which there is vertical recharge, denoted by R, of 10 cm/yr equivalent to $3.215 \cdot 10^{-9}$ m/s. The groundwater divide, a line of symmetry, occurs at $x = 0$. The base of the aquifer is impermeable.

Figure 7-1 (b) shows conditions related to solute transport. The aquifer initially is pristine, and concentrations equal zero. For the first five years, a relative concentration of 1.0 is loaded over the interval 40 m < x < 80 m at the water table. The solute source is removed in year 5, and the concentration along this segment immediately drops to zero. The contaminant migrates within the aquifer via advection and dispersion. Throughout the domain, porosity, denoted by n, is 0.35, the longitudinal dispersivity, α_L, and transverse vertical dispersivity, α_T, are 0.5 m and 0.005 m, respectively, and the effective molecular diffusion coefficient, D_m, is $1.34 \cdot 10^{-5}$ cm^2/s, equivalent to $1.34 \cdot 10^{-9}$ m^2/s.

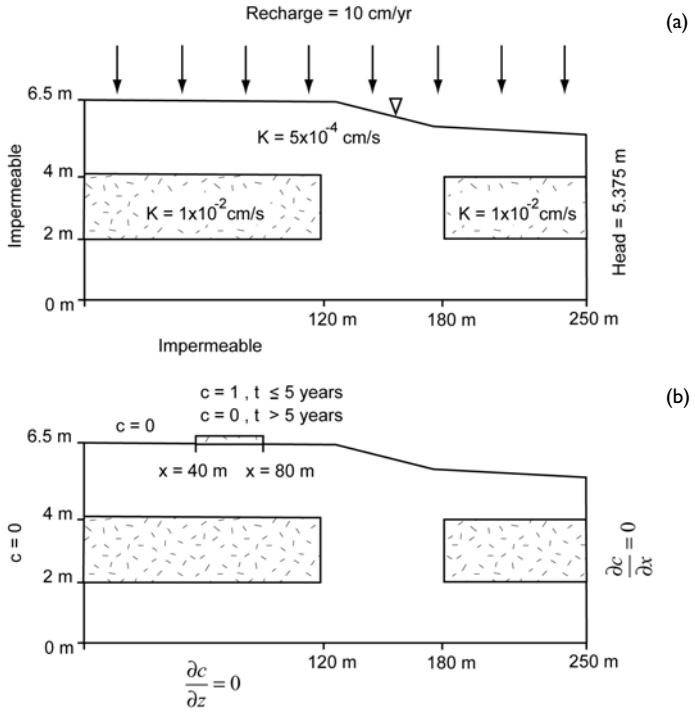


Figure 7-1: Definition of the flow-field problem (a) and the transport-of-solute problem (b).

FLUID FLOW: DOMAIN EQUATIONS AND BOUNDARY CONDITIONS

Governing equations for fluid flow and solute transport were specified in separate PDE, Coefficient Form application modes in COMSOL Multiphysics.

Steady groundwater flow generally is expressed with a conservation equation built with Darcy's law (Ref. 4, Ref. 5):

$$\nabla \cdot (K\nabla h) + R = 0$$

where K is hydraulic conductivity (L/T); x_i is spatial distance in direction i (L); R is the volumetric rate of recharge to water table per unit volume of aquifer (T^{-1}), and the dependent variable h is hydraulic head (L). Hydraulic head, a function of pressure and gravitational potential, is defined

$$h = h_p + y \tag{7-1}$$

where h_p is pressure head (L); and y is elevation (L). Equation 7-1 states the driving force for groundwater flow at field scales is h. For any given water particle, h equals the height of the water column h_p above the particle plus the particle's elevation y. It should be pointed out here that y is the name assigned to the independent variable x_i for the vertical direction.

The equations for groundwater flow and solute transport are linked by the average linear velocity v, or seepage velocity:

$$v_i = -\frac{K}{n}\frac{\partial h}{\partial x_i} \tag{7-2}$$

where n is porosity (L^3/L^3), or the fraction of the aquifer containing water. n appears in the denominator of Equation 7-2 because only a portion of a given aquifer block is available for flow.

The boundary conditions for the groundwater flow problem are shown in Figure 7-1 (a) and stated below. A zero flux Neumann condition represents the symmetry boundary at $x = 0$ m and the impermeable boundary at $y = 0$ m as follows:

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = 0$$

Hydraulic head is specified at $x = 250$ m with a Dirichlet condition:

$$h(x, t) = h_0$$

Representing the water table is slightly more complicated. A Neumann boundary is used to model the known recharge:

$$-K\frac{\partial h}{\partial y} = R$$

Specifying that this flux is entirely vertical requires multiplication by the y component of the normal vector **n** in COMSOL Multiphysics.

An important advantage of specifying a flux condition on the water table is the opportunity to fine tune the model setup. If the flow problem is well posed, h naturally equals y at the water table, because h_p is zero (that is, atmospheric pressure) at a free surface. In this model, the water table geometry is first determined by educated guess and is fine tuned manually in successive simulations until there is a good match between elevations and hydraulic head predictions on the boundary (Ref. 2).

SOLUTE TRANSPORT: DOMAIN EQUATIONS, BOUNDARY CONDITIONS, AND INITIAL CONDITIONS

Solute transport typically is time dependent for geologic problems and is described with the advection-dispersion equation (Ref. 4, Ref. 5):

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j} + v_i C\right) = \frac{\partial C}{\partial t}$$

where D_{ij} is the hydrodynamic dispersion tensor (L^2/T); C is the dissolved concentration (M/L^3); v_i is the average linear velocity (defined above); and t is time.

The dispersion tensor defines solute spreading by mechanical mixing and molecular diffusion. Equations for the tensor entries are:

$$D_{ii} = \alpha_L\frac{v_i^2}{|v|} + \alpha_T\frac{v_j^2}{|v|} + D^*$$

$$D_{ij} = D_{ji} = (\alpha_L - \alpha_T)\frac{v_i v_j}{|v|} + D^*$$

where D_{ii} are the principal components of the dispersion tensor (L^2/T); D_{ij}, D_{ji} are the cross terms of the dispersion tensor (L^2/T); the subscript L denotes longitudinal dispersivity (L); the subscript T denotes transverse dispersivity (L); $|v| = \sqrt{v_x^2 + v_y^2}$ is the magnitude of the velocity vector (L/T); and D^* represents effective molecular diffusion D_m in saturated porous media, (L^2/T), where $D^* < D_m << D_{ii}$ and typically is neglected.

The boundary and initial conditions for solute transport, shown in Figure 7-1 (b), are expressed below. Dirichlet conditions are used at the water table, where $C(x,h,t) = 0$, except for the segment 40 m $< x <$ 80 m in which

$$C = \begin{cases} C_0, & 0 < t < t_0 \\ 0, & t > t_0 \end{cases}$$

where the relative concentration C_0 is 1.0 through year 5 (t_0). After the solute source is removed, the concentration along this segment drops to zero. This model implements the time dependence of the source using a logical expression (a logical and function) in the COMSOL Multiphysics boundary settings.

The Dirichlet condition at the left boundary is

$$C(0, y, t) = 0$$

A Neumann condition is needed for the zero gradient boundaries:

$$\left.\frac{\partial h}{\partial x}\right|_{x = 250} = \left.\frac{\partial h}{\partial y}\right|_{y = 0} = 0$$

Finally, the initial condition specifies that the aquifer is pristine, when

$$C(x, y, 0) = 0$$

Results and Discussion

FLUID FLOW

Figure 7-2 provides hydraulic heads estimated with the COMSOL Multiphysics steady-state groundwater flow simulation. The hydraulic heads and streamlines shown in Figure 7-2 correspond nicely to the benchmark results provided by Sudicky (Ref. 2). The slight differences between the two plots are attributable to meshing: the mesh size varies naturally with the geometry.

The water table geometry determined for the simulation (see Figure 7-2) nearly duplicates the benchmark geometry obtained in Ref. 2. The good match between the flow fields is expected because the initial water table geometry used with COMSOL Multiphysics was designed to closely resemble the benchmark geometry. In the simulations reported here, therefore, only nuances of geometry were resolved through iteration. Figure 7-3 provides residuals from the geometry fitting; that is, the fractional

difference between h and y along the final water table boundary. As Figure 7-3 illustrates, the error in the geometry settings is 1% or less.

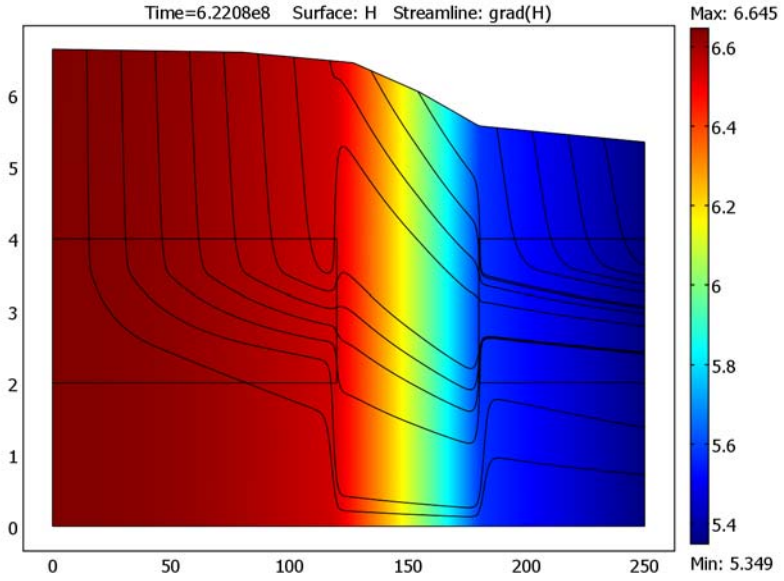


Figure 7-2: COMSOL Multiphysics estimates of hydraulic head and flow lines. The solution reproduces the results in Ref. 2.

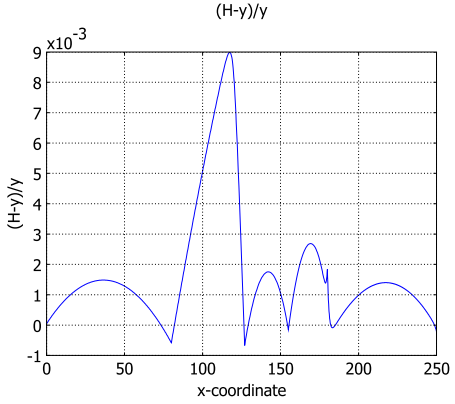


Figure 7-3: Fractional error in water table geometry computed using hydraulic head predicted by COMSOL Multiphysics, H, and water table elevation, y.

SOLUTE TRANSPORT

Solute transport solutions from the model are almost identical to the ones presented in Ref. 2. This is clearly shown in the contour intervals for three times in Figure 7-4. The minor variation between the COMSOL Multiphysics and benchmark solutions results from different mesh densities. In 1989, Sudicky concluded that the results illustrated in Ref. 2 are relatively free of numerical dispersion, as the low concentration contours closely follow the flow pattern. The surface plot for COMSOL also displays this property, in that even the lowest concentrations in Figure 7-4 still follow the irregular flow lines of Figure 7-2.

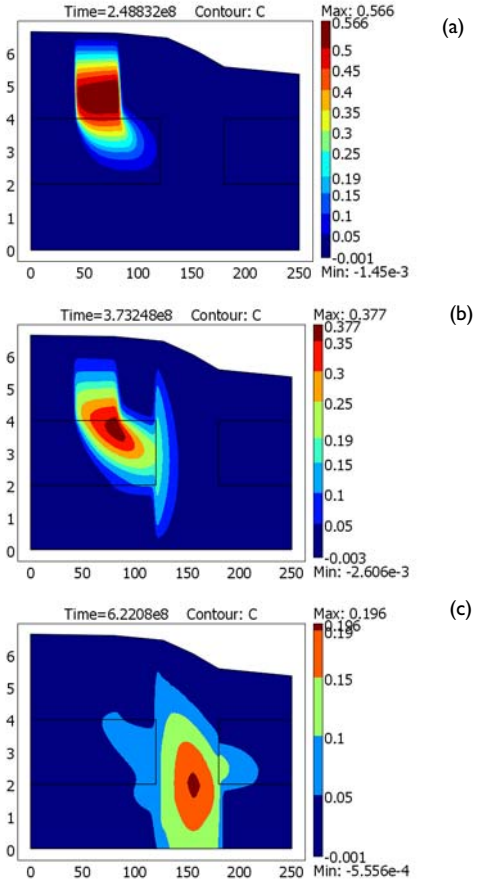


Figure 7-4: Plume concentrations calculated with COMSOL Multiphysics at three times: (a) t = 8 years, (b) t = 12 years, and (c) t = 20 years.

The results from this model show that COMSOL Multiphysics is an effective tool for simulating fluid flow and solute transport in the heterogeneous porous media and highly irregular flow fields that are common to field scale applications.

References

1. P.K.M. van der Heijde, "Model Testing: A Functionality Analysis, Performance Evaluation, and Applicability Assessment Protocol," *Groundwater Models for Resources Analysis and Management*, A.I. El-Kadi (ed.), CRC Press, Lewis Publishers, Boca Raton, FL, pp. 39–58, 1995.

2. E.A. Sudicky, "The Laplace transform Galerkin technique: application to mass transport in groundwater," *Water Resour. Res.*, vol. 25, no. 8, pp. 1833–1846, 1989.

3. C. Zheng and P. Wang, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems*, University of Alabama, 239 pp, 1998.

4. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing Company, 764 pp, 1972.

5. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, New York, 210 pp, 1979.

Model Library path: `COMSOL_Multiphysics/Geophysics/groundwater_flow`

Modeling Using the Graphical User Interface

1. Start COMSOL Multiphysics.
2. In the **Model Navigator** click the **Multiphysics** button.
3. Select **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form** and type `H` in the **Dependent variables** edit field.
4. Click the **Add** button.
5. Select **PDE, Coefficient Form** again.
6. Change the name of the dependent variable to `C` in the **Dependent variables** edit field.
7. Click the **Add** button.
8. Click **OK**.

GEOMETRY MODELING

1 Shift-click the **Line** button on the Draw toolbar on the left.

2 In the **Line** dialog box, enter the following data; when done, click **OK**.

PROPERTY	EXPRESSION
X	0 250 250 180 155 127 80 0
Y	0 0 5.35 5.575 6.045 6.455 6.603 6.645
Style	Closed polyline (solid)

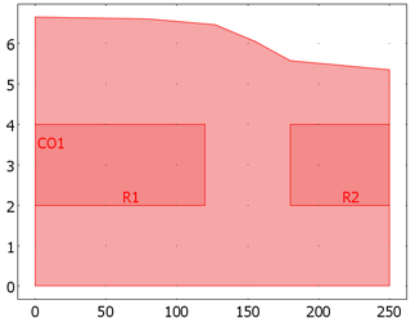
3 Double-click the **EQUAL** button on the status bar below the drawing area, to turn off the default "axis equal" setting. Click the **Zoom Extents** button on the Main toolbar. This way you make full use of the drawing area at the cost of losing the view of the geometry's actual proportions.

4 Shift-click the **Rectangle/Square** button on the Draw toolbar. In the **Rectangle** dialog box, specify the rectangle R1 according to the following table; when done, click **OK**.

PROPERTY	R1	R2
Width	120	70
Height	2	2
Base	Corner	Corner
x	0	180
y	2	2

5 Repeat the previous step for the rectangle R2.

The model geometry is now complete, and should look like that in the figure below (press Ctrl+A to get the same view).



Model geometry. Note the different scales on the horizontal and vertical axes.

OPTIONS AND SETTINGS

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

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

NAME	EXPRESSION	DESCRIPTION
R	3.215e-9	Vertical recharge
H_in	5.3486	Hydraulic head at right boundary
K1	5e-6	Hydraulic conductivity, sand
K2	0.0001	Hydraulic conductivity, lenses
C_in	1	Relative concentration, solute source
n	0.35	Porosity
alpha_L	0.5	Longitudinal dispersivity
alpha_T	0.005	Transverse vertical dispersivity
D_m	1.34e-9	Effective molar diffusion coefficient

3 Click **OK**.

PHYSICS SETTINGS

Subdomain Expressions

1 On the **Options** menu, point to **Expressions** and then click **Subdomain Expressions**.

2 Enter the following expressions in the **Subdomain Expressions** dialog box:

NAME	EXPRESSION IN SUBDOMAIN 1	EXPRESSION IN SUBDOMAIN 2 AND 3
vx	-K1*Hx/n	-K2*Hx/n
vy	-K1*Hy/n	-K2*Hy/n
absv	sqrt(vx^2+vy^2)	sqrt(vx^2+vy^2)
Dxx	alpha_L*vx^2/ absv+alpha_T*vy^2/absv+D_m	alpha_L*vx^2/ absv+alpha_T*vy^2/absv+D_m
Dyy	alpha_L*vy^2/ absv+alpha_T*vx^2/absv+D_m	alpha_L*vy^2/ absv+alpha_T*vx^2/absv+D_m
Dxy	(alpha_L-alpha_T)*vx*vy/absv	(alpha_L-alpha_T)*vx*vy/absv

3 Click **OK**.

Subdomain Settings—Darcy's Law

1 From the **Multiphysics** menu, choose **1 PDE, Coefficient Form (c)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 Select Subdomain 1, then set **c** equal to -K1. All the other coefficients should be 0.

4 Select Subdomains 2 and 3. Set **c** equal to `-K2`. All the other coefficients should be `0`.

5 Click **OK**.

Boundary Conditions—Darcy's Law

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

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

SETTINGS	BOUNDARIES 1–3, 5	BOUNDARIES 7, 8, 10, 11, 15	BOUNDARIES 16–18
Type	Neumann boundary condition	Neumann boundary condition	Dirichlet boundary condition
q	0	0	
g	0	`-ny*R`	
h			1
r			`H_in`

Subdomain Settings—Advection-Dispersion Equation

1 From the **Multiphysics** menu, choose **2 PDE, Coefficient Form (c2)**.

2 From the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Select all subdomains, then enter coefficients according to the following table:

COEFFICIENT	VALUE
c	`Dxx Dxy Dyy`
a	0
f	0
da	1
α	`-vx -vy`
β	0 0
γ	0 0

4 Click **OK**.

Boundary Conditions—Advection-Dispersion Equation

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

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

SETTINGS	BOUNDARIES 1, 3, 5, 8, 10, 11, 15	BOUNDARY 2	BOUNDARY 7	BOUNDARIES 16, 18	BOUNDARY 17
Type	Dirichlet boundary condition	Neumann boundary condition	Dirichlet boundary condition	Neumann boundary condition	Neumann boundary condition
q		0		0	0
g		0		K1*Hx/n*C	K2*Hx/n*C
h	1		1		
r	0		C_in*(40<=x&& t<=5*360*86400)		

MESH GENERATION

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

2 On the **Global** page, select the **Custom mesh size** button.

3 In the **Resolution of narrow regions** edit field, type 4 to specify the minimum number of mesh layers. For an elongated geometry like the one in this model, tuning this parameter is often an effective way to obtain a good mesh.

4 Click **Remesh**.

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

COMPUTING THE SOLUTION

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

2 In the **Solver Manager** dialog box, click the **Solve For** tab.

3 Select **PDE, Coefficient Form (c)**, then click **Solve**.

4 Select **PDE, Coefficient Form (c2)**, then click **OK**.

5 Open the **Solver Parameters** dialog box.

6 From the **Solver** list, select **Time dependent**.

7 In the **Times** edit field, type `360*86400*range(0,20)`. Click **OK**.

8 Click the **Restart** button to compute a new solution.

POSTPROCESSING AND VISUALIZATION

Use the first sequence of commands to plot Figure 7-2 on page 275:

1 From the **Postprocessing** menu, choose **Plot Parameters**.

2 Click the **Surface** tab.

3 On the **Surface Data** page, select **PDE, Coefficient Form (c)>H** from the **Predefined quantities** list.

4 Click the **Streamline** tab.

5 Select the **Streamline plot** check box.

6 On the **Streamline Data** page, select **PDE, Coefficient Form (c)>grad(H)** from the **Predefined quantities** list.

7 Click the **Specify start point coordinates** button and enter the following values:

x	15	30	45	60	75	90	130	145	160	175	190	205	220	235
y	5	5	5	5	5	5	5	5	5	5	5	5	5	5

8 Click the **Line Color** tab, then click the **Color** button. In the **Streamline Color** dialog box, select black and then click **OK**.

9 Click the **Advanced** button. Set the **Maximum number of integration steps** to 40000, then click **OK**.

10 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

You can also plot the plume concentrations in Figure 7-4 on page 276:

1 Open **Plot Parameters** dialog box again.

2 Click the **Surface** tab and select **PDE, Coefficient Form (c2)>C** from the **Predefined quantities** list on the **Surface Data** page.

3 Click the **Contour** tab and select **PDE, Coefficient Form (c2)>C** from the **Predefined quantities** list on the **Contour Data** page.

4 In the **Contour levels** area, click the **Vector with isolevels** button and enter `0.05 0.1 0.15 0.19 0.25 0.30 0.35 0.4 0.45 0.5` in the edit field.

5 Click the **General** tab, select the **Contour** check box, and clear the **Streamline** check box. Click **OK**.

6 To get a good view of the solution, double-click **EQUAL** on the status bar and then click the **Zoom Extents** button on the Main toolbar.

To plot this concentration for a different time you can select the time you want in the **Solution at time** list on the **General** page in the **Plot Parameters** dialog box (for Figure 7-4 (a) select **2.48832e8**, for Figure 7-4 (b) select **3.73248e8**, and for Figure 7-4 (c) select **6.2208e8**, that is, the concentration after 8, 12, and 20 years).

A Rock Fracture Flow Model

Introduction

A potential flow model describing fluid movement in a rock fracture uses the Reynolds equation, also known as the "cubic law" equation

$$\nabla \cdot \left(\frac{\rho g}{12\mu} a^3 \nabla H \right) = 0$$

which involves the following variables:

- Fluid density, ρ
- The gravitational constant, g
- The fluid's dynamic viscosity, μ
- The fracture's aperture or width, $a(x, y)$
- The scaled pressure, $H = H(x, y)$, also called hydraulic head

This model uses interpolation of aperture data defined in a text file.

Model Definition

The definition of that last variable, hydraulic head is

$$H = z + \frac{p}{\rho g}$$

where z equals the height and p represents fluid pressure.

After eliminating the constant factor in the diffusion coefficient, you end up with the equation

$$\nabla \cdot (a^3 \nabla H) = 0$$

Notice that you cannot eliminate the aperture expression a^3 because this example assumes that a is a nonconstant function of x and y, and thus it falls under the influence of the divergence operator.

Modeling in COMSOL Multiphysics

COMSOL Multiphysics does not include an application mode for potential flow, but you can use the Diffusion application mode for this model; the PDE solved here is identical to the Reynolds equation. You must make one minor mental adjustment here: In the user interface the hydraulic head is referred to as the concentration. You can however rename the dependent variable as `h` when adding the application mode in the Model Navigator.

The computational domain is rectangular and well inside the sampled aperture data matrix. Set a hydraulic head of 20 mm at the upper boundary and 0 mm at the lower boundary. This creates a pressure difference of 20 mm that drives the fluid flow. Both the left and right boundaries have insulation/symmetry boundary conditions.

The COMSOL installation includes a text file, `aperture_data.txt`, containing the sample aperture data for this model in the form of a 100-by-100 matrix. This synthetically generated data set corresponds to an aperture with a fractal dimension of 2.6. You import the aperture data to the COMSOL Multiphysics user interface by defining an interpolation function, which you then use as the aperture a in the cubic-law equation.

Results

The plot in Figure 7-5 shows the flux using colored surface data and the hydraulic head as the *z*-coordinate (height).

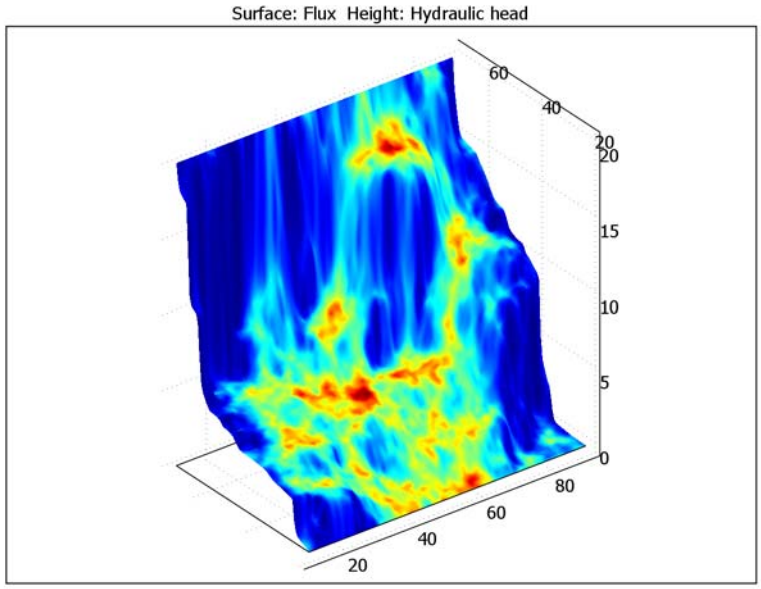


Figure 7-5: The flux and the hydraulic head.

The plot in Figure 7-6 on page 286 provides a visualization of the aperture data.

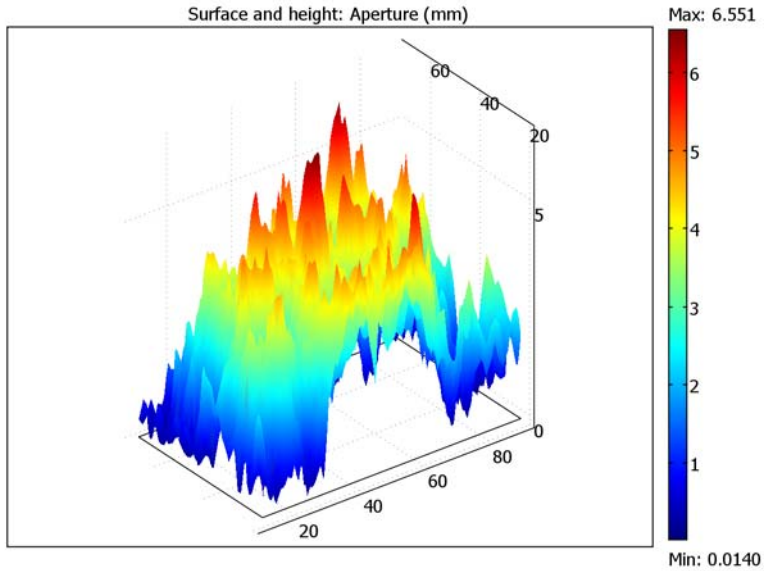


Figure 7-6: The interpolated aperture data shown as a combined surface and height plot.

Model Library path: `COMSOL_Multiphysics/Geophysics/rock_fracture`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** in the **Space dimension** list.
2. From the **Application Modes** tree, select **COMSOL Multiphysics>Convection and Diffusion>Diffusion>Steady-state analysis**.
3. Change the entry in the **Dependent variables** edit field to `H` and the **Application mode name** to `reynolds`. Make sure **Lagrange - Quadratic** is selected in the **Element** list.
4. Click **OK**.

OPTIONS AND SETTINGS

Because the Diffusion application mode assumes that the dependent variable is a concentration, the units in the user interface will be incorrect for this model's application. Therefore, begin by turning the unit system off.

1. From the **Physics** menu, choose **Model Settings**.
2. From the **Base unit system** list, select **None**.
3. Click **OK**.

Define the interpolation function for the aperture data:

1. From the **Options** menu, choose **Functions**.
2. In the **Functions** dialog box, click the **New** button.
3. In the **New Function** dialog box, type `aperture` in the **Function name** edit field.
4. Click **Interpolation** and select **File** in the **Use data from** list.
5. Click **Browse** and browse to `/models/COMSOL_Multiphysics/Geophysics/aperture_data.txt` in the COMSOL installation directory.
6. Select the **Store data in model** check box to make the model MPH-file self-contained. The possible drawback with this option is that you need to recreate the function if you modify the data file.
7. Click **Open** to select this file and close the **Open Data** dialog box and then click **OK** to close the **New Function** dialog box.
8. Optionally, select the **Use space coordinates as default function arguments** check box. If you choose this option, you can leave out the arguments when calling `aperture` in the subsequent modeling instructions.
9. Click **OK**.

GEOMETRY MODELING

1. Shift-click the **Rectangle/Square** button on the Draw toolbar.
2. In the **Rectangle** dialog box, specify the **Width** as `80` and the **Height** as `50`, and locate the lower-left corner at **x** equal to `10` and **y** equal to `20`. Click **OK** to create the rectangle R1.
3. Click the **Zoom Extents** button on the Main toolbar to adjust the coordinate system with respect to the size of the rectangle.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

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

SETTINGS	SUBDOMAIN 1
D (isotropic)	`aperture(x,y)^3`
R	0

Boundary Conditions

1 Open the **Boundary Settings** dialog box and enter boundary conditions as below:

SETTINGS	BOUNDARIES 1, 4	BOUNDARY 2	BOUNDARY 3
Boundary condition	Insulation/Symmetry	Concentration	Concentration
H_0		0	20

2 Click **OK**.

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box.

2 Select the **Adaptive mesh refinement** check box.

3 Click the **Adaptive** tab.

4 Set the **Maximum number of refinements** to 10 and the **Maximum number of elements** to 10000. This number might be too high depending on the amount of memory in your system. Users uncertain of available memory should start with a lower number.

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

6 Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

1 Open the **Plot Parameters** dialog box from the **Postprocessing** menu.

2 Click the **Surface** tab. On the **Surface Data** page, select **Diffusion (reynolds)>Diffusive flux, h** from the **Predefined quantities** list.

3 Still on the **Surface** page, click the **Height Data** tab. Select the **Height data** check box and then select **Diffusion (reynolds)>Concentration, h** from the **Predefined quantities** list.

4 Clear the **Color legend** check box.

5 On the **General** page, open the **Title** dialog box. Click the right button to specify the title manually and type `Surface: Flux  Height: Hydraulic head`.

6 Click **OK** to close the **Title** dialog box, and then click **Apply** to create the plot in Figure 7-5 on page 285.

7 To view the aperture data, return to the **Surface** page. On both the **Height Data** and **Surface Data** pages, type `aperture(x,y)` in the **Expression** edit field.

8 Select the **Color legend** check box.

9 On the **General** page, open the **Title** dialog box. In the **Title** edit field, type `Surface and height: Aperture (mm)`.

10 Click **OK** twice to close the dialog boxes and create the plot in Figure 7-6 on page 286.

8

Heat Transfer Models

The following models illustrate heat transfer using the Conduction application mode. Heat transfer also takes part in many multiphysics models. For more information about the heat transfer application modes and introductory models, see "Heat Transfer" on page 167 in the *COMSOL Multiphysics Modeling Guide*.

Heating with a Moving Laser

Introduction

Laser beams are commonly used to locally heat the surface of various substrates, for example, in laser welding or thermal annealing such as on layered silicon devices. The laser beam typically moves over a surface in a periodic fashion to produce the desired localized heating. In the case of layered silicon devices, each layer is very thin, making the modeling of the penetration depth caused by the moving laser a strongly time-dependent problem.

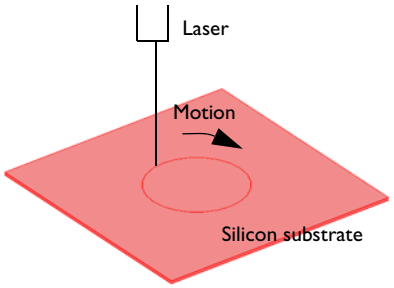


Figure 8-1: A moving laser heats a thin silicon substrate.

This example models the localized transient heating caused by a laser beam that moves in circles over a silicon substrate. The beam's penetration depth, which you can describe with an absorption coefficient, depends on the ambient temperature. The geometry under study represents the top layer of a silicon device. The model examines the penetration depth and the influence of the laser motion on the transient temperature distribution.

This model considers the laser beam as having an infinitesimal width and thus treats it as a line heat source. As such it is not meaningful to study the maximum temperature because it is mesh dependent. However, the overall heat flux and temperature distribution on a macroscopic level are both accurate.

Model Definitions

The model simulates the substrate as a 3D object (Figure 8-1) with these dimensions:

- Thickness: 1 mm
- Width: 10 mm-by-10 mm

It handles the variation of laser intensity with penetration depth using a 1D geometry that represents the substrate's thickness.

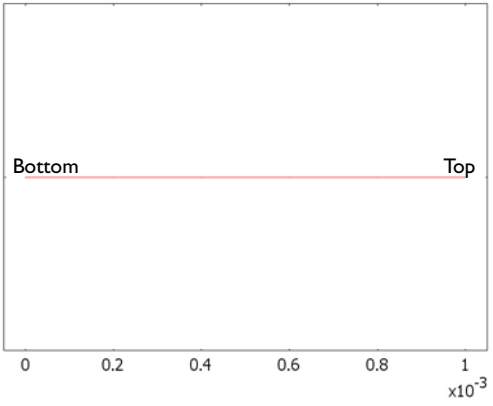


Figure 8-2: The 1D model geometry.

The model makes use of the Conduction application mode to describe the transient heat transfer in the 3D geometry. The transient energy-transport equation for heat conduction is

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-\underline{k} \nabla T) = Q$$

where ρ is the density, C_p is the specific heat capacity, $\underline{k}$ is the thermal conductivity tensor, and Q is the heat source term, which you here set to zero (this case models the source in a different way).

The material properties are those of silicon, using an anisotropic conductivity of $(k_{xx}, k_{yy}, k_{zz}) = (163, 163, 16)$ in units of W/(m·K), a density of 2330 kg/m^3, and a specific heat capacity of 703 J/(kg·K).

For the model, assume the boundaries are insulating.

In the 1D geometry, this model uses the Weak Form, Subdomain application mode to model the laser penetration. In the equation describing the penetration

$$\frac{\partial I}{\partial x'} = -k_{\text{abs}} I$$

I represents the relative laser intensity (the variable in the Weak Form, Subdomain application mode), x' represents the 1D coordinate, and k_{abs} is the absorption coefficient. The absorption coefficient can depend on the temperature, and the expression used in this model is

$$k_{\text{abs}} = 8 \cdot 10^3 \text{ m}^{-1} - 10 \text{ (m·K)}^{-1}(T - 300 \text{ K})$$

The volumetric heat source term, Q, in the 3D geometry is then

$$Q = P_{\text{in}} k_{\text{abs}} I$$

where P_{in} is the total power of the incoming laser beam.

Both of these equations are included in the Weak Form, Subdomain application mode, where they become one equation:

```
I_test*(Ix-k_abs*I)+k_abs*I*P_in*T_test
```

The first part of this expression describes the penetration equation, and the second part comes from the heat-source term in the 3D Heat Transfer application mode.

At the left boundary, apply a homogeneous Neumann condition, and at the right boundary set the relative intensity, I, to unity. The total incoming laser power, P_{in}, is 50 W.

The model implements the heat source's motion when coupling the 3D temperature variable, T, to the 1D equation. It does so with a subdomain extrusion coupling variable using a general transformation. A time-dependent transformation expression results in a moving heat source. This case describes a circular repeating motion using the transformation expressions

$$x = R\sin(\omega t), \qquad y = R\cos(\omega t), \qquad z = x'$$

where x, y, and z correspond to the 3D coordinates, and x' represents the 1D coordinate. Furthermore, R is the radius of circular motion, ω is the angular velocity, and t is time. The model uses the parameter values $R = 0.02$ m and $\omega = 10$ rad/s, the latter value corresponding to a period of roughly 0.628 s for the laser motion.

This method—using a separate geometry and equation to model the source term—is very useful because it provides that term directly at the test-function level. Furthermore, it models the source motion separately with the transformation

expressions, making it simple to alter. It is indeed the best way to model a moving point or line source.

The 3D model makes use of an extruded triangular mesh, which has a fine resolution close to the laser incident line and is coarse elsewhere. This results in a high-resolution solution with minimum computation requirements. The mesh results in around 10,000 elements and 6200 degrees of freedom.

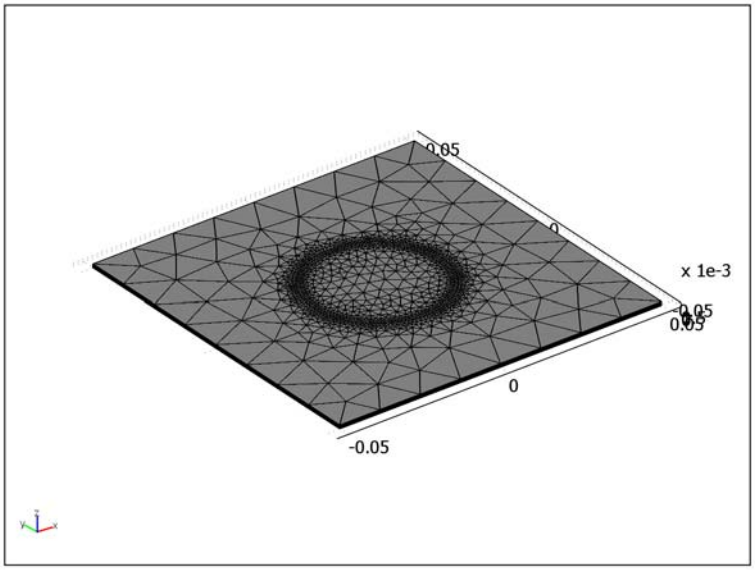


Figure 8-3: The 3D mesh produced by extruding a 2D triangular mesh, refined along the circular laser incident line.

Figure 8-4 depicts the temperature distribution at the laser-beam incident surface.

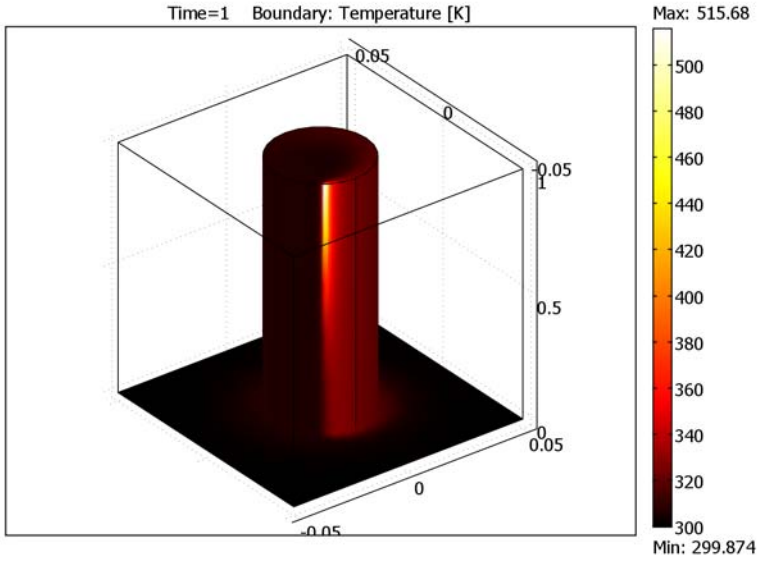


Figure 8-4: Temperature distribution after 1 s of laser heating.

The figure clearly shows a hot spot where the laser beam is located at a specific time. Furthermore, the results show a cold side and a warm side next to the vertical line below the laser beam. The warm side represents the area where the beam has just swept through.

A better way to study these effects is by plotting the temperature at the top surface along the circular laser-beam incident pattern as in Figure 8-5.

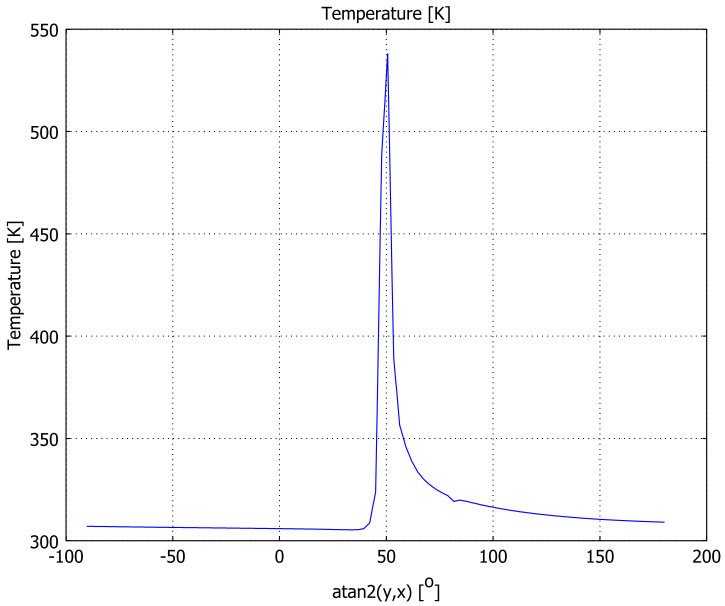


Figure 8-5: Temperature distribution along the laser-beam incident trajectory on the top surface after 0.7 s.

Here the laser beam moves from right to left, and the warm side is on the right side of the peak. Locally the temperature reaches around 510 K, but this value is completely mesh dependent. Nevertheless, the temperature distribution just a few mesh elements away represents the real temperature quite well.

Finally, Figure 8-6 shows beam penetration into the substrate. The heating at the bottom of the substrate is practically zero.

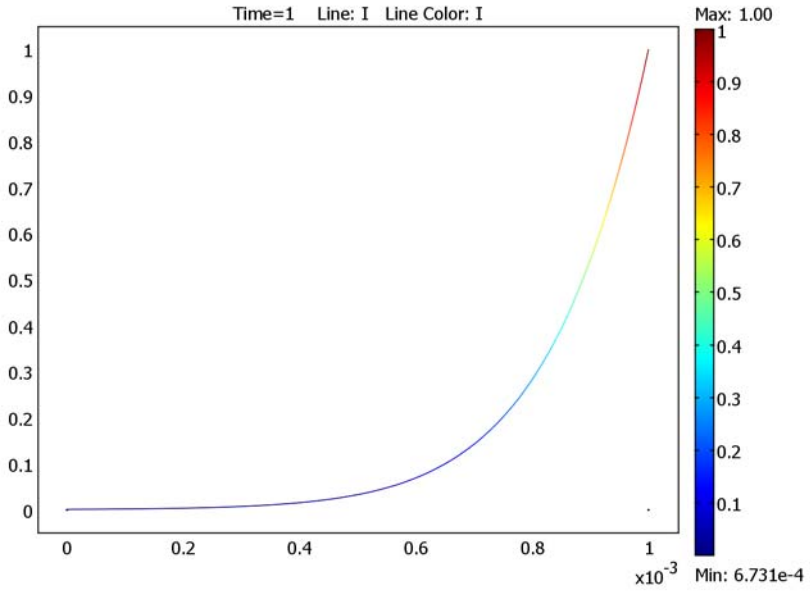


Figure 8-6: Relative laser-beam intensity as a function of sample depth.

Model Library path: `COMSOL_Multiphysics/Heat_Transfer/laser_heating`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **3D** in the **Space dimension** list and click the **Multiphysics** button.
2. Select **Heat Transfer>Conduction>Transient analysis** in the list of application modes (in the **COMSOL Multiphysics** folder if the license contains additional modules).
3. Select **Lagrange - Linear** in the **Element** list and click **Add**.
4. Click **Add Geometry** and select **1D** from the **Space dimension** list. Click **OK** to close the dialog box.

5 Select **COMSOL Multiphysics>PDE Modes>Weak Form, Subdomain>Time-dependent analysis** in the list of application modes.

6 Enter `I` in the **Dependent variables** edit field.

7 Click **Add**.

8 Click **OK** to exit the **Model Navigator** and begin modeling.

OPTIONS AND SETTINGS

In the **Constants** dialog box enter the following names and expressions. The descriptions are optional.

NAME	EXPRESSION	DESCRIPTION
`P_in`	`50[W]`	`Laser beam power`
`r`	`2[cm]`	`Radius of trajectory circle`
`omega`	`10[rad/s]`	`Angular velocity`

GEOMETRY MODELING 3D

1 Click the **Geom1** tab to go to the 3D geometry.

2 Open the **Work-Plane Settings** dialog box in the **Draw** menu. Click **OK** to get a default *xy* work plane at $z = 0$.

3 Select **Draw>Specify Objects>Square** to create a square with the width `0.1` m, centered at the origin (select **Center** from the **Base** list). When done, click **OK**.

4 Select **Draw>Specify Objects>Circle** to create a circle with the radius `0.02` m, centered at the origin. When done, click **OK**.

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

MESH GENERATION 3D

1 Open the **Mesh>Free Mesh Parameters** dialog box.

2 Select **Coarser** from the **Predefined mesh sizes** list.

3 On the **Boundary** page select Boundaries 5–8 and enter `1e-3` in the **Maximum element size** edit field.

4 Click **OK** to close the dialog box.

5 Click the **Initialize Mesh** button to generate the mesh.

6 Select **Mesh>Extrude Mesh** and enter `1e-3` in the **Distance** edit field.

7 On the **Mesh** page enter `5` for the **Number of element layers** and click **OK**.

GEOMETRY MODELING 1D

1 Click the **Geom2** tab to go to the 1D geometry.

2 Specify a line from `0` to `1e-3`, then click the **Zoom Extents** button.

MESH GENERATION 1D

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

2 On the **Boundary** page select Boundary 2. Enter `1e-5` for the **Maximum element size** and `1.1` for the **Element growth rate**.

3 Click **OK** to close the dialog box.

4 Click the **Initialize Mesh** button to generate the mesh.

PHYSICS SETTINGS 3D

Subdomain Settings

1 Click the **Geom1** tab to go to the 3D geometry.

1 Open the **Physics>Subdomain Settings** dialog box and select both subdomains.

2 Click **Load** and select **Silicon** from the **Basic Material Properties** folder in the **Materials/Coefficients Library** dialog box. Click **OK** when done.

3 Select **k (anisotropic)** and enter `163`, `163`, and `16` for the diagonal elements k_{xx}, k_{yy}, and k_{zz}, respectively.

4 On the **Init** page enter `300` for the initial temperature.

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

Boundary Conditions

Use the default **Thermal insulation** boundary condition for all exterior boundaries.

Coupling Variables

1 Select **Options>Extrusion Coupling Variables>Subdomain Variables**.

2 Select both subdomains and define a variable with the **Name** `T` and the **Expression** `T`. Select to use a **General transformation** and make sure the source transformation reads **x:** `x`, **y:** `y`, **z:** `z`.

3 On the **Destination** page select **Geom2** from the **Geometry** list and **Subdomain** from the **Level** list. Select the check box in front of Subdomain 1 and apply the destination transformation
x: `r*sin(omega*t)`, **y:** `r*cos(omega*t)`, **z:** `x`.

4 Click **OK** to close the dialog box.

PHYSICS SETTINGS 1D

Subdomain Settings

1 Click the **Geom2** tab to go to the 1D geometry.

2 Open the **Physics>Subdomain Settings** dialog box and select Subdomain 1.

3 On the **Weak** page enter `(Ix-I_abs)*I_test+I_abs*P_in*T_test` in the **weak** edit field and `0` in the **dweak** edit field.

4 On the **Init** page enter `1` for the **Initial value I(t_0)**.

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

Boundary Settings

1 Open the **Physics>Boundary Settings** dialog box,

2 Enter `0` in the **constr** edit field for Boundary 1, then enter `1-I` in the same edit field for Boundary 2.

3 Click **OK** to close the dialog box.

Scalar Expressions

In the **Scalar Expressions** dialog box make the following entries; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
k_abs	8e3[1/m]-10[1/(m*K)]*(T-300[K])	Absorption coefficient
I_abs	k_abs*I	Relative absorption

The unit warnings appear because the coupling variable `T` and the Weak Form, Subdomain variable `I` have no associated units; you can ignore these warnings.

COMPUTING THE SOLUTION

1 In the **Solver Parameters** dialog box, make the following changes; when done, click **OK**.

EDIT FIELD	VALUE
Times	range(0,0.02,1)
Absolute tolerance	1
Linear system solver	Direct (UMFPACK)

2 Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

1. If you are still in the 1D geometry, click the **Geom1** tab and then the **Postprocessing Mode** button to switch to postprocessing in 3D.

   The default plot shows the temperature distribution in five slices through the substrate.

2. Open the **Plot Parameters** dialog box. Clear the **Slice** check box and select the **Boundary** check box. On the **Boundary** page select **Thermal** from the **Color table** list. Click **OK** to see a boundary plot of the temperature.

3. Because the substrate is very thin you can get a better view of it by rescaling the *z*-axis. Select **Options>Axes/Grid Settings** and clear the **Axis equal** check box. After clicking **OK** to close the dialog box, click the **Zoom Extents** button on the Main toolbar.

4. To see what goes on inside the silicon substrate, hide the boundaries that are in the way. To do so, open the **Suppress Boundaries** dialog box from the **Options** menu and suppress Boundaries 1, 2, 4, 5, and 12. Then click the **Postprocessing Mode** button once again.

   To see the temperature distribution along the trajectory, proceed with the following steps:

5. Open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

6. On the **General** page, pick a time from the **Solutions to use** list (the plot in Figure 8-5 corresponds to the selection **0.7**).

7. On the **Line/Extrusion** page, select Edges 13, 16, and 19.

8. In the **x-axis data** area, click first the lower option button and then the **Expression** button.

9. In the **X-Axis Data** dialog box, type `atan2(y,x)` in the **Expression** edit field to get the usual angular coordinate, φ, along the first axis.

10. From the **Unit** list select ^{o}, then click **OK** to close the **X-Axis Data** dialog box.

11. Finally, click **OK** in the **Domain Plot Parameters** dialog box to see the plot.

Heat-sink Experiments Using the Component Library

Introduction

The most common method for investigating a process or system is to first study the individual components in detail. You would probably start by setting up detailed models for the various components and then try to merge them in some way to describe the system as a whole. With COMSOL Multiphysics you can merge individual models to investigate how they interact as components in a system.

This exercise illustrates the use of the component library to merge different types of heat sinks with a heating device. The resulting models give an estimate of the thermal resistance of each heat sink and of the temperature distribution in the heating device. The model set up is similar to the benchmarking method for heat sinks used by Alpha Company Ltd. in Japan.

The models defined here are rather simple as they use a semi-empirical expression for the heat transfer coefficient between the heat sink and the air that flows over it. It is also possible to simulate the air flow in detail and thus the coupled heat transfer-flow problem in COMSOL Multiphysics, but this is outside the scope of this specific example.

The purpose of this example is to guide you through the procedure for merging different components into a single model of a system.

Model Definition

In this study, four different heat sinks from Alpha Company Ltd. are combined with one heating device. All the heat sinks have a base of 19 mm-by-19 mm and a height of

10 mm. The following figure shows the geometry of the heat sinks, all of which are made of aluminum 6063.

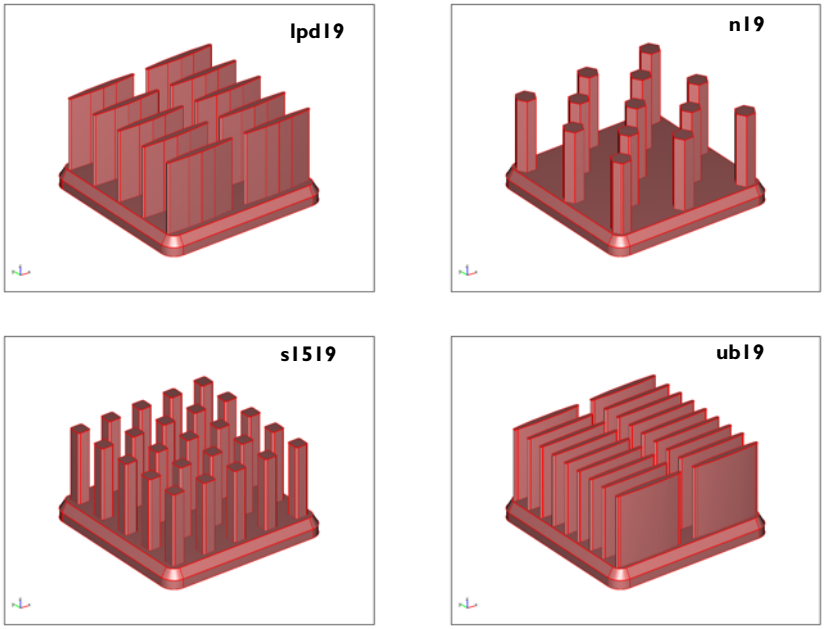


Figure 8-7: The four heat sinks are the types lpd19, n19, s1519, and ub19, all from Alpha Company Ltd.

The heating device measures 12.7 mm-by-12.7 mm and is 3 mm thick. It consists of an aluminum block with three heating elements made of steel. The next figure shows its geometry.

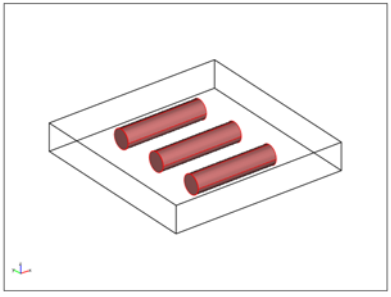


Figure 8-8: The heating device consists of three heating elements embedded in an aluminum block.

The physics inside the heat sinks is described by a heat balance where heat flux takes place by conduction. The thermal conductivity of aluminum 6063 is available in the material properties database in COMSOL Multiphysics.

The boundary condition at the top surface of the heat sinks sets the heat flux perpendicular to the boundary proportional to the temperature difference between the heat sink and the surrounding air according to the following equation:

$$-k\nabla T \cdot \mathbf{n} = h(T - T_{\mathrm{amb}}) \qquad (8\text{-}1)$$

The heat transfer coefficient, h, is obtained using a semi-empirical expression as a function of temperature and distance from the leading edge of the heat sink, in this case as a function of x in the next figure. In the previous equation, k denotes the thermal conductivity, T equals the temperature, and $\mathbf{n}$ is the normal vector to the boundary. The boundary conditions at the bottom of the heat sink describe an influx of heat from the device being cooled.

The physics in the heating device is described by a heat balance, with the flux given by conduction, and with a heat-source term in each of the heating elements. The heating elements are made of steel, while the aluminum block is made of aluminum 6063. The thermal transport properties are available in the material properties database.

The boundary conditions describe thermal insulation at all boundaries except for the top surface, which is in contact with a heat sink. At this boundary the temperature is equal to that of the heat sink.

The top surface of the heating device has the dimensions of 12.7 mm-by-12.7 mm, while the bottom surface of the heat sink is 19 mm-by-19 mm. After the merger of one of the heat sinks and the heating device, the part of the bottom surface of the heat sink that does not make contact with the heating device is thermally insulated as shown in Figure 8-9.

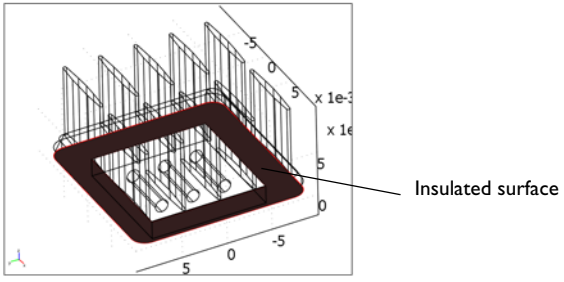


Figure 8-9: The surface is the part of the heat sink that is insulated.

Once the two components are merged, all physics and boundary conditions are obtained from the components except for the insulation boundary condition shown in Figure 8-9. This boundary condition is actively defined in the model of the entire system.

Results

Figure 8-10 shows the calculated thermal resistance for the four heat sinks when they are merged with the heating device. The thermal resistance is calculated as

$$\text{thermal resistance} = \frac{(T_{\text{contact}} - T_{\text{amb}})}{P} \tag{8-2}$$

where T_{contact} denotes the temperature in the middle of the contact surface between the heat sink and the heating device, and P equals the total heating power of 5 W. The definition of the thermal resistance is taken from Alpha Company, Ltd.

The models seem to overestimate the thermal resistance of the n19 heat sink but are otherwise in decent agreement with the experiments reported by Alpha Company, Ltd.

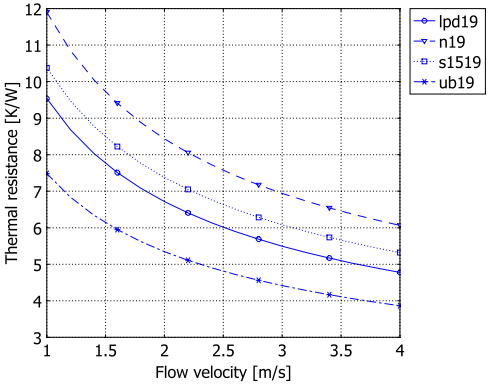


Figure 8-10: Thermal resistance as a function of the rate of air flowing over the heat sink.

The next figure shows the temperature distribution in the lpd19 heat sink in the cases where it is modeled by itself with a constant heat flux at the bottom surface, and then when the heating device is attached at the bottom. In both cases the heating power is 5 W and the flow rate of the cooling air is 4 m/s. The results are very similar except for the almost circular-shaped isosurface that is present in the merged model. In all cases the thermal resistance is slightly larger for the heat sink when attached to the

heating device compared to the standalone model, where a constant heat flux is set at the base surface. This is an expected behavior because the flux is limited to the contact surface in the model of the entire system.

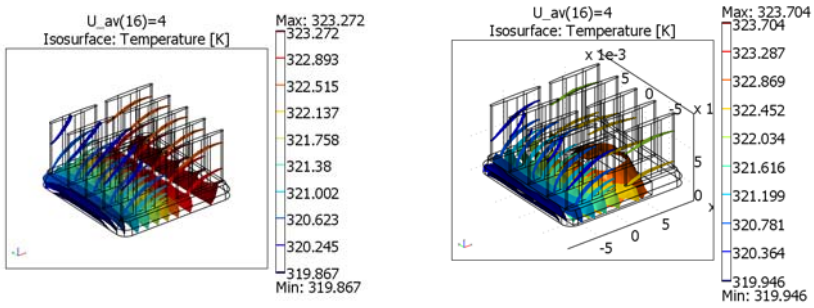


Figure 8-11: Temperature distribution in the standalone model of a lpd19 heat sink and in the model merged with the heating device (right).

The n19 heat sink displays a higher thermal resistance, which results in a maximum temperature of roughly 329 K, which is slightly higher than that for the lpd19 heat sink. The s1519 heat sink displays a lower resistance than that of the n19 but a resistance higher than that for the lpd19. The heat sink denoted ub19 is the one with the best cooling performance in this study. Under the same conditions as shown in the previous figure it gives a maximum temperature of approximately 317 K.

In experiments performed by Alpha Company Ltd. the difference in performance between the lpd19, n19, and s1519 heat sinks is very small, smaller than the simulations in this study. However, this might be caused by the fact that the n19 and s1519 heat sinks are better inducers of turbulence, which improves the cooling performance. This is in line with the measured pressure losses, which are higher for the n19 and s1519. In addition, both of these models show a nonlinear dependence on the pressure drop as a function of flow, a behavior typical for turbulent flow. The experiments and the models both agree that the ub19 heat sink has the best performance under the testing conditions.

Model Library path: `Component_Library/heat_sink_lpd19`

---

1 Start COMSOL Multiphysics.

2 In the **Model Navigator**, select **3D** from the **Space dimension** list.

3 Choose the application mode **COMSOL Multiphysics>Heat Transfer>Conduction**.

4 Click **OK**.

GEOMETRY MODELING

1 From the **File** menu, select **Import>CAD Data From File**.

2 Choose the **COMSOL Multiphysics file** file type and select the file `heat_sink_lpd19.mphbin`. Click **Import**.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Constants** dialog box.

2 Enter the following constants for later use (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
T_amb	25[degC]	Ambient temperature
m_norm	3.590681[cm^3]*2700[kg/m^3]	Mass of clad
U_av	1[m/s]	Average velocity
m_hs	2.9[g]	Mass of device
fact	m_norm/(m_norm-m_hs)	Velocity scaling
P	5[W]	Total heating power

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

4 In the **Scalar Expressions** dialog box, enter the following names, expressions, and (optionally) descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
L_in	x+9.5005[mm]	Inlet distance
U_avn	U_av*fact	Average scaled velocity
C1	10^(0.8616*log10((T+T_amb)[1/K]/2)-3.7142)	
C2	(0.1949*(log10((T+T_amb)[1/K]/2))^2-1.3494*log10((T+T_amb)[1/K]/2)+2.8469)^0.33	
C3	(350.9[K]/T)*U_avn*L_in/(-8e-12*(T[1/K])^2+4e-8*T[1/K]+5e-6)[m^2/s]	

NAME	EXPRESSION	DESCRIPTION
h_hs	(1[W/(m*K)]/L_in)*C1*C2* (0.332*flc2hs(5e5-C3,1e5)*C3^0.5+ 0.0296*flc2hs(C3-5e5,1e5)*C3^0.8)	Heat transfer coefficient
q	P/area	Heat flux

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

6 In the **Boundary Integration Variables** dialog box, select Boundary 3.

7 Create a boundary integration variable with the **Name** `area` defined by the **Expression** 1. Leave the **Integration order** at 4 and the **Global destination** check box selected. When done, click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Select Subdomain 1.

3 Click the **Load** button to open the **Materials/Coefficients Library** dialog box.

4 In the **Materials** area, open the **Basic Material Properties** library, select **Aluminum 6063-T83**, and then click **OK**.

5 Click the **Init** tab. In the **Initial value** area, set **T(t_0)** to `T_amb`.

6 Click the **Element** tab. From the **Predefined elements** list, select **Lagrange - Linear** to use linear elements for the temperature field.

7 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

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

SETTINGS	BOUNDARY 3	BOUNDARIES 1, 2, 4–118
Boundary condition	Heat flux	Heat flux
q_0	q	0
h	0	h_hs
T_{inf}	0	T_amb

If the highlighting of inconsistent units is active, notice that COMSOL Multiphysics indicates that the unit for the expression q is inconsistent. This is due to the integration coupling variable involved in computing the area. You can disregard this warning.

MESH GENERATION

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

COMPUTING THE SOLUTION

1. From the **Solve** menu, open the **Solver Parameters** dialog box.
2. From the **Solver** list, select **Parametric**.
3. In the **Parameter names** edit field, type `U_av`.
4. In the **Parameter values** edit field, type `range(1,0.2,4)`.
5. Click **OK** to close the dialog box. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 8-11 follow these instructions:

1. From the **Postprocessing** menu open the **Plot Parameters** dialog box. On the **General** page clear the **Slice** check box. Select the **Isosurface** check box.
2. Click the **Isosurface** tab. In the **Isosurface levels** area set the **Number of levels** to `10`.
3. Click **OK** to close the dialog box and plot the isosurfaces.

Continue to model the second component, which is the heating device being cooled by the heat sink.

Model Library path: `Component_Library/heating_device`

---

1. Start COMSOL Multiphysics.
2. In the **Model Navigator** select **3D** in the **Space dimension** list.
3. In the list of application modes select **COMSOL Multiphysics>Heat Transfer>Conduction**.
4. Click **OK**.

GEOMETRY MODELING

1. Select **Work-Plane Settings** from the **Draw** menu. Click **OK**.
2. Shift-click the **Rectangle/Square (Centered)** button on the Draw toolbar. In the **Width** field enter `12.7e-3`, and set the **Base** to **Center**.
3. Click **OK**.
4. Click the **Zoom Extents** button on the Main toolbar to center the geometry.

5 From the **Draw** menu, select **Extrude**. Set the **Distance** to `-2e-3`, then click **OK**.

6 From the **Draw** menu, select **Work-Plane Settings**. In the **Plane** area, click the **y-z** option button. Click **OK**.

7 Click the **Projection of All 3D Geometries** button on the Draw toolbar.

8 Draw a circle of radius $0.7 \cdot 10^{-3}$ centered at the point $(0, -0.001)$.

9 Select the circle by left-clicking on it. Press Ctrl+C to make a copy of the object.

10 Press Crtl+V, set `-3.5e-3` as its displacement in the *x* direction, and click **OK**.

11 Press Crtl+V again, and this time use `3.5e-3` as the *x* displacement. Click **OK**.

12 Select the three circles by holding down the shift key and clicking on each of them.

13 From the **Draw** menu, select **Extrude**. Set the **Distance** to `6e-3`, then click **OK**.

14 Click the **Move** button on the Draw toolbar. Set the distance in *x* direction to `-3e-3`, then click **OK**.

15 Select all objects (press Ctrl+A) and then click the **Union** button on the **Draw** toolbar.

OPTIONS AND SETTINGS

1 From the **Options** menu, open the **Constants** dialog box.

2 Enter the following constants for later use (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
h_hd	200[W/(m^2*K)]	Heat transfer coefficient
T_out	40[degC]	Outer temperature
P_he	5[W]/3	Power per heating element

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

4 In the **Subdomain Integration Variables** dialog box, select Subdomain 4.

5 Create a subdomain integration variable with the **Name** `volume` defined by the **Expression** `1`. Leave the **Integration order** at the default value `4` and the **Global destination** check box selected.

6 Click **OK** to close the dialog box.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Select Subdomains 2–4.

3 Click the **Load** button to open the **Materials/Coefficients Library** dialog box.

4 In the **Materials** area, open the **Basic Material Properties** library, select **Steel AISI 4340**, and then click **OK**.

5 In the **Q** edit field, type `P_he/volume`.

6 Choose Subdomain 1, then click the **Load** button.

7 From the **Basic Material Properties** library, select **Aluminum 6063-T83**, then click **OK**.

8 Click the **Init** tab. Select all subdomains, then type `T_out` in the **$T(t_0)$** edit field in the **Initial value** area.

9 Click the **Element** tab, then select **Lagrange - Linear** for all subdomains.

10 Click **OK** to close the dialog box.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Specify boundary conditions as in the following table; when done, click **OK**.

SETTINGS	BOUNDARY 4	BOUNDARIES 1–3, 5
Boundary condition	Heat flux	Thermal insulation
q_0	0	
h	`h_hd`	
T_{inf}	`T_out`	

MESH GENERATION

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

COMPUTING THE SOLUTION

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

Now merge the two components into a single COMSOL Multiphysics model.

Model Library path: `COMSOL_Multiphysics/Heat_Transfer/dev_merge_lpd19`

---

1 Start COMSOL Multiphysics.

2 In the **Model Navigator** select **3D** in the **Space dimension** list.

3 Click **OK**.

4 From the **File** menu, select **Open Component Library**.

5 Choose the **heating device** component, then click the **Merge** button.

6 In the **Merge Component** dialog box, click the **Merge** button.

The component is now inserted into Geometry 1.

7 From the **File** menu, select **Open Component Library**.

8 This time choose the **heat sink lpd19** component, then click the **Merge** button.

9 Click the **Merge** button again to merge the components into a single geometry with a single application mode.

10 To mate the two objects, go to the **Draw** menu and choose **Create Pairs**.

11 In the **Create Pairs** dialog box, select both objects and then click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 Click the **Init** tab. Select all subdomains, then type `T_amb` in the **$T(t_0)$** edit field in the **Initial value** area.

3 Click the **Element** tab, then select **Lagrange - Linear** for all subdomains.

4 Click **OK** to close the dialog box.

Boundary Conditions

1 From the **Physics** menu, open the **Boundary Settings** dialog box.

2 Select Boundary 3, then change the **Boundary condition** to **Thermal insulation**.

3 Click **OK** to close the dialog box.

MESH GENERATION

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

COMPUTING THE SOLUTION

1 From the **Solve** menu, open the **Solver Parameters** dialog box.

2 From the **Solver** list, select **Parametric**.

3 In the **Parameter names** edit field, type `U_av`.

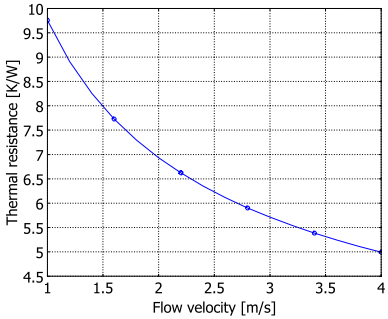
4 In the **Parameter values** edit field, type `range(1,0.2,4)`.

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

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

To generate Figure 8-10 follow these steps:

1. From the **Postprocessing** menu, open the **Domain Plot Parameters** dialog box.
2. On the **Point** page, select Point 226.
3. In the **Expression** edit field, type `(T-T_amb)/P_he`.
4. Click the **Line Settings** button. Choose **Circle** as **Line marker**, then click **OK**.
5. Click **OK** to close the dialog box and generate the first graph.
6. Click the **Edit Plot** toolbar button on the Figure window.
7. In the **Edit Plot** dialog box, edit the plot title and axis labels; when done, click **OK**.



8. Repeat the merging process to create similar plots for the other three heat sinks from Alpha Company Ltd.: types n19, s1519, and ub19.

9

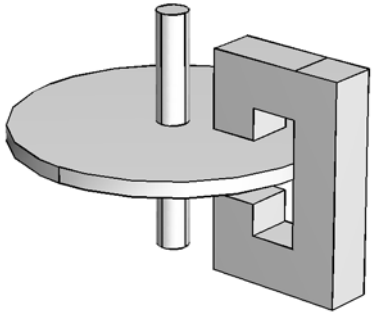
Multidisciplinary Models

Multidisciplinary models combine finite element analysis with other computational engineering tools and applications such as control system design, signal processing, state-space modeling, and dynamic simulations. Typically, the finite element model is embedded in the multidisciplinary model to detail physical processes.

Magnetic Brake

Introduction

A magnet brake in its simplest form consists of a disk of conductive material and a permanent magnet. The magnet generates a constant magnetic field, in which the disk is rotating. When a conductor moves in a magnetic field it induces currents, and the Lorentz forces from the currents slow the disk.



Model Definition

For a disk rotating with angular velocity ω about the z-axis, the velocity $\mathbf{v}$ at a point (x, y) is given by

$$\mathbf{v} = \omega(-y, x, 0).$$

When the disk is inserted in the air gap and it encounters the magnetic field $\mathbf{B}_0$, the configuration induces a current density $\mathbf{j}$ according to Lorentz' equation

$$\begin{cases} \mathbf{E} + \mathbf{v} \times (\mathbf{B} + \mathbf{B}_0) = \dfrac{1}{\sigma d}\mathbf{j} \\ \nabla \times \mathbf{E} = 0 \\ \nabla \times \mathbf{B} = \mu \mathbf{j}. \end{cases}$$

These equations use the following variables and material properties:

- $\mathbf{B}$ represents the magnetic field
- $\mathbf{E}$ is the electric field
- μ is the permeability
- σ is the electric conductivity
- d is the plate's thickness

This example uses the Dirichlet boundary condition $\mathbf{B} = 0$.

In this model, the magnetic flux $\mathbf{B}$ has only a vertical component, and the currents and electric field have no z-components. Solving for $\mathbf{B}$ gives the following scalar partial differential equation:

$$-\nabla \cdot \left(\nabla B + \mu \sigma d \omega (B + B_0) \begin{pmatrix} y \\ -x \end{pmatrix} \right) = 0$$

where B is the z-component of $\mathbf{B}$ and B_0 equals the z-component of $\mathbf{B}_0$.

Now consider how the system evolves over time. The induced torque slows the disc down, and you must set up an ordinary differential equation (ODE) to model the angular velocity ω.

To obtain the time derivative of the angular velocity ω, compute the torque arising from the induced currents. For a small surface element, the force equals

$$d\mathbf{F} = \mathbf{j} \times (\mathbf{B} + \mathbf{B}_0) dx dy$$

and integrating over the disk gives the total torque:

$$\mathbf{M} = \int_{\text{Disk}} \frac{1}{\mu} \mathbf{r} \times \{ (\nabla \times \mathbf{B}) \times (\mathbf{B} + \mathbf{B}_0) \} dx dy \, .$$

In this case, $\mathbf{M}$ has only a z-component with the value

$$M = \int_{\text{Disk}} \frac{1}{\mu} \left(y \frac{\partial B}{\partial x} - x \frac{\partial B}{\partial y} \right) \cdot (B + B_0) dx dy \, .$$

Thus the ODE for the angular velocity ω can be formulated as

$$J \frac{d\omega}{dt} = M \, ,$$

where the moment of inertia J for a disk with radius r equals

$$J = m\frac{r^2}{2} = \frac{\rho d r^4 \pi}{2}.$$

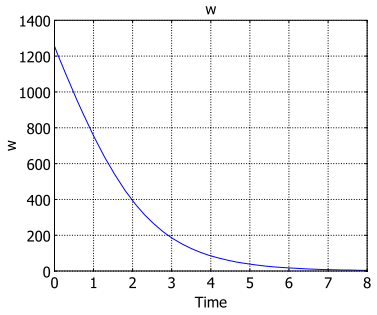
Modeling in COMSOL Multiphysics

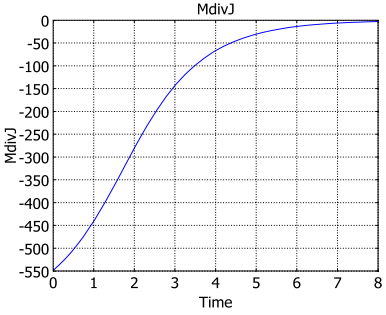
The models show different ways to solve this problem:

1. Start by determining the magnetic field for a given angular velocity.
2. Continue by exporting to Simulink getting a time-dependent solution. Simulink models the additional ODE for the angular velocity of the disk. For each time step in Simulink, COMSOL Multiphysics solves a stationary PDE for the magnetic field given the current angular velocity.
3. Finish by doing the same thing entirely within COMSOL Multiphysics using coupling variables and an additional ODE for the angular velocity. Now COMSOL Multiphysics solves for the angular velocity and the magnetic field simultaneously. The discretized problem is a differential-algebraic equation system (DAE).

Results

There is agreement between the results from the Simulink simulation and the results from COMSOL Multiphysics. In the plots for ω and $d\omega/dt$ against time, $d\omega/dt$ is proportional to the torque on the disk.





Model Library path: `COMSOL_Multiphysics/Multidisciplinary/magnet_brake_simulink`

MODEL NAVIGATOR

1. Select **2D** in the **Space dimension** list.
2. In the list of application modes, open the **COMSOL Multiphysics>PDE Modes** folder and then the **PDE, Coefficient Form** node.
3. Select **Stationary analysis**.
4. Type `B` in the **Dependent variables** edit field.
5. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu, choose **Constants**.
2. Enter the following constants; when done, click **OK**.

NAME	EXPRESSION
K	mu*5.99e7*0.02
w	2*pi*200
J	8960*0.02*0.1^4*pi/2
mu	4e-7*pi
B0_2	0.1

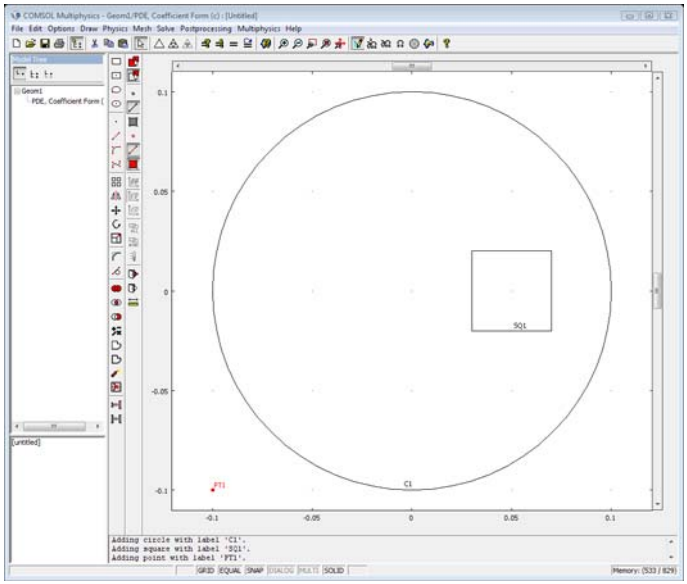
The variable `w` represents the fixed angular velocity ω. The variable `K` is the product of μ, σ, and d.

GEOMETRY MODELING

1. In the **Draw** menu, point to **Specify Objects** and then click **Circle**.
2. In the **Circle** dialog box, type `0.1` in the **Radius** edit field and keep the center in the origin.
3. Click **OK**.
4. In the **Draw** menu, point to **Specify Objects** and then click **Square**.
5. In the **Square** dialog box, type `0.04` in the **Width** edit field. In the **Position** area, select **Center** in the **Base** list, and enter `0.05` and `0` in the **x** and **y** edit fields, respectively.
6. Click **OK**.
7. In the **Draw** menu, point to **Specify Objects** and click **Point**.
8. In the **Point** dialog box, type `-0.1` and `-0.1` in the **x** and **y** edit fields, respectively.
9. Click **OK**.

10 Click the **Zoom Extents** button.

You will use the point at (–0.1, –0.1) to introduce an additional scalar state variable corresponding to the angular velocity in the final version of this model.



PHYSICS SETTINGS

Boundary Conditions

Use the default Dirichlet boundary conditions.

Subdomain Settings

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

2 Enter PDE settings as shown in the following table:

SETTINGS	SUBDOMAINS 1, 2
c	1
a, f, d_a	0
α	K*w*y -K*w*x
γ	-K*w*B0*y K*w*B0*x

3 Click **OK** to close the dialog box.

Expression Variables

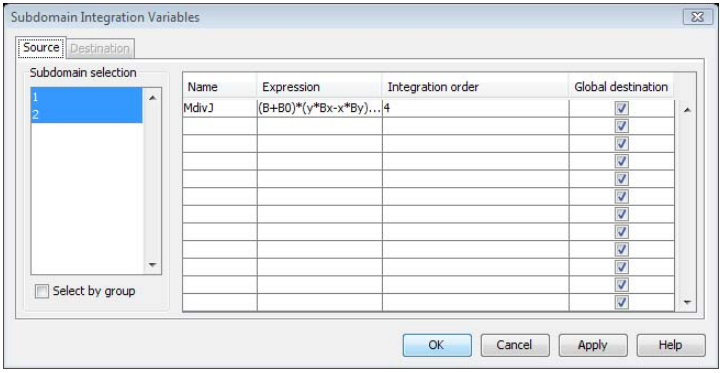
Define a variable B_0 (B0) in the two subdomains using an expression variable:

1. On the **Options** menu, point to **Expressions** and then click **Subdomain Expressions**.
2. Select Subdomain 1 and enter the name B0 in the **Name** column and 0 in the **Expression** column.
3. Select Subdomain 2 and enter the expression B0_2.
4. Click **OK**.

Coupling Variables

Define a coupling variable for the torque divided by the moment of inertia:

1. On the **Options** menu, point to **Integration Coupling Variables** and then click **Subdomain Variables**.
2. Select Subdomain 1 and 2 and enter the variable MdivJ in the **Name** column.
3. Enter the expression (B+B0)*(y*Bx-x*By)/mu/J. Keep the default integration order 4 and the default global destination.

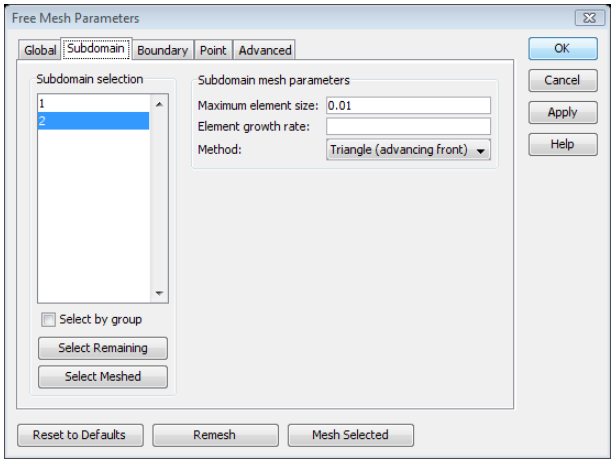


4. Click **OK**.

MESH GENERATION

1. Open the **Free Mesh Parameters** dialog box by selecting **Free Mesh Parameters** from the **Mesh** menu, click the **Custom mesh size** button and type in the 0.04 in the **Maximum element size** edit field.
2. Click the **Subdomain** tab.

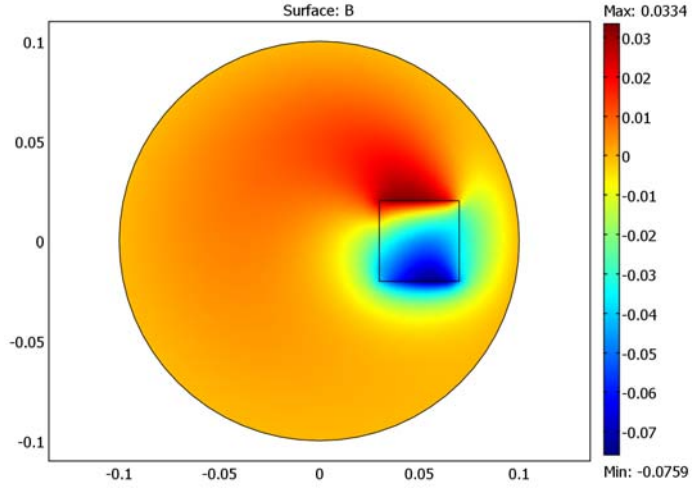
3 Select Subdomain 2 and type `0.01` in the **Maximum element size** edit field.



4 Click **OK** and then click the **Initialize Mesh** button.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to compute the solution.



Modeling Using the Programming Language—Fixed ω

1 Clear the FEM structure, set the variable name and choose quadratic elements:

```
clear fem
fem.dim = 'B';
fem.shape = 2;
```

2 Specify the constants `K`, `w`, `J`, `mu`, and `B0_2`:

```
fem.const = {...
  'K','mu*5.99e7*0.02',...
  'w','2*pi*200',...
  'J','8960*0.02*0.1^4*pi/2',...
  'mu','4e-7*pi',...
  'B0_2',0.1};
```

3 Create the geometry:

```
fem.geom = circ2(0.1)+square2(0.04,'pos',[0.05,0],'base','cent');
```

4 Specify the boundary conditions: homogeneous Dirichlet conditions at the edge of the disk (boundary elements 5, 6, 7, and 8):

```
fem.bnd.h = 1;
fem.bnd.r = 0;
fem.bnd.ind = {5:8};
```

5 Specify the PDE coefficients:

```
fem.equ.c = 1;
fem.equ.al = {{{'K*w*y' '-K*w*x'}}};
fem.equ.ga = {{{'-K*w*B0*y' 'K*w*B0*x'}}};
fem.equ.expr = {'B0' {'0' 'B0_2'}};
```

6 Specify the integration coupling variable MdivJ from Subdomains 1 and 2:

```
clear el
el.elem = 'elcplscalar';
el.var = {'MdivJ'};
el.g = {'1'};
clear src
src.expr{1} = {'(B+B0)*(y*Bx-x*By)/mu/J'};
src.ipoints{1} = {'4'};
src.ind{1} = {'1' '2'};
el.src{1} = {{},{},src};
el.geomdim = {{}};
el.global = {'1'};
fem.elemcpl = {el};
```

7 Generate the mesh:

```
fem.mesh = meshinit(fem,'hmax',0.04,'hmaxsub',[2 0.01]);
```

8 Solve the problem using the stationary solver and plot the solution:

```
fem.xmesh = meshextend(fem);
fem.sol = femstatic(fem);
postplot(fem,'tridata','B','tribar','on',...
```

```
'trirefine',10,'axisequal','on');
```

Exporting to Simulink—Time-Dependent ω

This example begins in the same way as the previous model, except the solution of the time-dependent problem is obtained using Simulink instead of extended multiphysics.

Note: This section requires that you run COMSOL Multiphysics with MATLAB and Simulink.

Set up Problem for Fixed ω

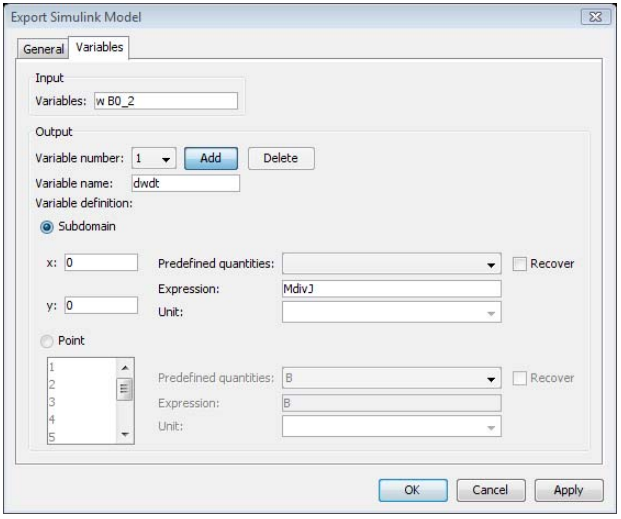
1. Make sure you are running COMSOL Multiphysics with MATLAB, and that you have installed Simulink along with MATLAB.
2. First set up the problem for fixed ω as described from page 319 or on page page 322 if you are using the programming language.

Export the Model to Simulink

1. On the **File** menu, point to **Export** and then click **Simulink Model** to open the **Export Simulink Model** dialog box.
2. Select **Export>Simulink** on the **File** menu.
3. Enter `magnet_struct` as the model name. Use **General static** as the Simulink block type.
4. Click the **Variables** tab and type `w B0_2` in the **Variables** edit field in the **Input** area. To add the variable `dwdt` at the origin, click **Add**, type `dwdt` in the **Variable name** edit

field, and make sure that the **Subdomain** button is selected. Type `0` in both the **x** and **y** edit fields, and type `MdivJ` in the **Expression** field.

This creates a structure that the COMSOL Multiphysics block in Simulink can use to run the COMSOL Multiphysics model as part of the Simulink simulation.



5 Open a Simulink model that can use the COMSOL Multiphysics model by typing `magnet_break_mdl`. As an alternative you can enter the Simulink model by following the instructions in the following section.

USING THE PROGRAMMING LANGUAGE

You can also perform the Simulink export on the MATLAB command line.

1 Start by exporting the FEM structure to MATLAB by selecting **Export>FEM Structure** on the **File** menu. If you are using the programming language to enter the model you can ignore this step.

2 Then type the command.

```
magnet_struct = femsim(fem,'input',{'w' 'B0_2'},...
'output',{{'MdivJ' [0 0]'}},...
```

```
'outnames',{'dwdt'},'static','on')
```

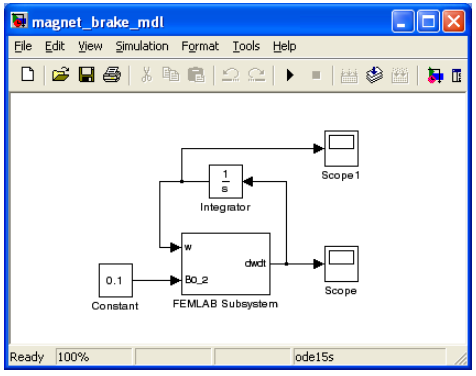
This creates a structure which the COMSOL Multiphysics block within Simulink can use to run the COMSOL Multiphysics model as part of the Simulink simulation.

The syntax `{'MdivJ' [0 0]'}` means that the output `dwdt` is computed by evaluating the expression `MdivJ` in the point (0, 0). Use the syntax of the `postinterp` command to specify outputs in this way.

3 Open a Simulink model that can use the COMSOL Multiphysics model by typing `magnet_break_mdl`. As an alternative you can enter the Simulink model by following the instructions in the following section.

DESIGN IN SIMULINK

Start Simulink and draw a model as in the following figure. You find the **COMSOL Multiphysics Subsystem** block in the **COMSOL Multiphysics** block library. To set up the input and the output ports, double-click the **COMSOL Multiphysics Subsystem** block and enter the **Simulink Structure** name `magnet_struct`.



1 Set the initial condition for the **Integrator** block to `2*pi*200`.

2 In the **Simulation Parameters** dialog box set the solver type to `ode15s`, set the relative tolerance to `1e-2` and the absolute tolerance to `1e-3`.

3 Start the simulation.

The scopes show graphs of ω and dω/dt against time that correspond to the plots on page 318.

Model Library path: `COMSOL_Multiphysics/Multidisciplinary/magnet_brake`

Modeling Using the Graphical User Interface —Time-Dependent ω

The modeling approach in this section uses the extended multiphysics feature to solve the time-dependent problem. Introduce a new variable `w`, active at a single point within the geometry using a Weak Form, Point application mode.

USING THE PREVIOUS MODEL

First set up the problem for fixed ω as described from page 319, but click the **Refine Mesh** button on the Main toolbar for a finer mesh. Without the export to Simulink, you can afford a finer mesh that increases the accuracy.

MODEL NAVIGATOR

1. Open the **Model Navigator** from the **Multiphysics** menu.
2. In the list of application modes, open the **COMSOL Multiphysics>PDE Modes** folder, and select **Weak Form**, **Point**.
3. Type `w` in the **Dependent variables** edit field.
4. Click **Add**.
5. Click **OK**.

OPTIONS AND SETTINGS

1. Open the **Constants** dialog box from the **Options** menu.
2. Select the variable `w` in the list and rename it `w0`. Later on, use this constant as initial value for `w`, the angular velocity.
3. Click **OK**.

PHYSICS SETTINGS

Point Settings

1. Open the **Point Settings** dialog box from the **Physics** menu.
2. Click the **Init** tab.
3. Select Point 1 and enter `w0` as initial value in the **$w(t_0)$** edit field.
4. Click the **Weak** tab.

5 Enter PDE settings as shown for the weak point mode.

WEAK TERM	POINT 1
weak	`w_test*MdivJ`
dweak	`w_test*w_time`
constr	0

6 Select Points 2 through 9 and clear the **Active in this domain** check box.

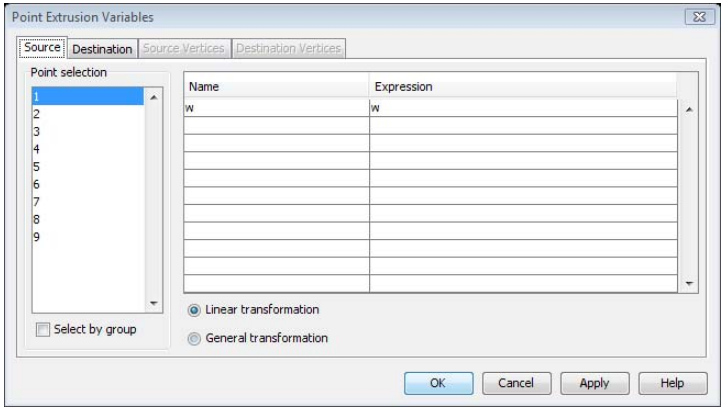
7 Click **OK**.

Defining Coupling Variables

The coupling variable `MdivJ` that integrates the torque has already been set up. You need to add a coupling variable that makes the angular velocity, `w`, available throughout the domain.

1 On the **Options** menu, point to **Extrusion Coupling Variables** and then click **Point Variables**.

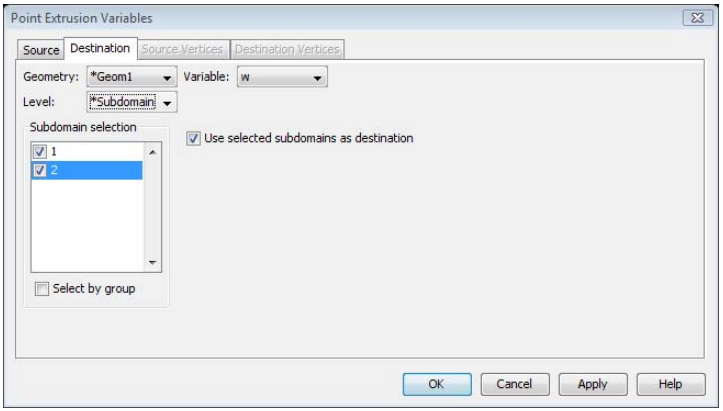
2 Select Point 1 and enter the variable name `w` and the expression `w`.



3 Click the **General transformation** button.

4 Click the **Destination** tab.

5 Select **Subdomain** in the **Level** list and then select the check boxes for Subdomains 1 and 2.



6 Click **OK**.

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box and select **Time dependent** in the **Solver** list.

2 Type `range(0,0.2,8)` in the **Times** edit field and then type `1e-3` in the **Relative tolerance** edit field and `1e-5` in the **Absolute tolerance** edit field.

3 Click the **Time Stepping** tab.

4 Select the **Time steps from solver** in the **Times to store in output** list.

5 Click **OK**.

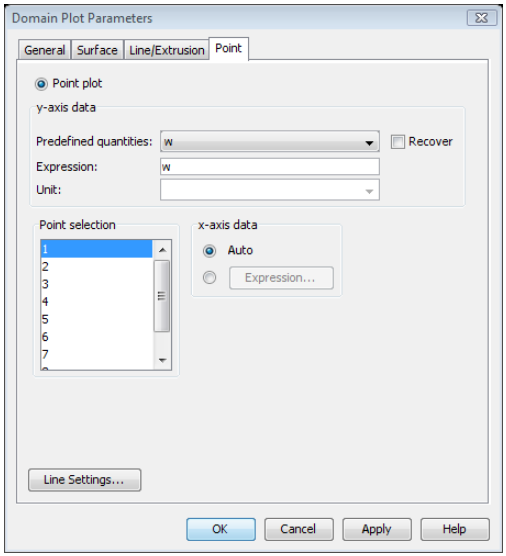
6 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Using the solution data, you can visualize the results in a number of ways:

- Click the **Animate** button to create an animation of the dissipation of B over time.
- For a graph of the ω against time, open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu. On the **General** page, select all the time steps in the list and

select **Point plot**. Click the **Point** tab, select Point1, and type `w` in the **Expression** edit field. Click **OK**.



- For a graph of $d\omega/dt$ against time, follow the same procedure as for ω but type `MdivJ` in the **Expression** edit field instead.

Process Control Using a PID Controller

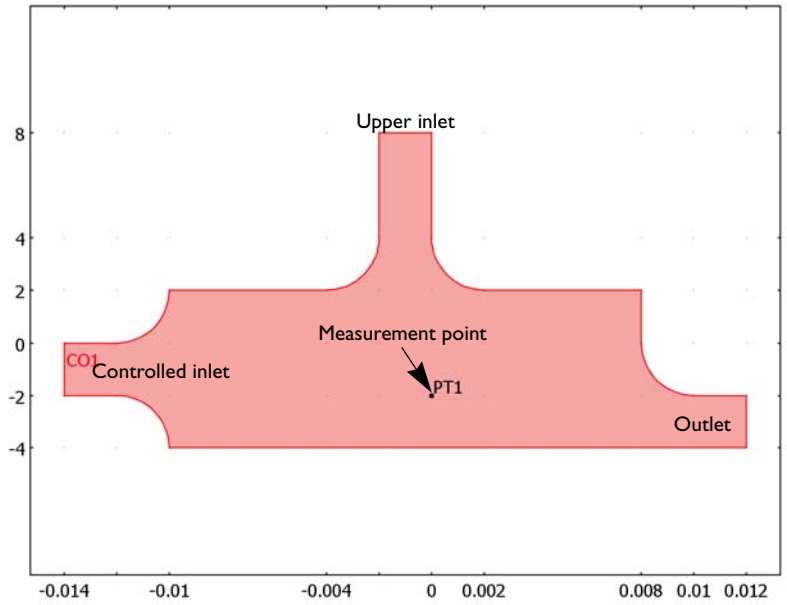
Introduction

In the chemical process industry it is often important to control a specific process. PID control (proportional-integral-derivative-control) is one way to achieve that, but it can be difficult to optimize the parameters in the PID algorithm. This example illustrates how you can implement a PID control algorithm to simulate a process control system and to find the optimal PID parameters.

This model is a generic example but could resemble the environment in a combustion chamber where the concentration at the ignition point is crucial. Two gas streams with different oxygen concentrations are mixed in the combustion chamber. The concentration is measured at the ignition point before complete mixing of the streams is reached. The control algorithm alters the inlet velocity of the gas with the lower oxygen content to achieve the desired total concentration at the ignition point.

Model Definition

The model geometry appears in the following figure. At the upper inlet, a gas stream with high oxygen content enters the reactor at a velocity of 10 mm/s, while a gas with a lower oxygen level enters from the left. The oxygen concentration is measured at a measurement point, and the inlet velocity of the less concentrated stream is altered by the PID control algorithm to achieve the desired concentration at that point.



The model uses the Navier-Stokes equations to describe the fluid flow and the Convection and Diffusion application mode for the mass balance.

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot [\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{F}$$
$$\nabla \cdot \mathbf{u} = 0 \tag{9-1}$$

$$\delta_{ts}\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - \mathbf{u} \cdot \nabla c \tag{9-2}$$

It is possible to formulate the boundary conditions for the mass-transport equation by assuming that you know the two inlet concentrations. In addition, assume that the reactant transport at the outlet is mainly driven by convection, that is, neglect diffusion in the main direction of the convective flow. An insulation/symmetry boundary condition describes all walls. The boundary conditions for the mass balance are:

BOUNDARY	CONSTRAINT
Upper inlet	$c = c_{\text{in,top}}$
Controlled inlet	$c = c_{\text{in,inlet}}$

BOUNDARY	CONSTRAINT
Outlet	$\mathbf{n} \cdot (-D\nabla c) = 0$
Walls	$\mathbf{N} \cdot \mathbf{n} = 0$

Here c is the concentration; $c_{\text{in,top}}$ and $c_{\text{in,inlet}}$ are the inlet concentrations (mol/m^3) for the upper and controlled inlets, respectively; D is the applied diffusivity (m^2/s); and $\mathbf{N}$ is the molar flux (mol/(m^2·s)).

The model uses the following boundary conditions for the fluid flow:

BOUNDARY	CONSTRAINT
Upper inlet	$\mathbf{u} = (0, -v_{\text{in,top}})$
Controlled inlet	$\mathbf{u} = (u_{\text{in}}, 0)$
Outlet	$p_0 = 0$
Inlet sections	$\mathbf{n} \cdot \mathbf{u} = 0$
Walls	$\mathbf{u} = 0$

Here $\mathbf{u}$ is the velocity vector (m/s), $v_{\text{in,top}}$ is the inlet velocity at the top inlet, and u_{in} is the PID controlled velocity. At the outlet, set the pressure to p_0 (Pa). No-slip boundary conditions describe all walls except the inlet sections where slip conditions apply, allowing for a smooth transition to a laminar velocity profile.

The PID control algorithm used to calculate u_{in} is

$$u_{\text{in}} = k_{\text{P}}(c - c_{\text{set}}) + k_{\text{I}}\int_0^t (c - c_{\text{set}})dt + k_{\text{D}}\frac{\partial}{\partial t}(c - c_{\text{set}}) \tag{9-3}$$

with the following parameters:

PARAMETER	VALUE
c_{set}	0.5 mol/m^3
k_{P}	0.5 m^4/(mol·s)
k_{I}	1 m^4/(mol·s^2)
k_{D}	10^{-3} m^4/mol

In practice, the derivative constant, k_{D}, is set to 0 in most cases as this parameter can be difficult to determine and the term may increase the fluctuations in the system.

Results

The two plots in Figure 9-1 show the oxygen concentration and the velocity stream lines in the chamber after approximately 0.01 s and 1.5 s, respectively. The figures show that the measured concentration depends strongly on the flow field. At start-up, when the inlet velocity of the stream entering from the left is very low, the sensor is entirely exposed to the highly concentrated stream, and as the left inlet velocity increases the opposite relation occurs.

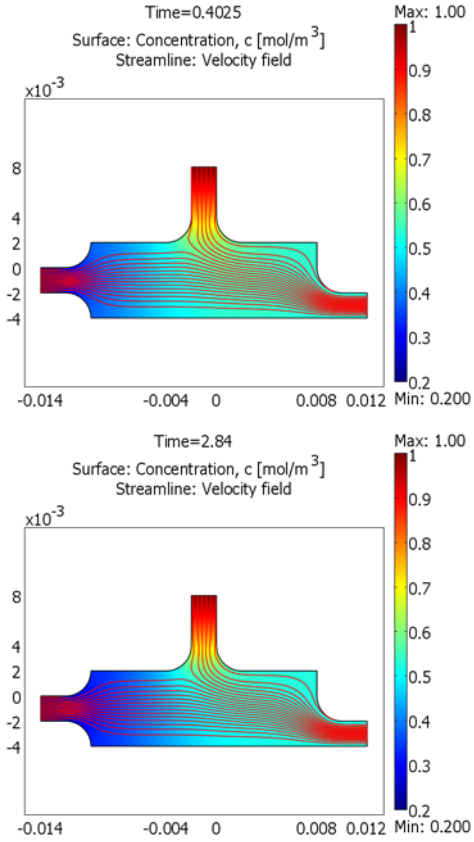


Figure 9-1: Oxygen concentration and velocity streamlines after approximately 0.01 s (top) and 1.5 s (bottom).

Figure 9-2 shows the inlet velocity and concentration in the measurement point as a function of time for two different values for the k_P parameter. The solid line represents the results for a k_P value of 0.5 $m^4/(mol \cdot s)$ while the dashed line corresponds to k_P

equal to 0.1 $m^4/(mol \cdot s)$. The results evaluated for the smaller k_P value oscillate more before stabilizing. Thus, it is clear that for this case the higher k_P value yields a more stable process control.

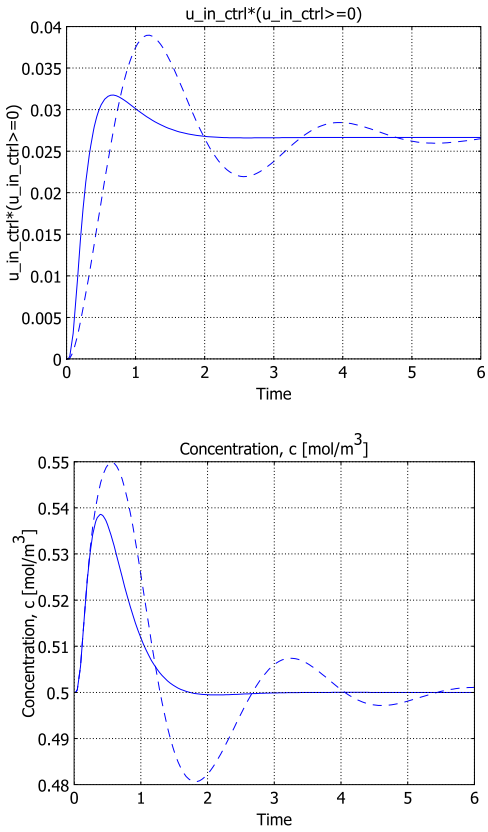


Figure 9-2: PID-controlled inlet velocity (top) and concentration in the measurement point (bottom) as a function of time for $k_P = 0.5$ $m^4/(mol \cdot s)$ (solid) and $k_P = 0.1$ $m^4/(mol \cdot s)$ (dashed).

Model Library path: `COMSOL_Multiphysics/Multidisciplinary/PID_control`

MODEL NAVIGATOR

1 Go to the **Model Navigator** and select **2D** from the **Space dimension** list.

2 In the list of application modes select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis**.

3 Click the **Multiphysics** button in the lower right corner, then click **Add**.

4 Similarly, add the **COMSOL Multiphysics>Convection and Diffusion>Convection and Diffusion>Transient analysis** application mode.

5 Click **OK**.

OPTIONS AND SETTINGS

Constants

1 Go to the **Options** menu and choose **Constants**.

2 Make the following entries in the **Constants** dialog box; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
v_in_top	0.01[m/s]	Velocity, upper inlet
cin_top	1[mol/m^3]	Concentration, upper inlet
cin_inlet	0.2[mol/m^3]	Concentration, controlled inlet
c00	0.5[mol/m^3]	Initial concentration, chamber interior
eta	3e-5[Pa*s]	Dynamic viscosity
rho	1.2[kg/m^3]	Density
D	1e-4[m^2/s]	Diffusivity
c_set	0.5[mol/m^3]	Setpoint concentration
k_P_ctrl	0.5[m^4/(mol*s)]	Proportional parameter
k_I_ctrl	1[m^4/(mol*s^2)]	Integral parameter
k_D_ctrl	1e-3[m^4/mol]	Derivative parameter

Grid Settings

1 Go to the **Options** menu and select **Axes/Grid Settings**.

2 On the **Axis** page enter **x-y limits** (expressed in the default length unit meters) for the axes as displayed below.

AXIS	VALUE
x min	-0.015
x max	0.015
y min	-0.01
y max	0.02

3 Click the **Grid** tab.

4 Clear the **Auto** check box and enter the following extra grid values:

GRID	VALUE
Extra x	-0.014 -0.012 -0.01 -0.004 -0.002 0 0.002 0.008 0.01 0.012
Extra y	-0.004 -0.002 0 0.002 0.004 0.008

5 Click **OK**.

GEOMETRY MODELING

1 When creating the geometry you alternate between using the **Line** and **2nd Degree Bézier Curve** tools located on the Draw toolbar to the left. For curved shapes use the curve tool, and for straight lines use the line tool. Click on the points given in the following table using the corresponding drawing tool. Use the coordinates displayed in the lower-left corner of the screen to find the points.

DRAW TOOL	POINTS (X, Y)
Line	(0.012,-0.002) (0.012,-0.004) (-0.01,-0.004)
Curve	(-0.01,-0.002) (-0.012,-0.002)
Line	(-0.014,-0.002) (-0.014,0) (-0.012,0)
Curve	(-0.01,0) (-0.01,0.002)
Line	(-0.004,0.002)
Curve	(-0.002,0.002) (-0.002,0.004)
Line	(-0.002,0.008) (0,0.008) (0,0.004)
Curve	(0,0.002) (0.002,0.002)
Line	(0.008,0.002) (0.008,0)
Curve	(0.008,-0.002) (0.01,-0.002)
Line	Right-click to close the geometry

2 To add the measurement point, click the **Point** button in the Draw toolbar to the left and click on the coordinates $(0, -2 \cdot 10^{-3})$.

3 Click the **Zoom Extents** button on the Main toolbar to center the geometry.

PHYSICS SETTINGS

Subdomain Settings—Incompressible Navier-Stokes

1 Go to the **Multiphysics** menu and select **Incompressible Navier-Stokes (ns)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 In the **Subdomain Settings** dialog box select Subdomain 1 and type `rho` in the **Density** edit field.

4 In the **Dynamic viscosity** edit field type `eta`. Click **OK**.

Boundary Conditions—Incompressible Navier-Stokes

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

2 In the **Boundary Settings** dialog box enter the following boundary conditions:

SETTINGS	BOUNDARY 1	BOUNDARY 7	BOUNDARIES 2, 3, 6, 8	BOUNDARIES 4, 5, 9–11, 13–17	BOUNDARY 12
Boundary type	Inlet	Inlet	Symmetry boundary	Wall	Outlet
Boundary condition	Velocity	Velocity	-	No slip	Pressure, no viscous stress
u_0	`u_in_ctrl* (u_in_ctrl>=0)`	0			
v_0	0	`-v_in_top`			
p_0					0

You will define `u_in_ctrl` as a scalar expression shortly.

3 Click **OK**.

Subdomain Settings—Convection and Diffusion

1 From the **Multiphysics** menu, choose **Convection and Diffusion (cd)**.

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

3 In the **D (isotropic)** edit field type `D` to define an isotropic diffusion coefficient.

4 In the **x-velocity** edit field type `u`.

5 In the **y-velocity** edit field type `v`.

6 Click the **Init** tab.

7 In the **c(t_0)** edit field enter the initial concentration `c00`, then click **OK**.

Boundary Conditions—Convection and Diffusion

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

2 In the **Boundary Settings** dialog box enter the following boundary conditions:

SETTINGS	BOUNDARY 1	BOUNDARIES 2–6, 8–11, 13–17	BOUNDARY 7	BOUNDARY 12
Type	Concentration	Insulation/ Symmetry	Concentration	Convective flux
c_0	`cin_inlet`		`cin_top`	

3 Click **OK**.

PID ALGORITHM SETUP

It is possible to specify the PID algorithm as a scalar expression. However, some of the terms in the algorithm require some additional specifications. The algorithm contains the concentration in the measurement point, the time derivative of the concentration in the point, and the time integration of the concentration difference between the measured and wanted concentrations.

1 Go to the **Options** menu and choose **Expressions>Scalar Expressions**.

2 Set the **Name** to `u_in_ctrl` and define the **Expression** as `nojac(k_P_ctrl*(conc-c_set)+k_I_ctrl*Int+k_D_ctrl*ctime)`. The `nojac` operator makes sure the above expression gives no Jacobian contribution. The resulting effect is the same as using nonideal weak constraints, namely a one-way coupling instead of the normal two-way coupling. Because of the use of a coupling variable, the unit becomes undefined for this variable and other quantities where you use it.

3 Click **OK**.

4 To specify the concentration and its time derivative in the point, go to the **Options** menu and choose **Integration Coupling Variables>Point Variables**.

5 Select Point 10 and enter `conc` in the **Name** edit field and `c` in the **Expression** edit field.

6 For the same point enter `ctime` in the **Name** edit field and `ct` in the **Expression** edit field. `ct` is the predefined expression for the time derivative of the concentration.

7 Click **OK**.

8 To specify the time integral of the concentration difference in the point, go to the **Physics** menu and open the **Global Equations** dialog box.

9 Type `Int` in the **Name (u)** edit field.

10 In the **Equation** edit field type `Intt-(conc-c_set)`.

11 Click **OK** to exit the **Global Equations** dialog box.

MESH GENERATION

1 Go to the **Mesh** menu and choose **Free Mesh Parameters**.

2 On the **Global** tab, select **Finer** in the **Predefined mesh sizes** list.

3 To reduce the number of elements along the curved boundaries, click the **Custom mesh size** button and type `0.5` in the **Mesh curvature factor** edit field.

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

COMPUTING THE SOLUTION

1 Go to the **Solve** menu and select **Solver Parameters**.

2 On the **General** page, set the **Times** vector to `range(0,0.04,6)`.

3 On the **Time Stepping** page, select **Time steps from solver** from the **Times to store in output** list to make all time steps the solver takes available for postprocessing.

4 Select **Intermediate** from the **Time steps taken by solver** list to give the solver some freedom to set its own time steps. Using this option restricts the solver to take at least one time step in each subinterval of the time list.

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

6 Click the **Solve** button on the Main toolbar to start the simulation.

POSTPROCESSING AND VISUALIZATION

The default visualization plots the magnitude of the velocity field at the end of the simulation interval. Follow the instructions below to reproduce the simultaneous plots of the oxygen concentration and the velocity stream lines at two different times presented in Figure 9-1 on page 334.

1 Go to the **Postprocessing** menu and choose **Plot Parameters** to open the **Plot Parameters** dialog box.

2 On the **General** page, select the solution near $t = 0.01$ s from the **Solution at time** list.

3 On the **Surface** page, click the **Surface Data** tab.

4 In the **Predefined quantities** list, select **Convection and Diffusion (cd)>Concentration, c**.

5 Click the **Streamline** tab.

6 Select the **Streamline plot** check box. In the **Predefined quantities** list on the **Streamline Data** tab keep the default selection, **Incompressible Navier-Stokes (ns)>Velocity field**.

7 From the **Streamline plot type** list select **Magnitude controlled**.

8 Click **Apply** to view the upper plot in Figure 9-1.

9 Return to the **General** tab, then select the solution near $t = 1.5$ s from the **Solution at time** list. Click **OK** to generate the lower plot in Figure 9-1.

To visualize the inlet velocity and the measured concentration as functions of time, use domain plots:

1 Open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

2 Click the **Point** tab.

3 Select Point 1 and enter `u_in_ctrl*(u_in_ctrl>=0)` in the **Expression** edit field.

4 Click **Apply**.

5 Click the **General** tab and select to plot in **New figure** in the **Plot in** list.

6 Click the **Point** tab, select Point 10, and select **Concentration, c** from the **Predefined quantities** list.

7 Click **OK**.

To see the above plots for different values of k_P, alter the k_P value and solve the model again without closing the plot frames:

1 Open the **Constants** dialog box from the **Options** menu and change the value of `k_P_ctrl` to `0.1 [m^4/(mol*s)]`.

2 Click the **Solve** button to solve the model for the new parameter value.

3 Open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

4 On the **General** page, select to plot in **Figure 2** and select the **Keep current plot** check box.

5 Click the **Point** tab and make sure Point 10 and **Concentration, c** are selected.

6 Click the **Line Settings** button. Set the **Line style** to **Dashed line**, then click **OK**.

7 Click **Apply** to generate the lower plot in Figure 9-2 on page 335.

8 On the **General** page, select to plot in **Figure 1**. Select the **Keep current plot** check box.

9 Click the **Point** tab, select Point 1, and type `u_in_ctrl*(u_in_ctrl>=0)` in the **Expression** edit field.

10 Click **OK** to close the dialog box and generate the upper plot in Figure 9-2.

Controlling Temperature

Introduction

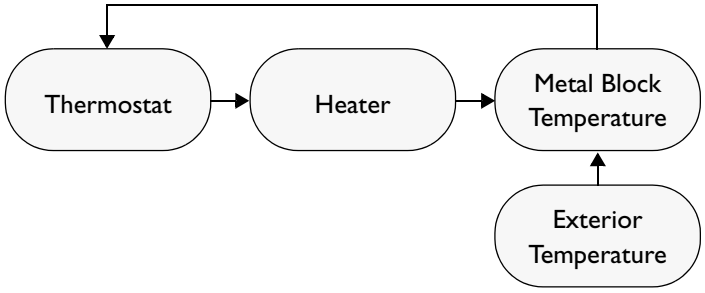
This example demonstrates controlling the temperature in a heated metal block using a thermal controller. You make the model in COMSOL Multiphysics and export it to Simulink, using an on-off controller.

Model Definition

The study of this thermal controller involves two distinct modeling situations:

- Taken as a whole, this dynamic system assumes only a small number of states, making it a good candidate for modeling and simulation with Simulink.
- One of the model's elements, the controller, contains a subsystem that involves heat distribution, which is described with a PDE, the heat equation. It is easy to break this portion of the problem down and model it in COMSOL Multiphysics.

The dynamic system consists of a metal block that exchanges heat with the environment. A heater and a thermostat switch are situated inside the glass-enclosed system. The system works as follows: The thermostat turns the heater on or off when the temperature becomes too low or too high.



The finite-element model of the metal block requires two inputs:

- The state of the heater, which can be On (1) or Off (0)
- The exterior temperature, T_{out}

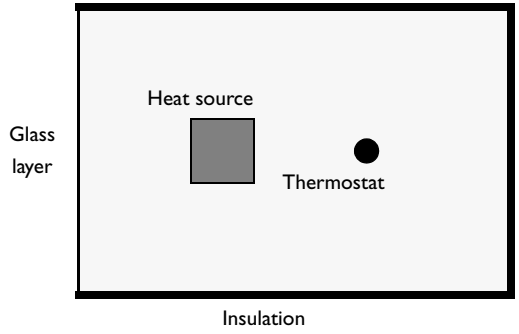
As its output, the model supplies the temperature at the thermostat's location.

The PDE describes the overall system's temperature distribution given the temperature of the heater and the exterior environment. If the heat transfer is so fast that the heat distribution is more or less constant (in space, not in time), a single state is sufficient. Otherwise, controlling the temperature requires modeling a PDE in COMSOL Multiphysics and then including those results in the Simulink environment as illustrated here.

The heat equation is:

$$\rho C\frac{\partial T}{\partial t} - \nabla \cdot (k\nabla T) = Q$$

The boundary conditions come from the level of insulation around the system. On well-insulated sides the temperature flux is zero, which gives the Neumann boundary condition $\mathbf{n} \cdot (k\nabla T) = 0$. The poorly insulated sides involve the Neumann condition $\mathbf{n} \cdot (k\nabla T) = k_g/l_g \cdot (T_{out} - T)$, where k_g and l_g are the thermal conductivity and the thickness of the glass sheet that separates the metal block and the exterior.



Because only the temperature distribution in the xy-plane is of interest, you can use a 2D model. For the units to make sense, think of the domain as having a depth (z direction) of 1 m.

Modeling in COMSOL Multiphysics

This model is based on the SI system, but to more appropriately represent the time scale of the problem, the time is counted in minutes. This means that you must scale all quantities with units that contain the basic unit of time by a factor 60 compared to their standard SI values. This model data in the following lists includes this conversion for the thermal conductivity k and the heat source Q.

Metal block:

- Dimensions $30 \times 20 \times 100$ cm $= 0.3 \times 0.2 \times 1$ m
- Density $\rho = 7.82 \cdot 10^3$ kg/m^3
- *Heat capacity* $C = 449$ J/(kg·K)
- *Thermal conductivity* $k = 82$ W/(m·K) $= 4.92 \cdot 10^3$ J/(m·min·K)

Glass sheet:

- *Thermal conductivity* $k_g = 0.9$ W/(m·K) $= 54$ J/(m·min·K)
- *Thickness* $l_g = 1$ mm $= 10^{-3}$ m

Heater:

- *Dimensions* $4 \times 4 \times 100$ cm $= 0.04 \times 0.04 \times 1$ m
- *Heat source* $Q = 2$ kW/$V_{\text{heater}} = 2 \cdot 10^3/(1 \cdot 0.04^2)$ W/m$^3 = 7.5 \cdot 10^7$ J/(m^3·min)

Do the modeling in COMSOL Multiphysics in two steps:

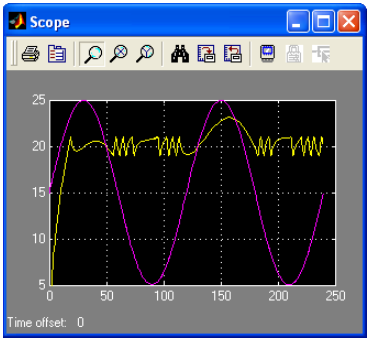
1. Set up a basic model of the steel plate for the Simulink export.
2. Make the model of the on-off controller in Simulink.

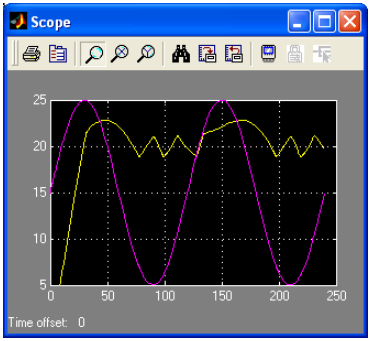
Results

The model uses Simulink to simulate the on-off controller. Simulink handles the nonlinear behavior of the on-off controller well. The PDE model for the plate is linear, you can do the Simulink export using the linearized state-space form to improve performance. You can also use the mode reduction facility of the Simulink export to improve performance in Simulink, but it only works for linear or linearized PDE models.

As an alternative approach, it is possible to model a PI controller, either in Simulink or using an ODE directly in COMSOL Multiphysics.

The following set of images shows the result of the Simulink simulation with the on-off controller. The left figure shows the thermostat temperature at node 3 and the right figure shows the result when the thermostat has been move to node 8.





Notice a few interesting details in the solutions. For instance, the distance between the thermostat and the exterior has an effect on the delay between the peaks of the two curves. Node 8 is farther from the exterior than node 3, so the delay is larger in the second plot than in the first.

Notice also the qualitative differences between the two simulations. This extra information comes as a bonus for solving a detailed heat-flow problem that accounts for the geometry and the heat-diffusion properties.

Model Library path: `COMSOL_Multiphysics/Multidisciplinary/thermal_controller_simulink`

Using the Graphical User Interface—No Controller

Before exporting the model description to Simulink, run a time-dependent simulation in COMSOL Multiphysics, running with the heater turned on with an initial temperature of 20 degrees in the plate.

MODEL NAVIGATOR

1. Select **2D** in the **Space dimension** list.
2. In the list of application modes, open **COMSOL Multiphysics>Heat Transfer** and then select **Conduction** and finally **Transient analysis**.

3 Use the default dependent variable name T. Make sure the **Lagrange - Quadratic** element type is selected in the **Elements** list.

4 Click **OK**.

GEOMETRY MODELING

1 In the **Draw** menu, point to **Specify Objects** and then click **Rectangle**.

2 In the **Rectangle** dialog box, type `0.3` and `0.2` in the **Width** and **Height** edit fields.

3 Click **OK**.

4 Click the **Zoom Extents** button.

5 In the **Draw** menu, point to **Specify Objects** and then click **Square**.

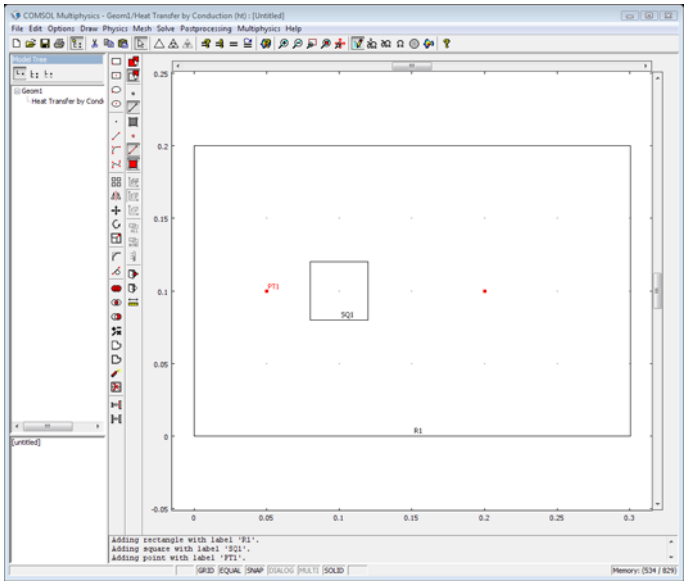
6 In the **Square** dialog box, type `0.04` in the **Width** edit field. In then **Position** area, select **Center** in the **Base** list and enter `0.1` and `0.1` in the **x** and **y** edit fields.

7 Click **OK**.

8 In the **Draw** menu, point to **Specify Objects** and then click **Point**.

9 In the **Point** dialog box, type `0.05 0.2` and `0.1 0.1` in the **x** and **y** edit fields, respectively, to create two points at (0.05, 0.1) and (0.2, 0.1).

10 Click **OK**.



OPTIONS AND SETTINGS

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

2 Enter the following constants:

NAME	EXPRESSION
HeatState	1
Tout	20

3 Click **OK**.

PHYSICS SETTINGS

Boundary Conditions

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

2 Enter the following boundary conditions:

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3, 8
Boundary condition	Heat flux	Thermal insulation
h	54/1e-3	
T_{inf}	Tout	

3 Click **OK**.

Subdomain Settings

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

2 Enter the following material properties:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
k (isotropic)	4.92e3	4.92e3
ρ	7.82e3	7.82e3
C_p	449	449
Q	0	7.5e7*HeatState

3 Click the **Init** tab.

4 Enter the following initial values:

SETTINGS	SUBDOMAINS 1, 2
$T(t_0)$	20

5 Click **OK**.

MESH GENERATION

To speed up the computation within Simulink, use a coarse mesh.

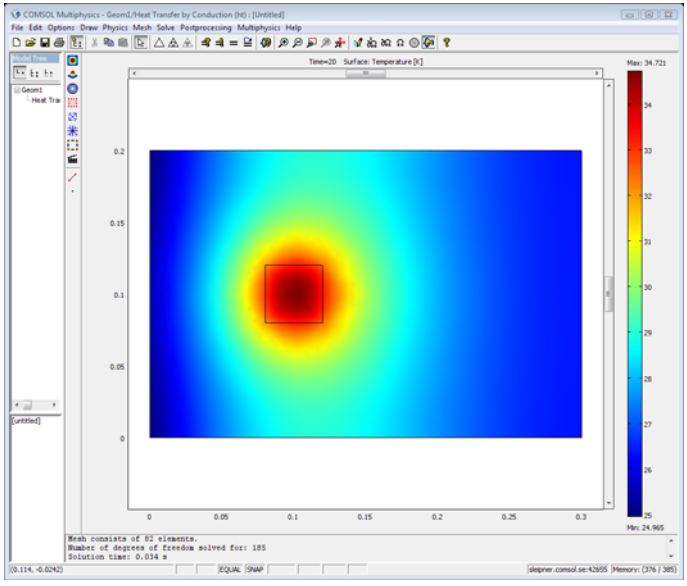
1. Open the **Free Mesh Parameters** dialog box, click the **Custom mesh size** button and enter `0.05` in the **Maximum element size** edit field.
2. Click **OK** to close the dialog box.
3. Initialize the mesh.

COMPUTING THE SOLUTION

Solve the heat equation using 21 equal steps for 20 minutes, starting at time = 0:

1. Open the **Solver Parameters** dialog box from the **Solve** menu.
2. Enter `range(0,20)` in the **Times** edit field.
3. Click **OK**.
4. Click the **Solve** button to start the simulation.

A plot of the surface temperature at Time = 20 appears as in this figure:



Exporting to Simulink—Temperature Control

The result of exporting a model from COMSOL Multiphysics to Simulink is a structure variable in the MATLAB workspace. To use the model in Simulink, simply drag the **COMSOL Multiphysics Subsystem** block to your Simulink model as described in "Modeling in Simulink" on page 350.

The following variables affect the temperature of the metal block:

- Exterior temperature, `Tout`
- The state of the heater, `HeatState`, which can have the values 1 or 0, corresponding to on or off

The output from the COMSOL Multiphysics model is the temperature in the block where the thermostat is located:

- Thermostat temperature, `Temp`

You need this variable to control the heater.

EXPORTING TO SIMULINK

1. Enter the model as described on page 345.
2. On the **File** menu, point to **Export** and then click **Simulink Model** to open the **Export Simulink Model** dialog box.
3. Enter `blocksct` in **Structure name** and change **Simulink block type** to **Linearized dynamic**. On the **Variables** tab, enter `HeatState Tout` in **Input**. To add the output variable Temp, click **Add** and enter **Variable name** `Temp`. Click **Point**, and select Point 3 in the list. Keep the **Expression** `T`. Click **OK**.
4. Open a Simulink model that can use the COMSOL Multiphysics model by typing in MATLAB

   ```
   thermal_controller_mdl
   ```

   As an alternative you can enter the Simulink model by following the instructions in the section "Modeling in Simulink" below.

USING THE PROGRAMMING LANGUAGE

1. Enter the model as described on page 345.
2. On the **File** menu, point to **Export** and then click **FEM Structure** to export the FEM Structure to MATLAB.
3. Type the command

```
blocksct = femsim(fem,'input',{'HeatState' 'Tout'},...
'output',{{'T' zeros(0,1) 'dom' 3}},...
'outnames',{'Temp'},'state','on');
```

This creates a structure which the COMSOL Multiphysics block within Simulink can use to run the COMSOL Multiphysics model as part of the Simulink simulation.

The syntax `{'T' zeros(0,1) 'dom' 3}` means that the output `Temp` is computed by evaluating the expression `T` in point 3. Use the syntax of the `postinterp` command to specify outputs in this way.

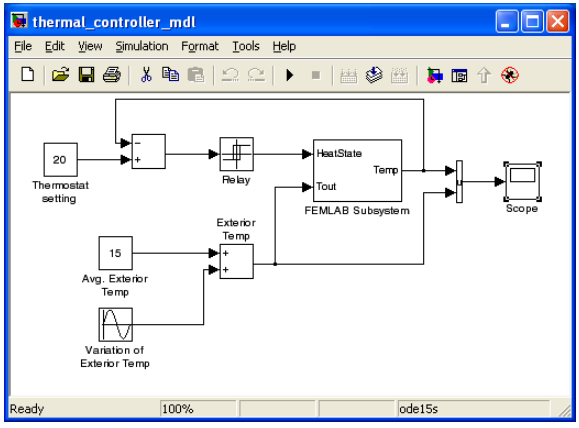
4 Open a Simulink model that can use the COMSOL Multiphysics model by typing

```
thermal_controller_mdl
```

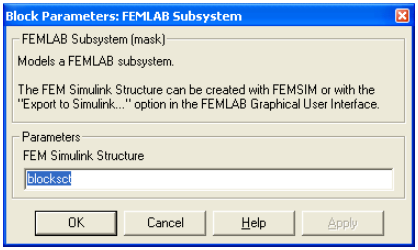
As an alternative you can enter the Simulink model by following the instructions below.

MODELING IN SIMULINK

1 Start Simulink by typing `simulink` in the MATLAB Command Window. Draw a model as shown below. You find the **COMSOL Multiphysics Subsystem** block under **COMSOL Multiphysics** in the Simulink block library. See the Simulink documentation for more information about creating models.

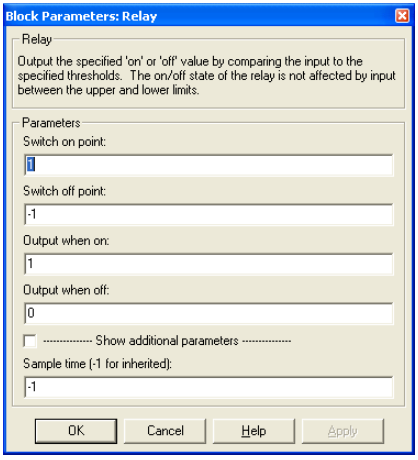


2 To set up the input and output ports of the **COMSOL Multiphysics Subsystem** block, double-click that block and set the structure name to `blocksct`. Click **OK**.

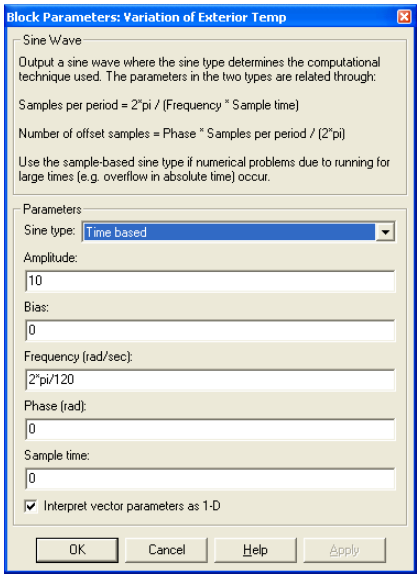


3 Specify the values of the constant blocks for **Thermostat Setting** and **Average Exterior Temperature** as in the previous figure.

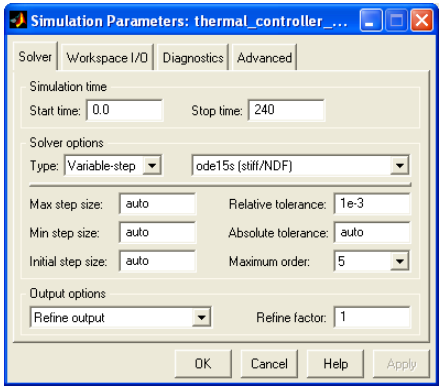
4 In the **Relay** block, enter the value `1` as the **Switch on point** and `-1` as the **Switch off point**.



5 In the **Sine Wave** block, set the amplitude to `10` and the frequency to `2*pi/120`, which corresponds to a period of 120 minutes.



6 Open the **Simulation Parameters** dialog box by making a selection from the **Simulation** menu. Set the **Stop time** to 240 minutes and the **Solver** to `ode15s`. The stability of discrete heat equations is known to put severe constraints on the time step of explicit methods. Thus you should select the `ode15s` solver (implicit) rather than the explicit integrators.



7 Now solve the system by selecting **Start** from the **Simulation** menu.

8 To view the temperature at node 3, double-click the **Scope** block.

9 Finally switch the thermostat from node 3 to node 8. On the **File** menu, point to **Export** and then click **Simulink Model** to open the **Export Simulink Model** dialog box.

10 Select Point 8 in the list. Click **OK**.

11 Restart the simulation in Simulink.

10

Multiphysics Models

Multiphysics models include the coupling of several dependent variables from different physics in the same model. Typical multiphysics applications include fluid-structure, thermal-structure, and thermal-electric couplings. In COMSOL Multiphysics, you can also build extended multiphysics models, which contain several kinds of physics and equations on more than one geometry. Extended multiphysics model can include any mix of 0D (ODEs or algebraic equations), 1D, 2D, and 3D geometries.

Free Convection

Introduction

This example describes a fluid flow problem with heat transfer in the fluid. An array of heating tubes is submerged in a vessel with fluid flow entering at the bottom. Figure 10-1 shows the setup.

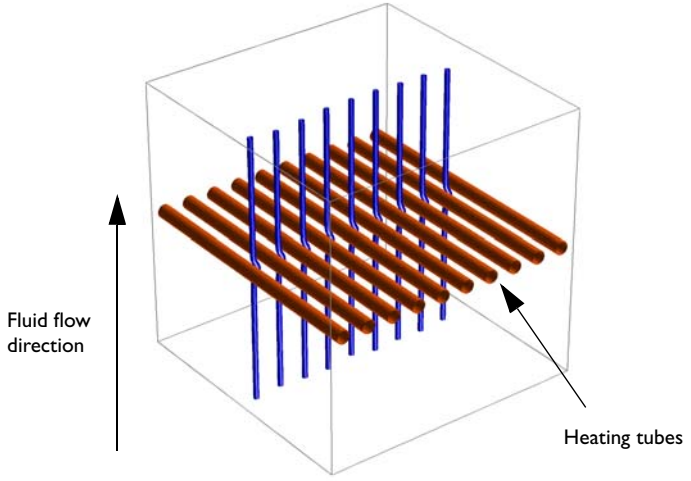


Figure 10-1: Heating tubes and direction of the fluid flow

Model Definition

The first consideration when modeling should always be the true dimension of the problem. Sometimes there are no variations in the third dimensions, and it can be extrapolated from the solution of a related 2D case. Neglecting any end effects from the walls of the vessel, the solution is constant in the direction of the heating tubes, therefore you can reduce the model to a 2D domain.

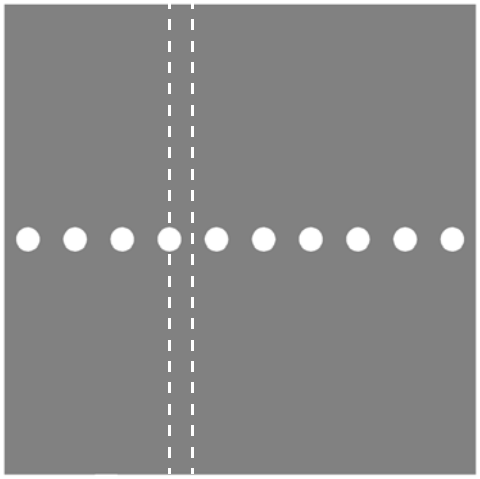


Figure 10-2: Using symmetry to reduce computation time and complexity. The model describes one section of the array of heating tubes (indicated by the dashed lines).

The next step is finding symmetries. In this case, using symmetry planes, it suffices to model the thin domain indicated in Figure 10-2.

GOVERNING EQUATIONS

This is a multiphysics model because it involves more than one kind of physics. The incompressible Navier-Stokes equations from fluid dynamics work together with a heat transfer equation. There are four unknown field variables (dependent variables):

- The velocity field components, u and v
- The pressure, p
- The temperature, T

They are all related through bidirectional multiphysics couplings.

The incompressible Navier-Stokes equations consist of a momentum balance (a vector equation) and a mass conservation and incompressibility condition:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \eta\nabla^2\mathbf{u} + \mathbf{F}$$

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

Here

- $\mathbf{u}$ is the velocity field.
- p is the pressure.
- $\mathbf{F}$ is a volume force.
- ρ is the fluid density.
- η is the dynamic viscosity.
- ∇ is the vector differential operator.

The heat equation is an energy conservation equation that says that the change in energy is equal to the heat source minus the divergence of the diffusive heat flux:

$$\rho C_p\left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) + \nabla \cdot (-k\nabla T) = Q$$

where C_p is the heat capacity of the fluid and ρ is fluid density. Q represents a source term. The velocity field comes from the incompressible Navier-Stokes equation.

Modeling in COMSOL Multiphysics

To build a model in COMSOL Multiphysics using the above equations, use two application modes: the Incompressible Navier-Stokes application mode for fluid flow and the Convection and Conduction application mode for heat transfer. The multiphysics couplings enter directly into the physics settings in the application modes.

In this model, the equations are coupled in both directions. First, add free convection to the momentum balance with the *Boussinesq approximation*. This approximation ignores variations in density with temperature, except that the variations give rise to a buoyancy force lifting the fluid. This force enters the $\mathbf{F}$ term in the incompressible Navier-Stokes equations.

At the same time, the heat equation must account for the velocity field. Using the predefined Fluid-Thermal Incompressible Flow coupled multiphysics entry, the velocity components from the incompressible Navier-Stokes equations appear automatically as the velocity field for the convective heat transfer in the Convection and Conduction application mode.

Results

The analysis of the coupled thermal-fluid model provides the velocity field, pressure distribution, and temperature distribution in the fluid. Figure 10-3 shows a postprocessing plot of the velocity field and the temperature. Without heating, you would expect an exit y-velocity that is slightly lower toward the left side, behind the heating tube (wake effect). In this case, however, you see that the y-velocity is higher on the left side. This is because of the buoyancy effect of the free convection.

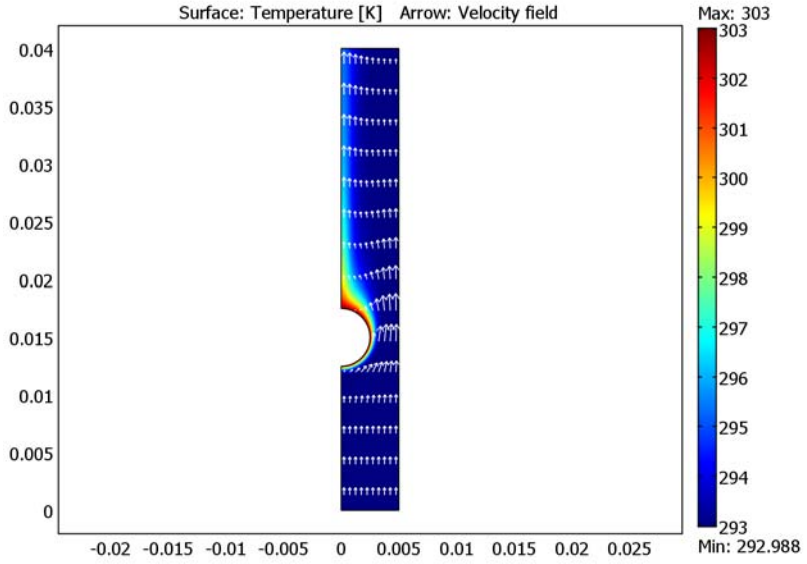


Figure 10-3: The velocity field and temperature distribution in the fluid.

Using integration to find the mean temperature at the outlet shows that the temperature increases roughly 0.75 K from the inlet to the outlet.

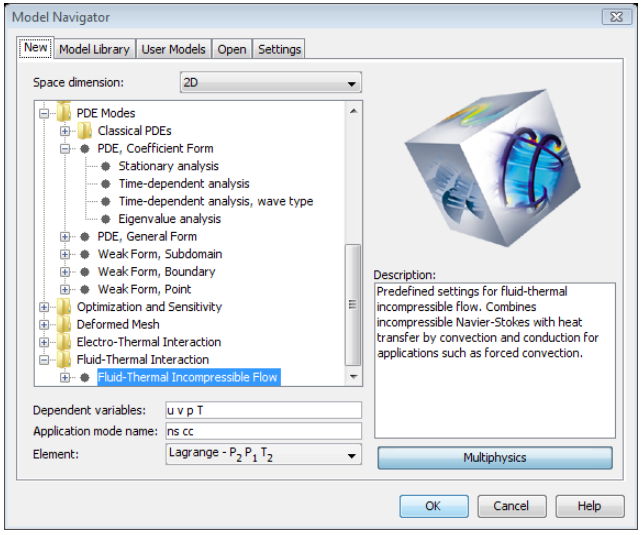
For further analysis, see “Time-Dependent Simulation” on page 372.

Model Library path: `COMSOL_Multiphysics/Multiphysics/free_convection`

MODEL NAVIGATOR

Use the following steps to create a new multiphysics model:

1. Click the **New** tab, and check that **2D** is selected in the **Space dimension** list. The space dimension must always be selected first, because the available application modes vary depending on the space dimension.
2. In the application modes list on the left, open the **COMSOL Multiphysics** folder, open the **Fluid-Thermal Interaction** folder, and then click **Fluid-Thermal Incompressible Flow**.
3. Click **OK** to close the **Model Navigator** and create a new model.



Selecting the Fluid-Thermal Incompressible Flow predefined multiphysics coupling in the Model Navigator.

OPTIONS AND SETTINGS

Later in this model you need the fluid properties of the water, the temperatures at the inlet and on the surface of the heating tubes, and the inlet velocity. It is convenient to enter this data as *constants* in the **Constants** dialog box. In this model, all values are given in SI units.

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

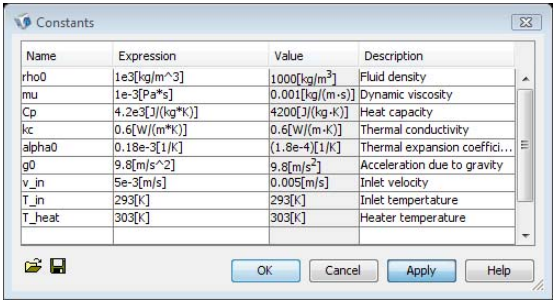
2 First add the density of the fluid:

Enter `rho0` in the **Name** field. Press the **Tab** key to move the cursor to the **Expression** field and enter `1e3[kg/m^3]`. The value is saved when you press **Enter**, click **Apply**, or otherwise leave the **Expression** field. In the **Description** column, type `Fluid density` (adding a description is optional).

3 Continue by adding the remaining properties.

NAME	EXPRESSION	DESCRIPTION
rho0	1e3[kg/m^3]	Fluid density
mu	1e-3[Pa*s]	Dynamic viscosity
Cp	4.2e3[J/(kg*K)]	Heat capacity
kc	0.6[W/(m*K)]	Thermal conductivity
alpha0	0.18e-3[1/K]	Thermal expansion coefficient
g0	9.8[m/s^2]	Acceleration due to gravity
v_in	5e-3[m/s]	Inlet velocity
T_in	293[K]	Inlet temperature
T_heat	303[K]	Heater temperature

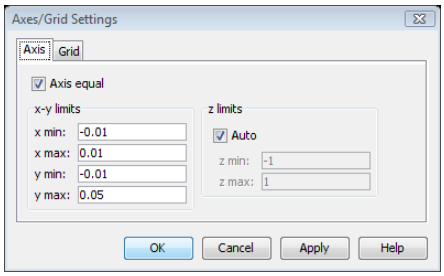
4 When you have entered all constants, click **OK**.



The model size is on the order of a few centimeters, while the area visible in the user interface is on the order of meters (remember that you are modeling in SI units). Before you start drawing the geometry, change the size of the visible drawing area and the grid spacing:

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

2 In the **Axes/Grid Settings** dialog box, type `-0.01`, `0.01`, `-0.01`, and `0.05` in the **x min**, **x max**, **y min**, and **y max** edit fields, respectively.



3 Click the **Grid** tab and then click to clear the **Auto** check box. Enter `0.005` in both the **x spacing** and **y spacing** edit fields.

4 Click **OK** to close the dialog box and apply the settings.

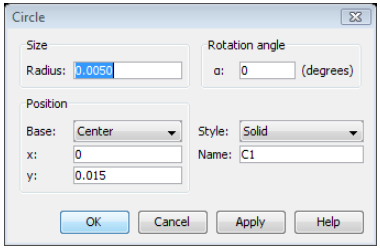
GEOMETRY MODELING

The next step is to create the model geometry. This is easy, involving only a rectangle and circle geometry object, subtracting one from the other.

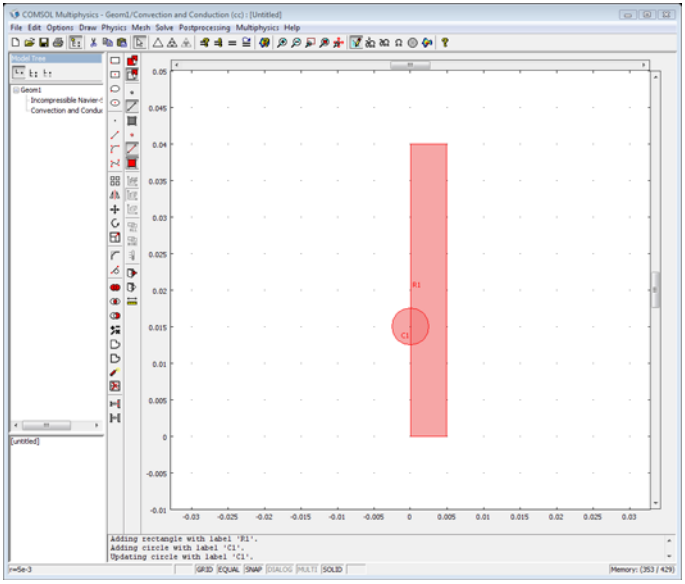
1 Draw a rectangle of width 0.005 and height 0.04, with the lower left corner at the origin. Click the **Rectangle/Square** toolbar button. It is the first button on the Draw toolbar, on the left side of the drawing area. Then click at (0,0) using the left mouse button, and drag the mouse to (0.005,0.04). Release the button.

2 Draw a circle with radius 0.005 centered at (0, 0.015). Click the fourth button on the Draw toolbar, **Ellipse/Circle (Centered)**. Then, using the *right* mouse button, click at (0, 0.015) and drag the mouse in any direction, keeping the button down, until the circle has a radius of 0.005. Using the right mouse button constrains the ellipse to a circle.

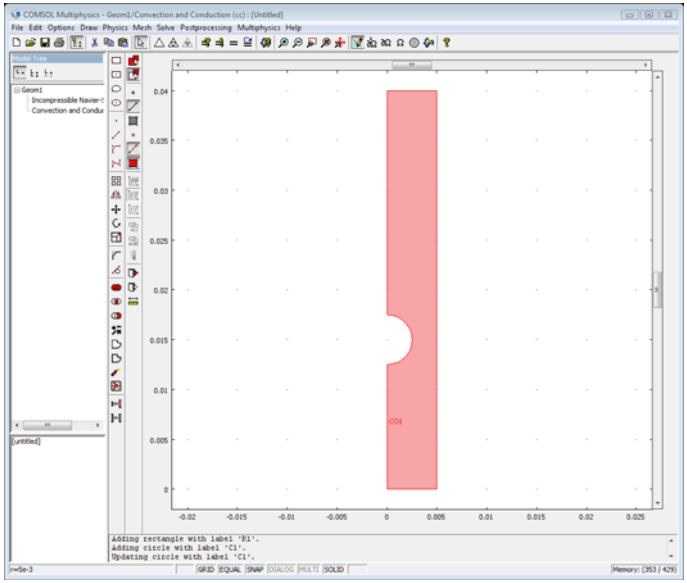
3 The desired radius of the circle is not 0.005, however, but is 0.0025. To fix this, double-click the circle object or select **Object Properties** from the **Draw** menu. In the **Circle** dialog box, enter `0.0025` as **Radius** and click **OK**.



4 Select both the circle and the rectangle. Either draw a rubber-band box around both them, or press the shortcut key Ctrl+A to select all objects.



5 Click the **Difference** button on the Draw toolbar and then the **Zoom Extents** button on the Main toolbar. The **Zoom Extents** button adjusts the axes settings so that the geometry fits nicely into the drawing area.



PHYSICS SETTINGS

Boundary Conditions

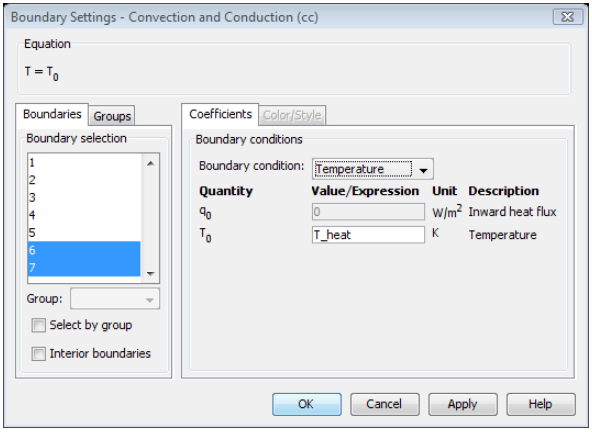
Specify the boundary conditions, first for the Convection and Conduction application mode and then for the Incompressible Navier-Stokes application mode.

1 From the **Physics** menu, choose **Boundary Settings**. This opens the **Boundary Setting** dialog box and transfers COMSOL Multiphysics to Boundary mode. The contents of this dialog box vary depending on the application mode.

2 Start by insulating all boundaries. This is the default boundary condition, so you do not need to change anything.

3 Select the inflow boundary by clicking at the corresponding edge in the geometry or by selecting Boundary 2 from the **Boundary selection** list. Select **Temperature** from the **Boundary conditions** list and type `T_in` in the **Temperature** edit field.

4 Select the heater that exists along Boundaries 6 and 7 from the **Boundary selection** list. Then select **Temperature** in the **Boundary conditions** list and type `T_heat` in the **Temperature** edit field.



Specifying a temperature of T_heat on Boundaries 6 and 7.

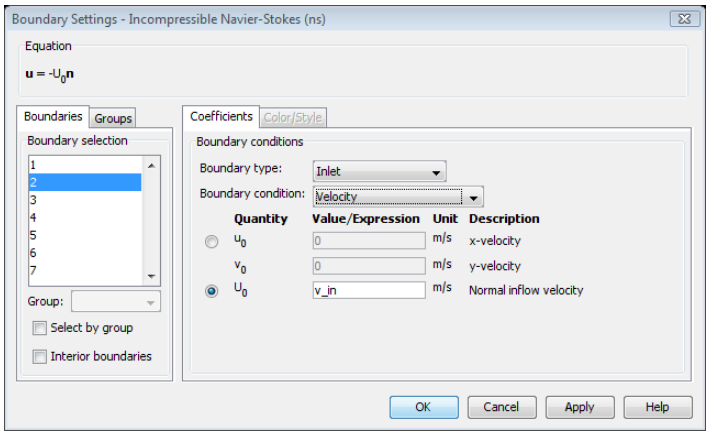
5 Click the outflow boundary (Boundary 4) and select **Convective flux** in the **Boundary conditions** list.

6 Click **Apply** to confirm the settings for the Convection and Conduction application mode.

7 Switch to the Incompressible Navier-Stokes application mode by selecting this mode from the **Multiphysics** menu. You can now open the corresponding **Boundary Settings** dialog box from the **Physics** menu (you can also use the Model Tree to access the settings for both applications modes).

8 Select any boundary in the **Boundary selection** list and then press Ctrl+A to select all boundaries in the list and then select the **Symmetry boundary** from the **Boundary type** list.

9 For the inflow boundary, select Boundary 2 and then choose **Inlet** from the **Boundary type** list and **Velocity** from the **Boundary condition** list. Type `v_in` in the **Normal inflow velocity** edit field.



Specifying the velocity in the normal direction.

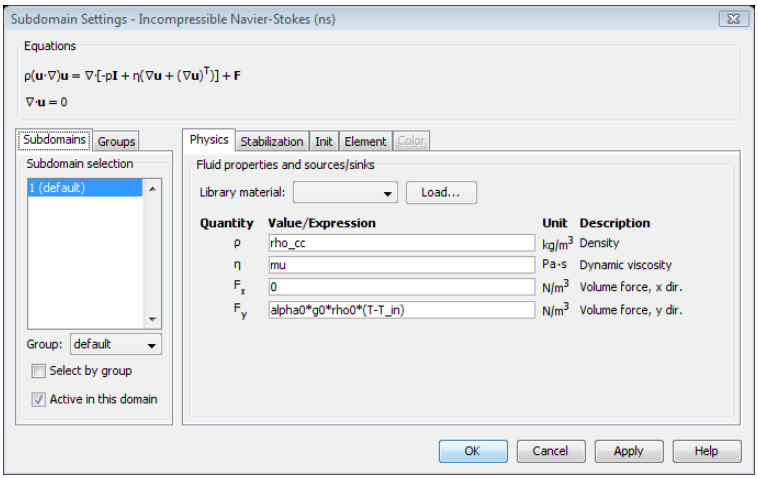
10 Continue by selecting the outflow boundary (Boundary 4). From the **Boundary type** list, select **Outlet**. The default condition **Pressure, no viscous stress** is correct.

11 Finally select Boundaries 6 and 7 and then select the type **Wall** and the condition **No slip**. Click **OK** to confirm your choices and close the dialog box.

Subdomain Settings

1 From the **Physics** menu, choose **Subdomain Settings** to open the **Subdomain Settings** dialog box and put the user interface in Subdomain mode.

2 Select the single subdomain, Subdomain 1, and use the already defined constants to set the density and the viscosity. Type `rho0` and `mu` in the **Density** and **Dynamic viscosity** edit fields, respectively.



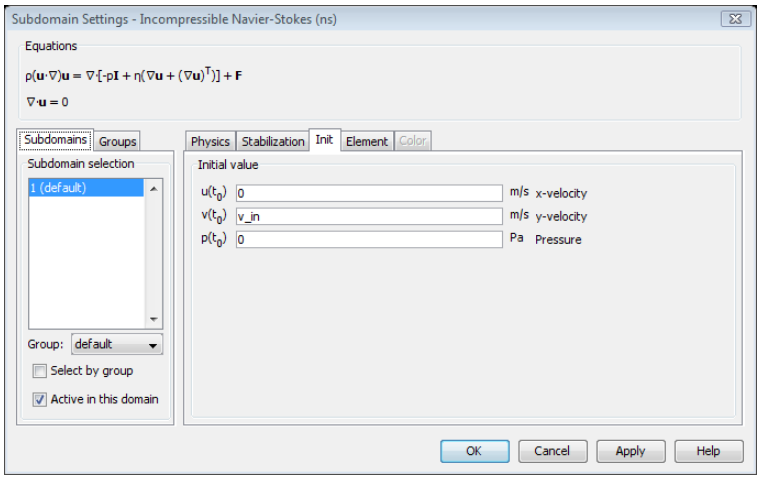
Providing fluid properties and a volume force in the Subdomain Settings dialog box.

3 To model the effect of temperature on the density of the fluid as a buoyancy force in the y direction, type `alpha0*g0*rho0*(T-T_in)` in the **Volume force, y dir.** edit field (F_y). Remember that T is the dependent variable from the Convection and Conduction application mode. Notice that an extended edit field displays the entire expression.

In the **Subdomain Settings** dialog box you can also set initial values. The Navier-Stokes equations are nonlinear and therefore require an educated guess as an initial solution to the nonlinear solver. A good initial value is necessary for the model to converge. The initial values also serve as initial conditions for the time-dependent solver. In this case, a constant velocity field v_{in} has sufficient quality.

1 Click the **Init** tab in the **Subdomain Settings** dialog box.

2 Set the initial value $\mathbf{v}(t_0)$ to `v_in`.



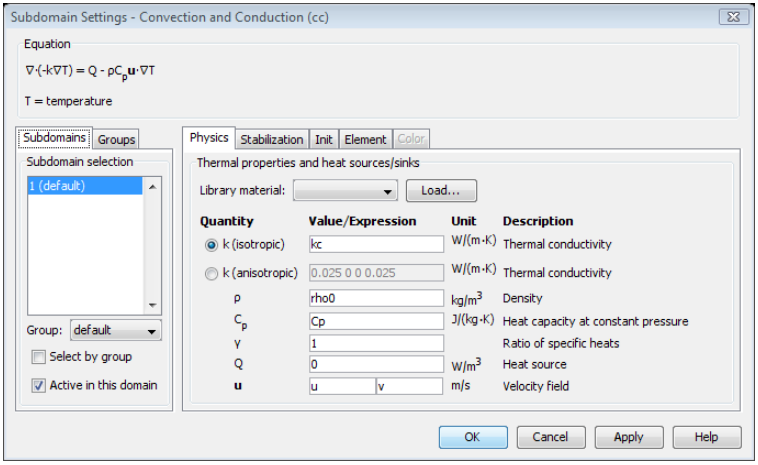
The initial values for the velocity components.

3 Click **OK**.

Continue with the subdomain settings for the Convection and Conduction application mode:

1 Use the **Multiphysics** menu to switch to the Convection and Conduction application mode.

2 From the **Physics** menu, choose **Subdomain Settings** to open the **Subdomain Settings** dialog box for the Convection and Conduction application mode.

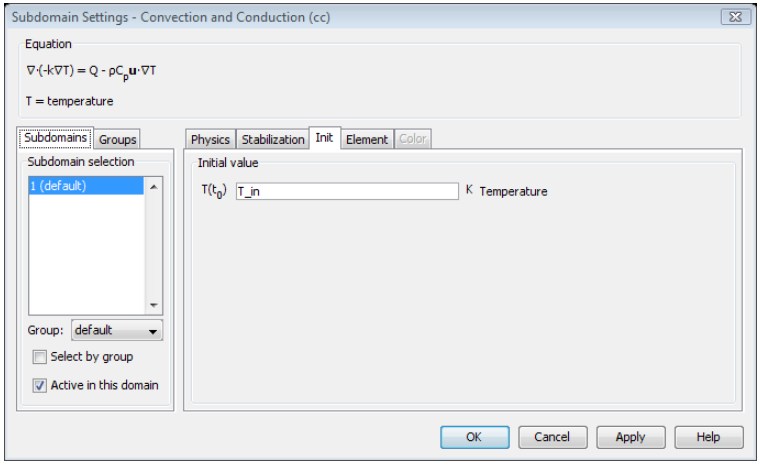


Specifying the thermal properties.

3 Type `kc`, `rho0`, and `Cp` in the **k (isotropic)**, ρ, and $\mathbf{C_p}$ edit fields, respectively.

Notice that `u` and `v` appear in the components of the **u** edit field for the velocity field. They are the dependent variables for the velocity components from the Incompressible Navier-Stokes application mode, which account for the convective transport of heat. This is the predefined multiphysics coupling that the Fluid-Thermal Incompressible Flow coupled multiphysics entry sets up automatically.

4 The temperature also needs an initial value. Use the inlet temperature as the starting temperature in the entire domain. Click the **Init** tab and enter `T_in` in the **$T(t_0)$** field. Then click **OK** to confirm all settings and close the dialog box.



The initial value for the temperature.

MESH GENERATION

In this model, use a predefined setting for a fine mesh:

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

2 In the **Free Mesh Parameters** dialog box, select **Finer** in the **Predefined mesh sizes** list.

3 Click **OK**.

4 Initialize the default mesh clicking the **Initialize Mesh** button on the Main toolbar.

5 Click the **Refine Mesh** button on the Main toolbar to refine the mesh once. This improves the accuracy of the solution.

COMPUTING THE SOLUTION

The required nonlinear solver is the default solver, so you start the solver directly.

From the **Solve** menu choose **Solve Problem**, or click the **Solve** button on the Main toolbar. Notice the solution progress window where you can monitor and stop the solution process. The solution converges quickly in this case.

As soon as the solution is ready, COMSOL Multiphysics displays a default plot. In this case, you get a surface plot of the velocity field.

POSTPROCESSING AND VISUALIZATION

In *postprocessing mode* you can select from many different plot types and set parameters for the different plots. Using the postprocessing utilities you can visualize the solution variables, their derivatives, and the space coordinates. Many frequently used expressions are predefined as *application mode variables*, directly available from lists in the **Plot Parameters** dialog box. Perform the following steps to create the plot in Figure 10-3:

1. Click the **Plot Parameters** button on the Main toolbar. This opens the **Plot Parameters** dialog box.
2. To obtain a surface plot with superimposed velocity vectors, select the **Surface** and **Arrow** check boxes in the **Plot type** area on the **General** page.
3. Click the **Surface** tab.
4. On the **Surface Data** page, select **Convection and Conduction (cc)>Temperature** from the **Predefined quantities** list.
5. Click the **Arrow** tab.
6. Select **Incompressible Navier-Stokes (ns)>Velocity field** from the **Predefined quantities** list on the **Subdomain Data** page.
7. In the **Arrow positioning** area, type 10 and 15 in the **x points** and **y points** edit fields, respectively.
8. Finally, in the **Arrow parameters** area, click the **Color** button to choose a suitable arrow color, for example, white. When you have selected a color, click **OK** to close the **Arrow Color** dialog box.
9. Click **OK**.

ADVANCED POSTPROCESSING

Integrating to Find the Mean Temperature

Because both the velocity and temperature vary along the outlet at the top, you must use additional postprocessing to get the mean temperature at the exit. The bulk temperature, or the "cup mixing temperature" is the temperature that the fluid has if it is collected in a cup at the outflow and is properly mixed. For this 2D example, assuming constant C_p and ρ, the cup mixing temperature is given by the following expression on Boundary 4 (the outlet):

$$\langle T \rangle = \frac{\int T(\mathbf{n} \cdot \mathbf{u}) ds}{\int (\mathbf{n} \cdot \mathbf{u}) ds}$$

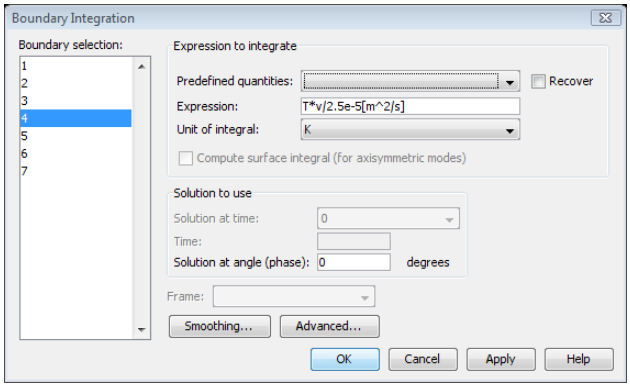
where **u** is the velocity vector and the **n** is the unit normal vector of the boundary.

1. To obtain the denominator, choose **Boundary Integration** from the **Postprocessing** menu.
2. Select Boundary 4.
3. In the **Expression** edit field, type `nx*u+ny*v`—or just `v`, because the outward normal vector on Boundary 4 is $\mathbf{e}_y$. Click **Apply**.

   The message log at the bottom of the main user interface shows the value of the denominator (the decimal sequence might differ slightly between platforms):

   ```
   Value of integral: 2.501098e-5 [m^2/s], Expression: v, Boundary: 4.
   ```

4. In the **Boundary Integration** dialog box, type `T*v/2.5e-5[m^2/s]` in the **Expression** edit field. This computes the resulting mean temperature.



5. Click **OK**. The result is displayed in the message log.

You should get a mean temperature of roughly 293.8 K, that is, a temperature rise of approximately 0.8 K between inlet and outlet.

Time-Dependent Simulation

This example is an extension of the stationary free convection model from the previous section. In the first step of modeling the heat transfer by forced and free convection, we found a steady-state solution. See “Modeling Using the Graphical User Interface” on page 360 on how to create and save the first part of the model.

The following section assumes that you start from the final state of the steady-state model.

LOADING A PREVIOUSLY SAVED MODEL

If you have previously saved the results from the first part of the model as a Model MPH-file, now load it into COMSOL Multiphysics (if you are continuing from the previous steady-state model, skip the following three steps):

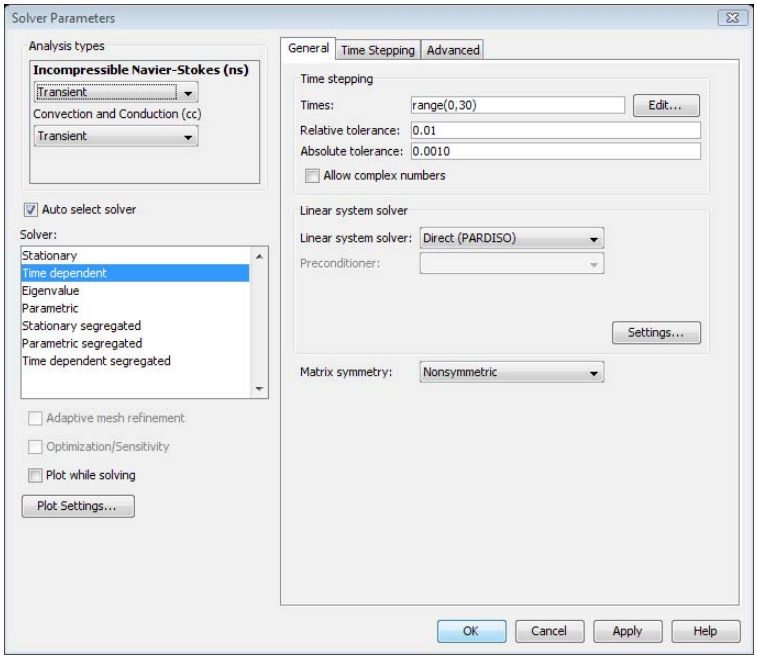
1. From the **File** menu, choose **Open**. You can also click the **Open** button on the main toolbar to load a Model MPH-file.
2. Browse to locate the Model MPH-file and select it.
3. Click **Open**.

COMPUTING THE SOLUTION

1. From the Solve menu, choose **Solver Parameters**.

   Before solving the model with the time-dependent solver, you must set the analysis type to transient for both application modes.
2. In the **Analysis types** area, select **Transient** from the lists of analysis types for both the **Convection and Conduction (cc)** application mode and the **Incompressible Navier-Stokes (ns)** application mode.
3. Click the **General** tab in the **Solver Parameters** dialog box.
4. The **General** page for the time-stepping algorithms is now active. The output times can be a vector, specifying for which times the solution should be saved for

postprocessing. Type `range(0,30)` in the **Times** edit field to specify that the solution will be sampled every second during 30 seconds.



Setting the parameters for the time-dependent analysis.

5 Click the **Time Stepping** tab.

6 Select **Free** from the **Time steps taken by solver** list. For this model, the time steps that the solver computes are more efficient than the default time steps used for the Incompressible Navier-Stokes application mode.

7 Click **OK** to confirm the choices.

8 Click the **Solve** button on the Main toolbar to start the time-dependent analysis.

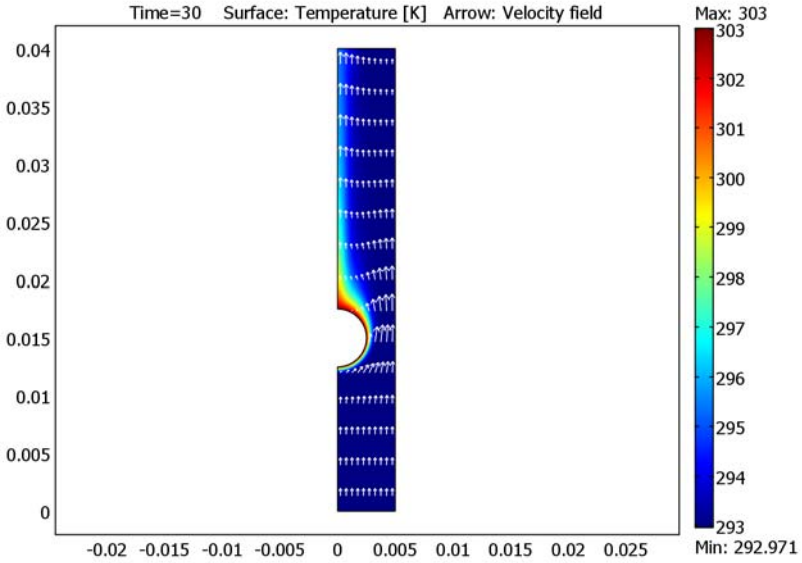
POSTPROCESSING AND VISUALIZATION

The plot shows the solution for the last time step using the same plot settings as before. Select which time step to display in the **Plot Parameters** dialog box:

1 Click the **Plot Parameters** button to open the **Plot Parameters** dialog box.

2 Click the **General** tab and select the time step that you want to see from the **Solution at time** list.

3 Click **Apply** to plot the solution at that time.



Magnetic Drug Targeting in Cancer Therapy

Introduction

Current research on methods to target chemotherapy drugs in the human body includes the investigation of bio-compatible magnetic nanocarrier systems. For example, magnetic liquids such as ferrofluids can play an important role as drug carriers in the human body (Ref. 1). As such, they can be used for drug targeting in modern locoregional cancer treatment. A remaining challenge for this medical application is the choice of clinical setting. Important parameters are optimal adjustment of the external magnetic field and the choice of ferrofluid properties.

Avoiding damage to healthy human cells from chemotherapy drugs imposes an upper limit in the treatment dose. This limit impedes the chances of successful treatment of the tumor cells. One objective of modern cancer research is therefore to concentrate chemotherapy drugs locally on tumor tissue and to weaken the global exposure to the organism.

This model of the ferrohydrodynamics of blood demonstrates a simple setup for investigating an external magnetic field and its interaction with blood flow containing a magnetic carrier substance. The model treats the liquid as a continuum, which is a good first step. You can extend this model by particle tracing, making it a multiscale model. The equations and theory are based on Maxwell's equations and the Navier-Stokes equations. You first solve Maxwell's equations in the full modeling domain formed by permanent-magnet, blood-vessel, tissue, and air domains. A magnetic volume force then couples the resulting magnetic field to a fluid-flow problem in the blood-vessel domain described by the Navier-Stokes equations.

Model Definition[1]

The model geometry represents a blood vessel, a permanent magnet, surrounding tissue, and air in 2D. Blood feeds into the vessel from the left in Figure 10-4. The velocity and pressure fields are calculated in the blood stream. COMSOL Multiphysics computes the magnetic field (magnetic vector potential) generated by the permanent

1. This model was provided by Dr. Daniel J. Strauss, The Institute for New Materials, Inc., www.inm-gmbh.de.

magnet. This magnetic field generates a magnetic volume force that affects the flow field in the blood vessel.

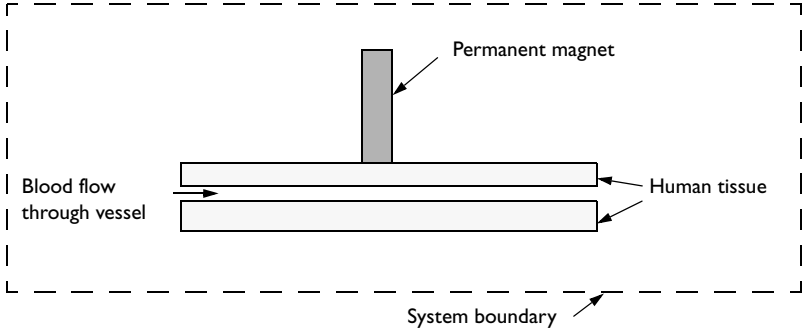


Figure 10-4: Geometric representation of the model.

MAGNETOSTATIC EQUATIONS

Because the magnetic part of this problem is static, Maxwell-Ampere's law for the magnetic field $\mathbf{H}$ (A/m) and the current density $\mathbf{J}$ (A/m^2) applies:

$$\nabla \times \mathbf{H} = \mathbf{J} \tag{10-1}$$

Furthermore, Gauss' law for the magnetic flux density $\mathbf{B}$ (Vs/m^2) states that

$$\nabla \cdot \mathbf{B} = 0\,. \tag{10-2}$$

The constitutive equations describing the relation between $\mathbf{B}$ and $\mathbf{H}$ in the different parts of the modeling domain read:

$$\mathbf{B} = \begin{cases} \mu_0\mu_{\mathrm{r,\,mag}}\mathbf{H} + \mathbf{B}_{\mathrm{rem}} & \text{permanent magnet} \\ \mu_0(\mathbf{H} + \mathbf{M}_{\mathrm{ff}}(\mathbf{H})) & \text{blood stream} \\ \mu_0\mathbf{H} & \text{tissue and air} \end{cases} \tag{10-3}$$

Here μ_0 is the magnetic permeability of vacuum (Vs/(A·m)); μ_r is the relative magnetic permeability of the permanent magnet (dimensionless); $\mathbf{B}_{\mathrm{rem}}$ is the remanent magnetic flux (A/m); and $\mathbf{M}_{\mathrm{ff}}$ is the magnetization vector in the blood stream (A/m), which is a function of the magnetic field, $\mathbf{H}$.

Defining a magnetic vector potential $\mathbf{A}$ such that

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \nabla \cdot \mathbf{A} = 0\,, \tag{10-4}$$

you finally, by substitution in Equation 10-1 through Equation 10-3, arrive at the following vector equation to solve:

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{J}$$

Simplifying to a 2D problem with no perpendicular currents, this equation reduces to

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{0} . \tag{10-5}$$

Note that this equation assumes that the magnetic vector potential has a nonzero component only perpendicularly to the plane, $\mathbf{A} = (0, 0, A_z)$.

An arc tangent expression with two material parameters α (A/m) and β (m/A) characterizes the induced magnetization $\mathbf{M}_{\mathrm{ff}}(x, y) = (M_{\mathrm{ff}x}, M_{\mathrm{ff}y})$ of a ferrofluid (Ref. 2):

$$M_x = \alpha \operatorname{atan}\left(\frac{\beta}{\mu_0} \frac{\partial A_z}{\partial y} \right)$$

$$M_y = \alpha \operatorname{atan}\left(\frac{\beta}{\mu_0} \frac{\partial A_z}{\partial x} \right)$$

For the magnetic fields of interest, it is possible to linearize these expressions to obtain

$$\begin{aligned} M_x &= \frac{\chi}{\mu_0} \frac{\partial A_z}{\partial y} \\ M_y &= -\frac{\chi}{\mu_0} \frac{\partial A_z}{\partial x} \end{aligned} \tag{10-6}$$

where $\chi = \alpha\beta$ is the magnetic susceptibility.

Boundary Conditions

Along a system boundary reasonably far away from the magnet (see Figure 10-4) you can apply a magnetic insulation boundary condition, $A_z = 0$.

FLUID FLOW EQUATIONS

The Navier-Stokes equations describe the time-dependent mass and momentum balances for an incompressible flow:

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{F}$$
$$\nabla \cdot \mathbf{u} = 0 \tag{10-7}$$

where η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ the velocity (m/s), ρ the fluid density (kg/m^3), p the pressure (N/m^2), and $\mathbf{F}$ a volume force (N/m^3).

With the assumption that the magnetic nanoparticles in the fluid do not interact, the magnetic force $\mathbf{F} = (F_x, F_y)$ on the ferrofluid for relatively weak fields is given by $\mathbf{F} = |\mathbf{M}|\nabla|\mathbf{H}|$. Using Equation 10-3, Equation 10-4, and Equation 10-6 then leads to the expressions

$$F_x = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial x \partial y}\right)$$
$$F_y = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x \partial y} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial y^2}\right)$$

To get the final expression for the volume force in the blood stream, multiply these expressions by the ferrofluid mass fraction, k_{ff}.

Boundary Conditions

On the vessel walls, apply no-slip conditions, $u = v = 0$. At the outlet, you can set an outlet pressure condition, $p = 0$. At the inlet boundary, specify a parabolic flow profile on the normal inflow velocity according to $4U_{\text{m}}s(1–s)$, where s is a boundary segment length parameter that goes from 0 to 1 along the inlet boundary segment and U_{m} is the maximal flow velocity. To emulate the heart beat, the inflow velocity follows a sinusoidal expression in time:

$$U_0 = 2U_{\text{m}}s(1-s)(\sin(\omega t) + \sqrt{\sin(\omega t)^2})$$

Selecting the angular velocity ω to be 2π rad/s gives a heart beat rate of 60 beats per minute. Figure 10-5 displays the resulting expression (normalized to unity).

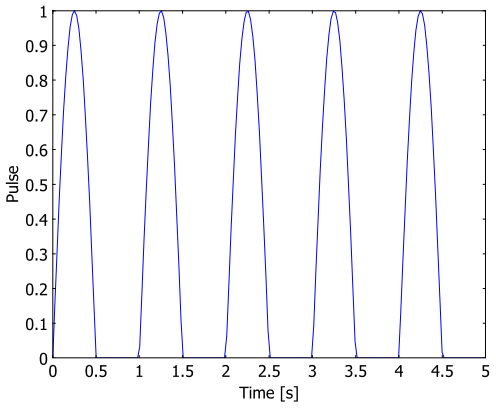


Figure 10-5: Simulated heart beat.

Model Data

Table 10-1 lists the relevant material properties for the model.

TABLE 10-1: MODEL DATA

QUANTITY	DESCRIPTION	VALUE
$\mu_{r,mag}$	Relative permeability, magnet	$5 \cdot 10^3$
B_{rem}	Remanent flux density, magnet	0.5 T
α	Ferrofluid magnetization-curve parameter	10^{-4} A/m
β	Ferrofluid magnetization-curve parameter	$3 \cdot 10^{-5}$ $(A/m)^{-1}$
ρ	Density, blood	1000 kg/m^3
η	Dynamic viscosity, blood	$5 \cdot 10^{-3}$ kg/(m·s)

Results

Figure 10-3 shows a detail from the plot of the magnetic field strength. The highest B-field strength clearly occurs inside the magnet. To see the low-level variations in the surrounding tissue and vessels, the plot does not show magnetic flux densities above 0.17 T. The geometric form of the magnet generates strong fields just outside of the rounded corners. Sharper corners generate even stronger local fields.

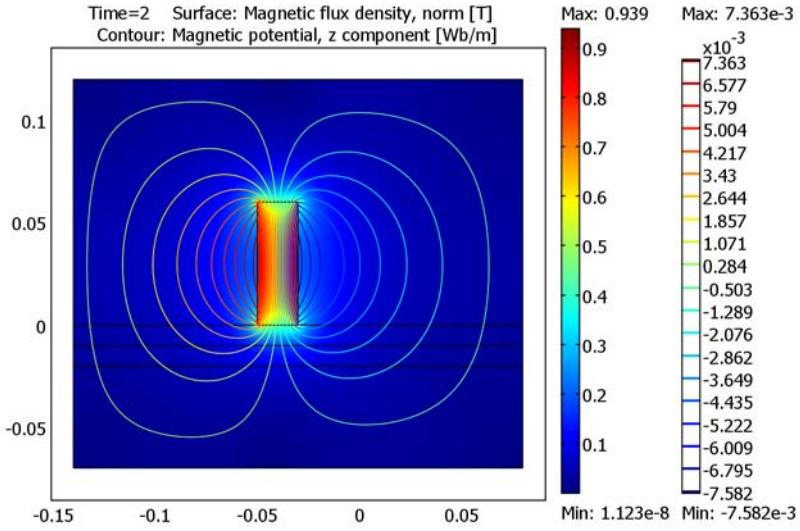


Figure 10-6: Magnetic vector potential and magnetic flux density, B field (white areas surpass the plot color range).

Figure 10-7 shows the velocity field at a heart beat where there is a maximum mean throughput in the vessel. At the left end there is a parabolic laminar flow profile.

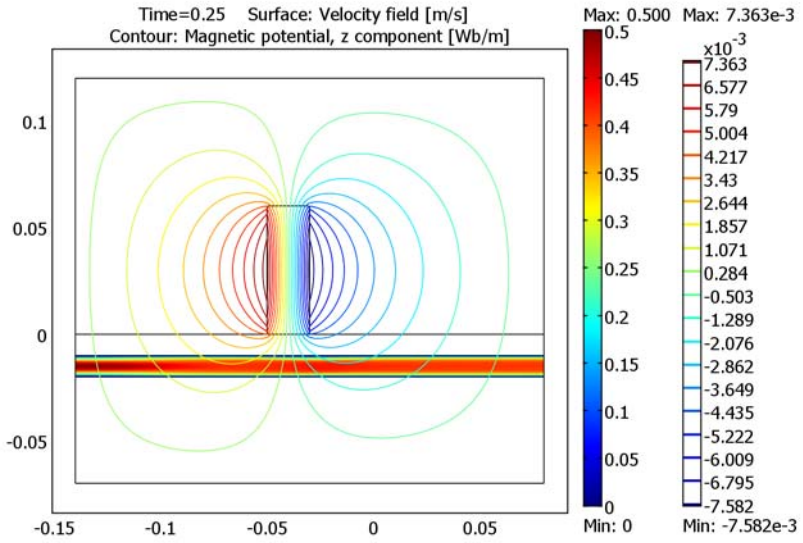


Figure 10-7: Velocity field at maximum blood throughput (t = 0.25).

Figure 10-8 reveals the velocity field between two heart beats, where the net throughput is zero.

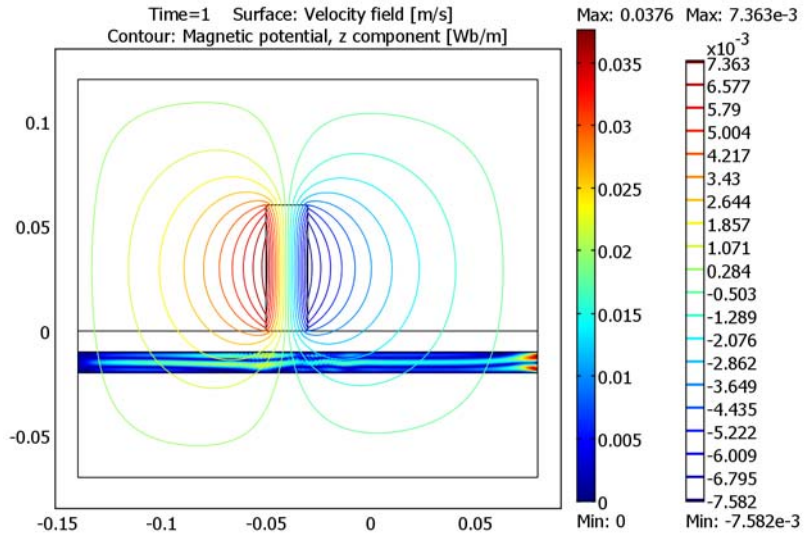


Figure 10-8: Velocity field at zero blood throughput (t = 1).

Modeling in COMSOL Multiphysics

EQUATIONS

To model Equation 10-5, use the Magnetostatics application mode in 2D. In the **Subdomain Settings** dialog box, choose the constitutive relation

$$\mathbf{B} = \mu_0\mu_r\mathbf{H} + \mathbf{B}_r$$

and make use of the fact that the remanent flux density $\mathbf{B}_r = \mu_0\chi\mathbf{M}$, where χ is the magnetic susceptibility.

STAGED SOLUTION

Because the magnetostatic problem is a stationary nonlinear problem that is independent of the fluid-flow problem, you need to solve that only once. You can therefore start by solving only Equation 10-5 with the stationary solver. Then proceed with solving only the fluid-flow problem, Equation 10-7, with the static magnetic

potential as input. Solve the fluid-flow problem using the time-dependent solver. This strategy reduces RAM memory allocation and speeds up the solution.

SOLVER SETTINGS

The convergence tolerance for the time-stepping algorithm should only be based on the truly time-dependent equations. The continuity equation (second line in Equation 10-7) is stationary and describes the pressure distribution. Therefore, you can exclude p from the time-stepping tolerance checks. To do so, select **Exclude algebraic** in the **Error estimation strategy** list on the **Time Stepping** page of the **Solver Parameters** dialog box.

FINITE ELEMENT SHAPE FUNCTIONS

This problem includes second-order space derivatives of A in some coefficients. To get acceptable accuracy, use third-order Lagrange elements in the Magnetostatics application mode. The default setting in this application mode is second-order elements.

References

1. P.A. Voltairas, D.I. Fotiadis, and L.K. Michalis, "Hydrodynamics of Magnetic Drug Targeting," *J. Biomech.*, vol. 35, pp. 813–821, 2002.

2. C.M. Oldenburg, S.E. Borglin, and G.J. Moridis, "Numerical Simulation of Ferrofluid Flow for Subsurface Environmental Engineering Applications," *Transport in Porous Media*, vol. 38, pp. 319–344, 2000.

3. R.E. Rosensweig, *Ferrohydrodynamics*, Dover Publications, New York, 1997.

Model Library path: `COMSOL_Multiphysics/Multiphysics/magnetic_drug_targeting`

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 Select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis**.

4 Click first the **Multiphysics** button and then the **Add** button.

5 From the list of application modes, select **COMSOL Multiphysics>Electromagnetics>Magnetostatics**. Click **Add**.

6 Click **OK**.

GEOMETRY MODELING

1 Click the **Rectangle/Square** button at the top of the Draw toolbar. Draw an arbitrary rectangle by clicking in the drawing area and dragging the mouse.

2 Double-click the rectangle.

3 Make the following changes in the dialog box; when done, click **OK**.

PROPERTY	VALUE
Width	0.02
Height	0.06
x	-0.05
y	0

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

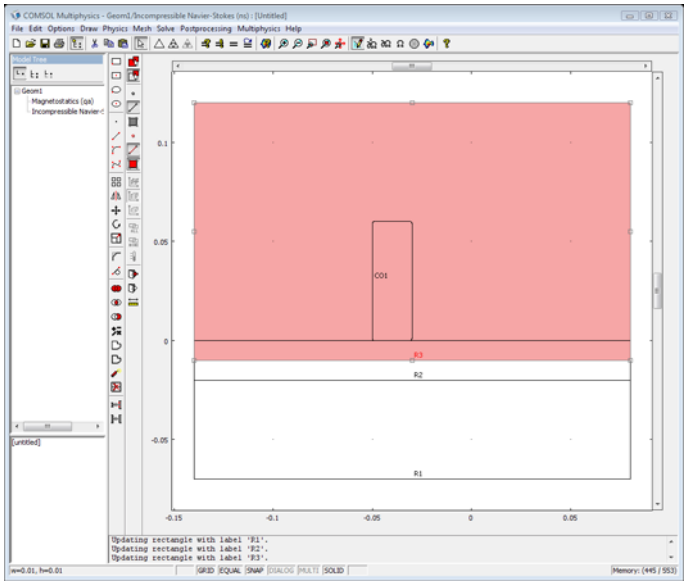
5 From the **Draw** menu, choose **Fillet/Chamfer**. Click on the rectangle R1 and select all four vertices by Ctrl-clicking them.

6 Type `1e-3` in the **Radius** edit field, then click **OK**.

7 Draw three additional arbitrary rectangles using the **Rectangle/Square** button and set the object properties like the first one according to the following table:

RECTANGLE	WIDTH	HEIGHT	BASE X	BASE Y
R1	0.22	0.05	-0.14	-0.07
R2	0.22	0.02	-0.14	-0.02
R3	0.22	0.13	-0.14	-0.01

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



OPTIONS AND SETTINGS

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

2 Enter constants with names, expressions (values and units), and descriptions (the descriptions are optional) according to the following table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
mur_mag	1	Relative permeability, magnet
B_rem	1[T]	Remanent flux density, magnet
alpha	1e4[A/m]	Ferrofluid magnetization-curve parameter
beta	3e-5[m/A]	Ferrofluid magnetization-curve parameter
chi_ff	alpha*beta	Magnetic susceptibility, ferrofluid
k_ff	0.1	Ferrofluid mass fraction in blood stream
rho	1000[kg/m^3]	Density, blood
eta	0.005[Pa*s]	Dynamic viscosity, blood
U_m	50[cm/s]	Maximum flow velocity
f	60[1/min]	Heart-beat rate
omega	2*pi[rad]*f	Pulse angular velocity

Scalar Expressions

1 On the **Options** menu, point to **Expressions** and then click **Scalar Expressions**.

2 Define the following expressions (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
mu0	mu0_qa	Permeability of vacuum
M_ffx	k_ff*(chi_ff/mu0)*Azy	Induced ferrofluid magnetization, x-component
M_ffy	-k_ff*(chi_ff/mu0)*Azx	Induced ferrofluid magnetization, y-component
F_ffx	k_ff*(Azx*Azxx+Azy*Azxy)* chi_ff/(mu0*(1+chi_ff)^2)	Ferrofluid volume force, x-component
F_ffy	k_ff*(Azx*Azxy+Azy*Azyy)* chi_ff/(mu0*(1+chi_ff)^2)	Ferrofluid volume force, y-component

3 Click **OK**.

PHYSICS SETTINGS

Application Mode Properties

Change the default element type to be a cubic Lagrange element:

1 From the **Multiphysics** menu, choose **Magnetostatics (qa)**.

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

3 In the **Application Mode Properties** dialog box, select **Lagrange - Cubic** in the **Default element type** list. Click **OK**.

Subdomain Settings—Magnetostatics

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

2 On the **Physics** page, select Subdomain 2.

3 Set the **Constitutive relation** to $\mathbf{B} = \mu_0\mathbf{H} + \mu_0\mathbf{M}$.

4 In the left and right **M** edit fields, enter `M_ffx` and `M_ffy`, respectively.

5 Select Subdomain 5, then set the **Constitutive relation** to $\mathbf{B} = \mu_0\mu_r\mathbf{H} + \mathbf{B}_r$.

6 In the μ_r edit field, enter `mur_mag`. In the right $\mathbf{B}_r$ edit field for the *y*-component of the remanent flux density, enter `B_rem`. Leave the corresponding *x*-component at zero.

7 Click **OK**.

Boundary Conditions—Magnetostatics

The default setting is magnetic insulation, so you do not have to make any changes. To be reassured, choose **Physics>Boundary Settings** and inspect the boundaries.

Subdomain Settings—Navier-Stokes

1 From the **Multiphysics** menu, choose **Incompressible Navier-Stokes (ns)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 Press Ctrl+A to select all five subdomains.

4 Clear the **Active in this domain** check box.

5 Select Subdomain 2 from the list and select the **Active in this domain** check box.

6 Specify the fluid properties according to the following table:

QUANTITY	VALUE/EXPRESSION
ρ	`rho`
η	`eta`
F_x	`F_ffx`
F_y	`F_ffy`

7 Click the **Artificial Diffusion** button to add streamline diffusion to the model. This is necessary because of the high Reynolds number flow.

8 In the **Artificial Diffusion** dialog box, make sure the **Streamline diffusion** check box is selected.

9 On the **Init** page, leave all initial conditions at zero.

10 Click **OK**.

Boundary Conditions—Navier-Stokes

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

2 Specify boundary conditions according to the following table:

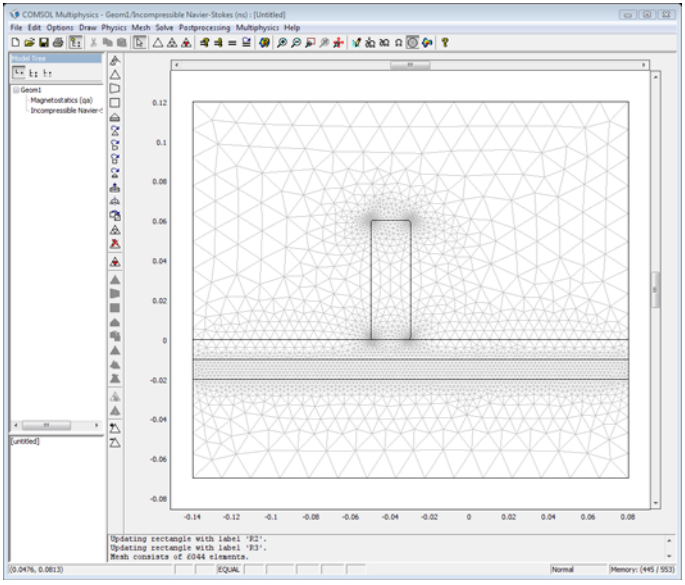
SETTINGS	BOUNDARY 3	BOUNDARIES 4, 6	BOUNDARY 16
Boundary type	Inlet	Wall	Outlet
Boundary condition	Velocity	No slip	Pressure, no viscous stress
U_0	`2*s*(1-s)*U_m*(sin(omega*t)+ sqrt(sin(omega*t)^2))`		
P_0			0

3 Click **OK**.

MESH GENERATION

1 Choose **Mesh>Free Mesh Parameters**, and in the dialog box that opens, click the **Subdomain** tab.

2 Select Subdomain 2 from the list and enter `0.002` in the **Maximum element size** edit field. Click **Remesh** and **OK**.



COMPUTING THE SOLUTION

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

2 On the **Solve For** page, select only **Magnetostatics (qa)**. Click **OK**.

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

4 On the **General** page, select **Stationary** from the **Analysis** list. Click **OK**.

5 Click the **Solve** button on the Main toolbar to compute the solution for A_z.

6 When the solver has finished, click the **Solver Manager** button.

7 On the **Initial Value** page, go to the **Values of variables not solved for and linearization point** area and click the **Current solution** option button.

8 On the **Solve For** page, select only **Incompressible Navier-Stokes (ns)**. Click **OK**.

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

10 On the **General** page, select **Transient** from the **Analysis** list and type `range(0,0.05,2)` in the **Times** edit field.

11 On the **Time Stepping** page, select **Exclude algebraic** from the **Error estimation strategy** list (see "Solver Settings" on page 384 for an explanation). Click **OK**.

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

The solution takes a few minutes to compute.

POSTPROCESSING AND VISUALIZATION

To generate Figure 10-6 on page 381, follow these instructions.

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

2 On the **General** page, select the **Surface** and **Contour** check boxes in the **Plot type** area.

3 Click the **Surface** tab. On the **Surface Data** page, select **Magnetostatics (qa)>Magnetic flux density, norm** from the **Predefined quantities** list.

4 On the **Contour** page, select **Magnetostatics (qa)>Magnetic potential, z component**.

5 Click **OK**.

To generate Figure 10-7 on page 382 and Figure 10-8 on page 383, proceed in the following way:

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

2 On the **General** page, select **0.25** from the **Solution at time** list.

3 Click the **Surface** tab. On the **Surface Data** page, select **Incompressible Navier-Stokes (ns)>Velocity field** from the **Predefined quantities** list.

4 Click **Apply** to generate the plot in Figure 10-7.

5 On the **General** page, change the entry in the **Solution at time** list to **1**.

6 Click **OK** to generate the plot in Figure 10-8.

To generate a movie, do as follows:

1 Open the **Plot Parameters** dialog box again and go to the **Animate** tab.

2 Click **OK** and wait for the movie to be generated (this step can take some time).

When the movie is finished, you can save it as an AVI or QuickTime file using the **Save** button in the movie window.

Marangoni Convection

Introduction

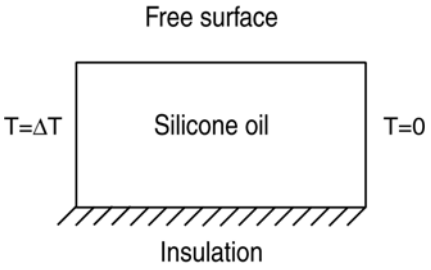
Marangoni convection occurs when the surface tension of an interface (generally liquid-air) depends on the concentration of a species or on the temperature distribution. In the case of temperature dependence, the Marangoni effect is also called thermo-capillary convection. It is of primary importance in the fields of:

- Welding
- Crystal growth
- Electron beam melting of metals

Direct experimental studies are not easy to carry out in these systems because the materials are often metals and temperatures are very high. One possibility is to replace the real system with an experimental setup using a transparent liquid at ambient temperatures.

Model Definition

This model describes the 2D stationary behavior of a vessel filled with silicone oil, for which the thermo-physical properties are known. The aim of the study is to compute the temperature field that induces a flow through the Marangoni effect. The model shows this effect using the simple geometry in the figure below.



GOVERNING EQUATIONS

A stationary momentum balance describes the velocity field and the pressure distribution (Navier-Stokes equations):

$$-\eta\nabla^2\mathbf{u} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{F}$$
$$\nabla\cdot\mathbf{u} = 0$$

The first term gives the rate of momentum gain by viscous transfer, the second by convection, and the third by pressure forces. The equation contains the following variables and properties:

- η is the dynamic viscosity (kg/(m·s)).
- $\mathbf{u}$ is the velocity vector (m/s).
- ρ is the density (kg/m^3).
- p is the pressure (Pa).

The $\mathbf{F}$ term is a source term representing external forces per unit volume.

To include the heating of the fluid, couple the fluid flow to an energy balance according to

$$\nabla\cdot(-k\nabla T + \rho C_p T\mathbf{u}) = Q$$

The expression within the brackets is the heat flux vector, containing a conductive and a convective part. The equation contains the following variables and properties:

- k is the thermal conductivity (W/(m·K)).
- T is the temperature (K).
- C_p is the heat capacity (J/(kg·K)).
- Q (W/m^3) represents a source term.

You can use the Boussinesq approximation to include the effect of temperature on the velocity field. In this approximation, variations in temperature produce a buoyancy force (or Archimedes' force) that lifts the fluid. Enter this force into the $\mathbf{F}$ term in the Navier-Stokes equation as:

$$\mathbf{F} = \begin{pmatrix} Fx \\ Fy \end{pmatrix} = \begin{pmatrix} 0 \\ \alpha g \rho\left(T - \frac{\Delta T}{2}\right) \end{pmatrix}$$

where α is the thermal expansion coefficient (1/K), g is the acceleration due to gravity (m/s^2), and ΔT is the temperature difference (K) between the right and left wall in the model geometry.

Equation 10-8 describes the forces that the Marangoni effect induces on the interface (liquid/air):

$$\eta\frac{\partial u}{\partial y} = \gamma\frac{\partial T}{\partial x} \tag{10-8}$$

where γ is the temperature derivative of the surface tension (N/(m·K)). This equation states that the shear stress on a surface is proportional to the temperature gradient (Ref. 1).

Modeling in COMSOL Multiphysics

To solve the momentum balance equations, use the Incompressible Navier-Stokes application mode. For the heat transfer by convection and conduction, use the Convection and Conduction application mode. There are two multiphysics couplings, one in each direction:

- The Boussinesq approximation means that an expression including temperature acts as a force in the y direction in the momentum balance.
- The convective heat transfer depends on the velocities from the momentum balance.

This means that you must solve the coupled system directly using the nonlinear solver.

To implement the condition that the shear stress is proportional to the temperature gradient on the surface, use a Weak Form, Boundary application mode where you can implement Equation using a weak formulation:

```
lm_test*(eta1*uy-gamma*Tx)+u_test*lm
```

The last term makes sure that this condition replaces the condition on the x-velocity from the Slip/Symmetry boundary condition in the Incompressible Navier-Stokes application mode.

It is also necessary to omit the Dirichlet boundary condition for T at the surface level to get consistent boundary conditions. To do this, adjust the boundary conditions on the equation system level.

Finally, to study the Marangoni effect, increase the temperature difference between the right and left wall in steps. With the restart option, the solver uses the previous solution as initial value providing fast convergence.

Results

The Marangoni effect becomes more pronounced as the temperature difference increases:

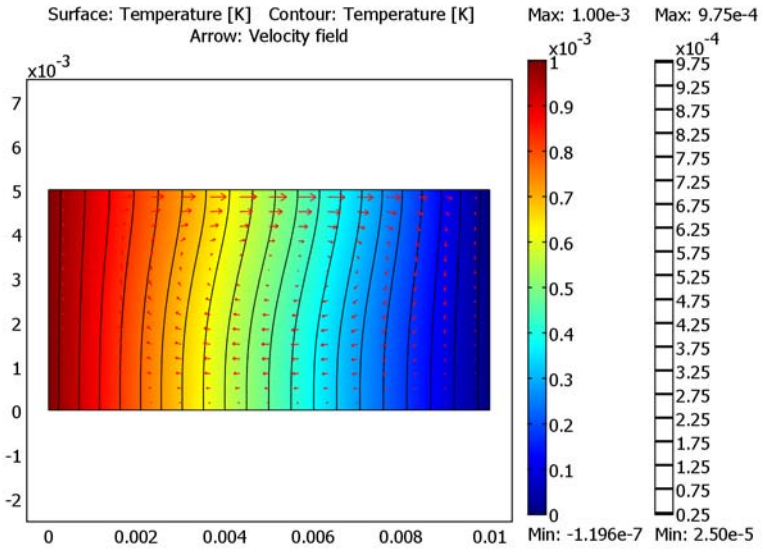


Figure 10-9: Marangoni convection with a temperature difference of 0.001 K.

For the very low temperature difference of 0.001 K, the temperature field is almost decoupled from the velocity field. Therefore, the temperature decreases almost linearly from left to right.

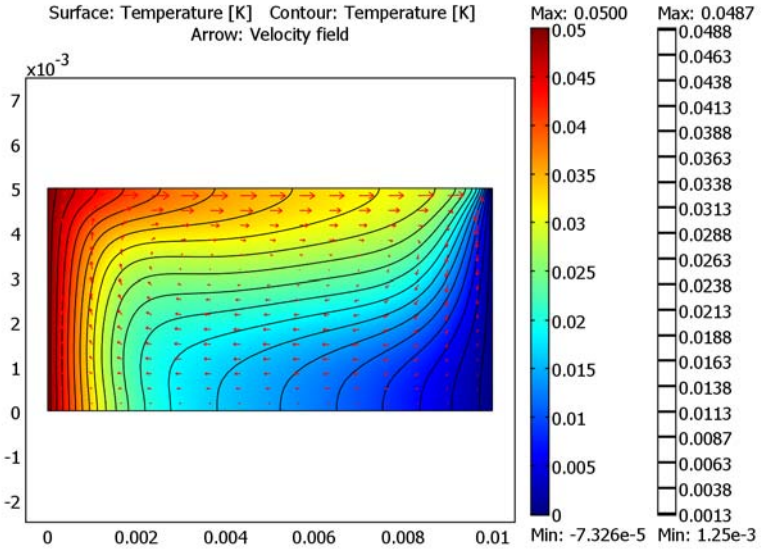


Figure 10-10: Marangoni convection with a temperature difference of 0.05 K.

For the temperature difference of 0.05 K notice how the Marangoni convection influences the flow of fluid and the distribution of temperature. The temperature is no longer decreasing linearly and you can clearly see the advection of the isotherms caused by the flow.

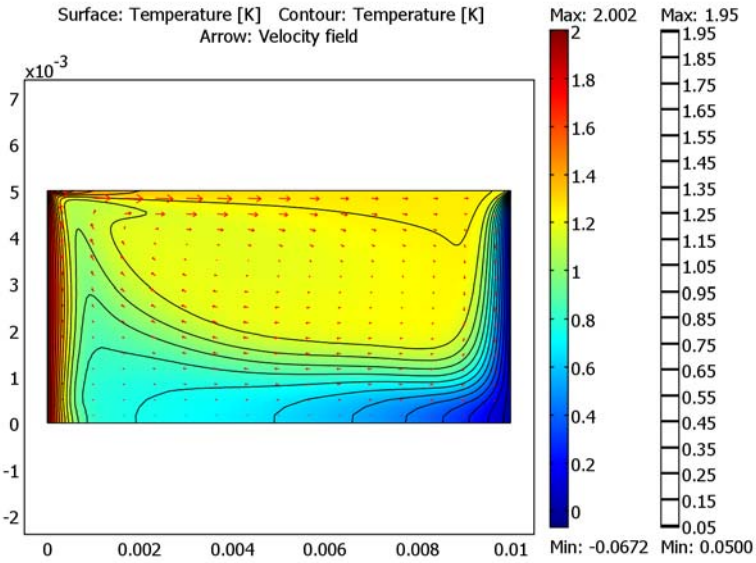


Figure 10-11: Marangoni convection with a temperature difference of 2 K.

At higher temperature differences (2 K in Figure 10-11 above), the physical coupling between the temperature and the velocity field is clearly visible. The heat conduction is small compared to the convection, and at the surface the fluid accelerates where the temperature gradient is high.

Reference

1. V.G. Levich, *Physicochemical Hydrodynamics*, Prentice-Hall, N.J., 1962.

Model Library path: `COMSOL_Multiphysics/Multiphysics/marangoni`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 Click the **Multiphysics** button.

3 In the **COMSOL Multiphysics>Fluid Dynamics** folder, select **Incompressible Navier-Stokes** and then **Steady-state analysis**. Make sure **Lagrange - P_2P_1** is selected in the **Element** list.

4 Click **Add**.

5 In the **Heat Transfer** folder, select **Convection and Conduction** and then **Steady-state analysis**. Make sure **Lagrange - Quadratic** is selected in the **Element** list.

6 Click **Add**.

7 In the **PDE Modes** folder, select **Weak Form, Boundary** and then **Stationary analysis**.

8 Type `lm` in the **Dependent variables** edit field.

9 Select **Lagrange - Linear** in the **Element** list.

10 Click **Add**.

11 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, define the following constants with names, expressions, and descriptions (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
deltaT	1e-3[K]	Temperature difference
gamma	-8e-5	Temperature derivative of the surface tension
rho1	760[kg/m^3]	Fluid density
eta1	4.94e-4[Pa*s]	Dynamic viscosity
k1	0.1[W/(m*K)]	Thermal conductivity
Cp1	2090[J/(kg*K)]	Heat capacity
alpha1	1.3e-3[1/K]	Thermal expansion coefficient
g	9.8[m/s^2]	Acceleration due to gravity

GEOMETRY MODELING

1 On the **Draw** menu, point to **Specify Objects** and then click **Rectangle**.

1 In the **Rectangle** dialog box, type `0.01` in the **Width** edit field and type `0.005` in the **Height** edit field.

2 Click **OK**.

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

PHYSICS SETTINGS

Boundary Conditions—Momentum Balance

1 From the **Multiphysics** menu, choose **Incompressible Navier-Stokes (ns)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 In the **Boundary Settings** dialog box, enter boundary conditions for the Incompressible Navier-Stokes mode according to the table below:

SETTINGS	BOUNDARIES 1, 2, 4	BOUNDARY 3
Boundary type	Wall	Symmetry boundary
Boundary condition	No slip	-

4 Click **OK**.

Point Settings—Momentum Balance

Set the pressure to zero in the point (0,0) to get a well-defined condition on the pressure:

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

2 In the **Point Settings** dialog box, select Point 1.

3 Select the **Point constraint** check box

4 Click **OK**.

Boundary Conditions—Heat Transfer

1 From the **Multiphysics** menu, choose **Convection and Conduction (cc)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 In the **Boundary Settings** dialog box, enter boundary conditions for the Convection and Conduction mode according to the table below:

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3	BOUNDARY 4
Boundary condition	Temperature	Thermal insulation	Temperature
T_0	`deltaT`		0

4 Click **OK**.

Boundary Conditions—Liquid/Air Interface

1 From the **Multiphysics** menu, choose **Weak Form, Boundary (wb)**.

2 From the **Physics** menu, choose **Boundary Settings**.

3 In the **Boundary Settings** dialog box, clear the **Active in this domain** check box for Boundaries 1, 2, and 4.

4 Click the **Weak** tab.

5 Select Boundary 3 and type `lm_test*(eta1*uy-gamma*Tx)+u_test*lm` in the **weak** edit field. This implements Equation 10-8, which states that the shear stress on a surface is proportional to the temperature gradient.

6 Click **OK**.

Boundary Conditions—Equation System Level

To get consistent boundary conditions, omit the Dirichlet boundary condition for T on the vertex connecting Boundary 1 and Boundary 3 and on the vertex connecting Boundary 4 and Boundary 3:

1 On the **Physics** menu, point to **Equation System** and then click **Boundary Settings**.

2 In the **Boundary Settings - Equation System** dialog box, click the **r** tab.

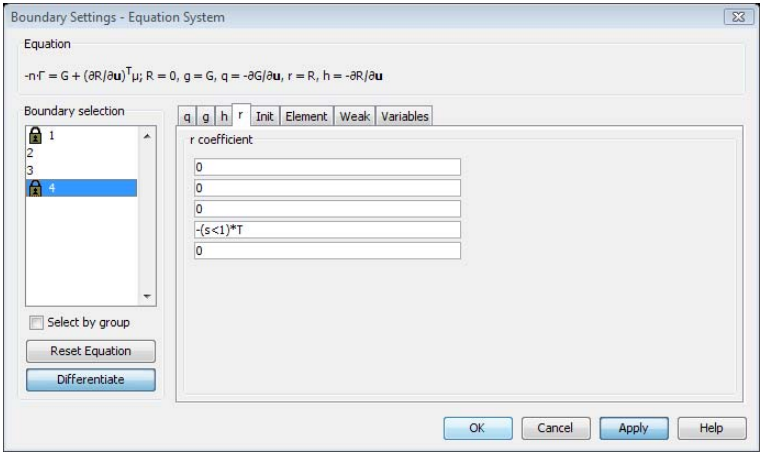
3 Select Boundary 1 and type `(s<1)*(T0_cc-T)` in edit field in row 4. `s` is the boundary parameterization variable, which varies from 0 to 1 in the direction of the boundary arrow. That means that `(s<1)` is 1 only at the vertex at the end of the boundary.

4 Click the **Differentiate** button to get the h coefficient.

5 Select Boundary 4 and type `-(s<1)*T` in the edit field in row 4.

6 Click the **Differentiate** button to get the h coefficient.

7 Click **OK**.



Subdomain Settings—Momentum Balance

1 From the **Multiphysics** menu, choose **Incompressible Navier-Stokes (ns)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 In the **Subdomain Settings** dialog box, select Subdomain 1 and enter the material properties and buoyancy force term below for the Incompressible Navier-Stokes application mode:

SETTINGS	SUBDOMAIN 1
ρ	`rho1`
η	`eta1`
F_y	`alpha1*g*rho1*(T-deltaT/2)`

4 Click **OK**.

Subdomain Settings—Heat Transfer

1 From the **Multiphysics** menu, choose **Convection and Conduction (cc)**.

2 From the **Physics** menu, choose **Subdomain Settings**.

3 In the **Subdomain Settings** dialog box, enter the material properties and velocities below for the Convection and Conduction mode:

SETTINGS	SUBDOMAIN 1
k (isotropic)	`k1`
ρ	`rho1`
C_p	`Cp1`
u	`u`
v	`v`

4 Click **OK**.

MESH GENERATION

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

2 In the **Free Mesh Parameters** dialog box, click the **Custom mesh size** button and type `1.1` in the **Element growth rate** edit field.

3 Click the **Boundary** tab.

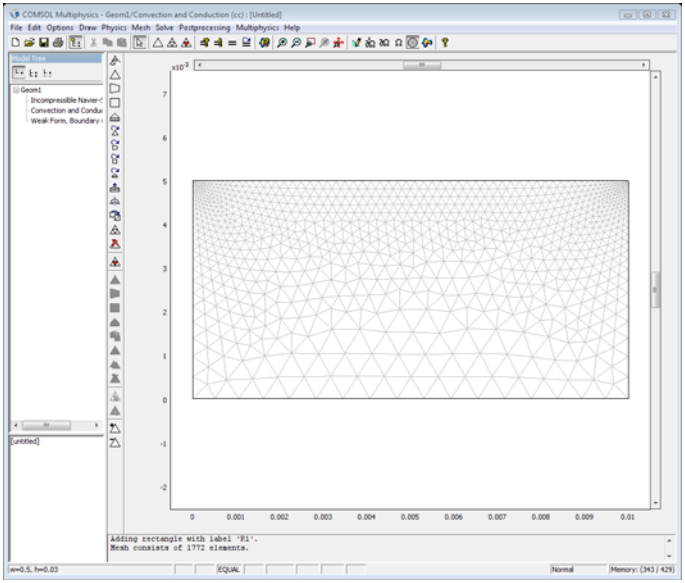
4 Select Boundary 3 and type `2e-4` in the **Maximum element size** edit field.

5 Click the **Point** tab.

6 Select Points 2 and 4 and type `4e-5` in the **Maximum element size** edit field.

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

These settings provide a finer mesh close to the liquid surface and especially toward the right end.



COMPUTING THE SOLUTION

First solve the problem with the small temperature difference, $\Delta T = 10^{-3}$ K, specified above. Click the **Solve** button to compute the solution. See the section "Postprocessing an Visualization" below on how to plot the temperature and velocity field.

Increase the temperature difference to 0.05 K to make the Marangoni effect more visible:

1 Set `deltaT` to `0.05[K]` in the **Constants** dialog box.

2 Click the **Restart** button.

Finally increase the temperature difference even more (to 2 K):

1 Set `deltaT` to `2[K]` in the **Constants** dialog box.

2 Click the **Restart** button

POSTPROCESSING AND VISUALIZATION

Show the temperature field as a surface plot with overlaid contours and the velocity field using arrows as in the results plots earlier in this model documentation:

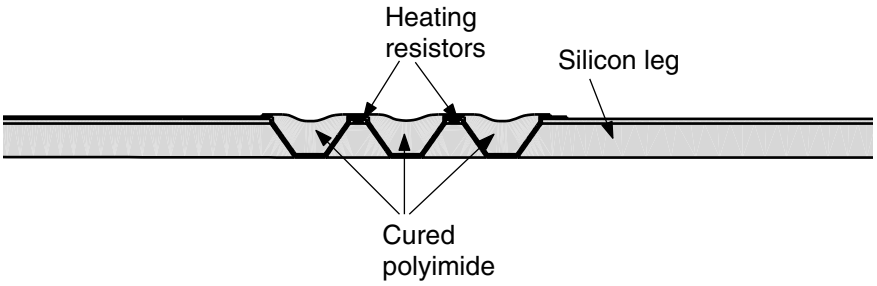
1. From the **Postprocessing** menu, choose **Plot Parameters**.
2. Under **Plot type** in the **Plot Parameters** dialog box, select the **Surface**, **Contour**, and **Arrow** check boxes.
3. Click the **Surface** tab.
4. On the **Surface Data** tab, select **Convection and Conduction (cc)>Temperature** in the predefined quantities list.
5. Click the **Contour** tab.
6. On the **Contour Data** tab, select **Convection and Conduction (cc)>Temperature** in the predefined quantities list.
7. In the **Contour color** area, click the **Uniform color** button and then click the **Color** button.
8. Select black in the **Contour Color** dialog box and click **OK**.
9. Click the **Arrow** tab.
10. Verify that the predefined quantity for the arrow data is the velocity field.
11. Click **OK**.

Simulation of a Microrobot[2]

Introduction

This example describes the modeling of one of the legs of a silicon microrobot in COMSOL Multiphysics. The image below shows the microrobot.

The microrobot uses a technique based on polyimide V-groove joints to get each of the legs to move. The polyimide has a relatively high coefficient of thermal expansion α, and this causes the leg to bend slightly when the polyimide is heated. Putting several V-grooves on each leg provides sufficient deflection (see the following figure).



See Ref. 1 for a more detailed description of the microrobot.

Model Definition

EQUATIONS

The model couples a Heat Transfer application mode to a Plane Strain structural application mode to simulate the bending.

The unknowns of the system are:

- u, the displacement along the x-axis
- v, the displacement along the y-axis
- T, the temperature

2. Model courtesy of Thorbjörn Ebefors, Dept. of Signals, Sensors and Systems (S3), Royal Institute of Technology (KTH), Stockholm, Sweden.

Time scales for the structural mechanics problem are much smaller than for the heat transfer problem so you can neglect them and analyze the structural model as a static model. The time dependence of the system is retained through the heat transfer equation. This assumption is well motivated and results in a shorter simulation time. The discretized system becomes a differential-algebraic equation system (DAE) containing the following equations:

- The principle of virtual work for plane strain condition states that:

$$\delta W = \int_V (-\varepsilon_{x\text{test}}\sigma_x - \varepsilon_{y\text{test}}\sigma_y - 2\varepsilon_{xy\text{test}}\tau_{xy} + \mathbf{u}_{\text{test}}^t \mathbf{F}_V) dV + \int_S \mathbf{u}_{\text{test}}^t \mathbf{F}_S ds + \int_S \mathbf{u}_{\text{test}}^t \mathbf{F}_S ds = 0$$

  where W is the total stored energy. The stress-strain relation including thermal expansion reads:

$$\sigma = D\varepsilon_{\text{el}} + \sigma_0 = D(\varepsilon - \alpha T)$$

  where α is the thermal expansion coefficient.

See "The Plane Strain Application Mode" on page 225 in the *COMSOL Multiphysics Modeling Guide* for details.

- The transient heat equation:

$$\rho C_P \frac{\partial T}{\partial t} + \nabla \cdot (k\nabla T) = Q(t)$$

  where ρ is the density, C_P is the heat capacity, k is the thermal conduction, and Q is the heat source.

MATERIAL PROPERTIES

To represent the model use several subdomains corresponding to the different parts. You need six property sets to define each part of the leg of the microrobot (Si, SiNa, Al, P, SiO, and pSi).

THERMAL LOAD

A heat source of $2{\cdot}10^{13}$ W/m^3, corresponding to 100 mW, is turned on in each of the two heating resistors during the first 10 ms of the 20 ms simulation.

BOUNDARY CONDITIONS

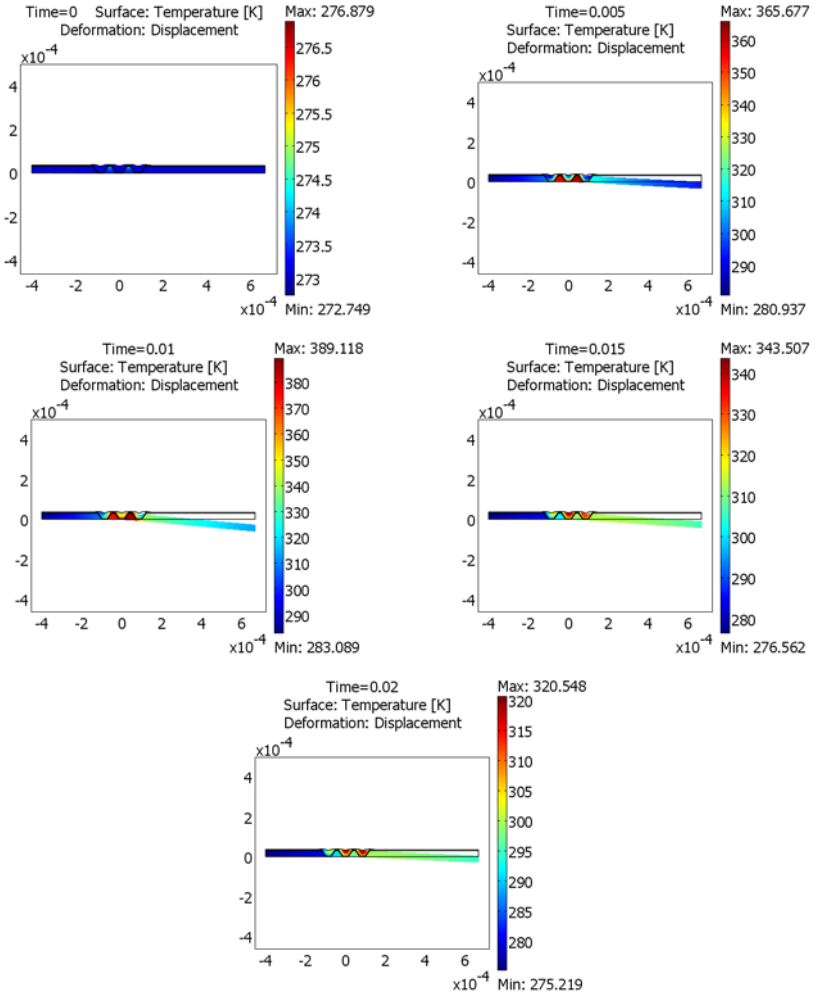
An important part of the simulation is the modeling of the cooling effect at the boundaries. Experiments have verified that most of the heat dissipates in the silicon structure (the "body" of the robot). Also, the experiments show a minor cooling effect at the tip of the leg.

Motivated by this, use a heat transfer coefficient of 10^6 W/(m^2·K) on the part of the leg connected to the rest of the robot, a coefficient of 10^5 W/(m^2·K) on the tip of the leg, and insulation on the rest of the structure. These values are somewhat arbitrary, but the simulation results have been calibrated with experimental data.

The boundary conditions for the structural mechanics part are simply constrained displacement at the left end of the robot leg and zero force on the rest of the structure.

Results and Discussion

As expected, the following plots show that the microrobot leg bends when there is a heat source and returns to its initial shape with the decrease of the temperature. The plot sequence shows the temperature increase from 0 s to 20 ms every 5 ms.



The animation shows how the temperature in the robot leg increases and how it bends downward, as expected. Note that the temperature should be interpreted as a deviation from the initial state, which is room temperature. After 10 ms, the power is turned off,

and the leg returns toward its undeformed initial state. It is of great interest to optimize the model, for example, the shape of the V-grooves and the power in each heating resistance, so that the bending process becomes as fast as possible.

Modeling in COMSOL Multiphysics

To model such a system with COMSOL Multiphysics you need to select two application modes: Heat Transfer and Plane Strain.

The coupling appears in the definition of the stress variables by adding the thermal strain.

The coupling is one-way only (from the heat source to the displacements due to the heat source).

Reference

1. T. Ebefors, "Polyimide V-groove Joints for Three-Dimensional Silicon Transducers." Ph.D. thesis, May 2000, Dept. of Signal, Sensors and Systems (S3), Royal Institute of Technology (KTH), Stockholm, Sweden.

Model Library path: `COMSOL_Multiphysics/Multiphysics/microrobot`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics or click the **New** button to open the **Model Navigator**.

2 Select **2D** from the **Space dimension** list.

3 Click the **Multiphysics** button.

4 Select the **COMSOL Multiphysics>Heat Transfer>Conduction** application mode and then **Transient analysis**.

5 Click **Add**.

6 Open the **Structural Mechanics** application modes folder and then the **Plane Strain** application mode, and select **Static analysis**.

7 Click **Add**.

8 Click **OK**.

GEOMETRY MODELING

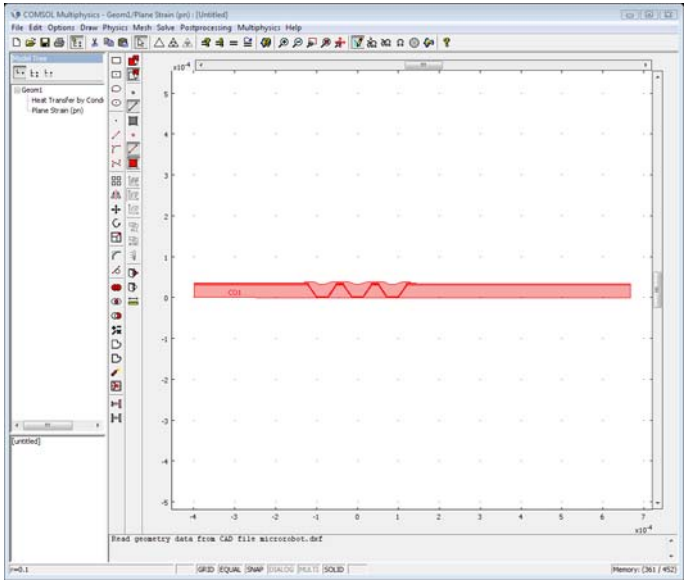
The geometry of this model is provided as a DXF file as it is quite complicated.

1 On the **File** menu, point to **Import** and then click **CAD Data From File**. Select **DXF file (*.dxf)** in the **Files of type** list.

2 Browse to `models/COMSOL_Multiphysics/Multiphysics` under the COMSOL installation directory.

3 Select `microrobot.dxf`. Click **Import**.

4 On the **Draw** menu, point to **Coerce To** and then click **Solid.**



PHYSICS SETTINGS

Because the microrobot legs are composed of several materials with different material properties, you have to define subdomain settings for each materials. Using subdomain expression variables makes it easier to enter the subdomain properties of the model.

Define the following parameters for the materials:

- The thermal conductivity `k_mat`
- The heat capacity `C_mat`
- The density: `rho_mat`

- Young's modulus: `E_mat`
- The Poisson ratio: `nu_mat`
- The thermal expansion coefficient: `al_mat`
- The heat source: `heat`

Expression Variables

Open the **Scalar Expressions** dialog box from the **Options** menu. Create a scalar expression with **Name** `dT`, **Expression** `T-273.15`, and **Description** `Temperature difference`.

Subdomain Expressions

1 On the **Options** menu, point to **Expressions** and then click **Subdomain Expressions**.

2 In the **Subdomain Expressions** dialog box, which you open from the **Physics** menu, enter the following material properties:

PROPERTY	SUBDOMAINS 1, 6, 10, 14	SUBDOMAINS 2, 7, 11, 15	SUBDOMAIN 3	SUBDOMAIN 4	SUBDOMAINS 5, 9, 13	SUBDOMAINS 8, 12
k_mat	140	15	238	0.16	1.4	20
C_mat	707	1000	900	2000	1000	707
rho_mat	2300	2865	1410	2700	2200	2300
E_mat	130e9	95e9	70e9	2e9	70e9	160e9
nu_mat	0.3	0.25	0.3	0.35	0.22	0.3
al_mat	2.5e-6	0.8e-6	23e-6	140e-6	0.5e-6	2e-6
heat	0	0	0	0	0	2e13

From left to right the material properties represent Si, SiN, Al, P, SiO, and pSi.

3 Click **OK**.

Model Settings

The default equation system form for models including the heat transfer application modes is the general form, but this is a linear problem, so you can use the coefficient form. This makes it easier to identify the thermal expansion coefficient in the equation system.

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

2 Select **Coefficient** from the **Equation system form** list.

3 Click **OK**.

Boundary Settings

1 In the **Physics** menu open the **Boundary Settings** dialog box.

2 Select Boundaries 1, 3, and 5.

3 Select the $\mathbf{R_x}$ and $\mathbf{R_y}$ check boxes. This locks the displacement to zero in both the *x* and *y* directions.

4 Click **OK**.

5 Change the application mode to **Heat Transfer by Conduction (ht)** in the **Multiphysics** menu.

6 Open the **Boundary Settings** dialog box from the **Physics** menu and enter the following settings:

SETTINGS	ALL BOUNDARIES EXCEPT 1, 3, 5, 95, 96	BOUNDARIES 1, 3, 5	BOUNDARIES 95, 96
Type	Thermal insulation	Heat flux	Heat flux
h		1e6	1e5

7 Click **OK**.

Subdomain settings

1 Change the application mode to **Plane Strain (pn)** in the **Multiphysics** menu.

2 In the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Enter following settings for the material properties on the **Material** page:

SETTINGS	ALL SUBDOMAINS
E	E_mat
ν	nu_mat
ρ	0

The density ρ is set to zero to remove all the dynamics in the model.

4 Click **OK**.

5 Change the application mode to **Heat Transfer by Conduction (ht)** in the **Multiphysics** menu.

6 Open the **Subdomain Settings** dialog box, and set the material properties for the Heat Transfer equation:

SETTINGS	ALL SUBDOMAINS
k (isotropic)	`k_mat`
ρ	`rho_mat`
C_p	`C_mat`
Q	`(t<1e-2)*heat`

Notice the logical expression `(t<1e-2)` in the heat source coefficient, which is used to get full heating power (`heat`) for 10 ms, and after that no power. When done, click **OK**.

Next, include the thermal strain in the stress variables definition:

7 On the **Physics** menu, point to **Equations System** and then click **Subdomain Settings**.

8 In the **Subdomain Settings - Equation System** dialog box for the equation system, click the **Variables** tab.

9 Select all the subdomains.

10 Change the normal stress variables definition according to the following table:

VARIABLE	DEFINITION

sx_pn	`E_pn*(1-nu_pn)*(ex_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*nu_pn*(ey_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*nu_pn*(-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))`

sy_pn	`E_pn*nu_pn*(ex_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*(1-nu_pn)*(ey_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*nu_pn*(-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))`

sz_pn	`E_pn*nu_pn*(ex_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*nu_pn*(ey_pn-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))+`
	`E_pn*(1-nu_pn)*(-al_mat*dT)/((1+nu_pn)*(1-2*nu_pn))`

These editings of the stress variables, indicated by the bold font in the previous table, specify the coupling between the heat-transfer problem and the structural mechanics problem.

11 Click **OK**.

MESH GENERATION

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

2 On the **Global** tab, click the **Custom mesh size** button and type `1.7` in the **Element growth rate** edit field. This reduces the mesh by allowing the element size to grow faster away from a region with small details.

3 Click the **Remesh** button to initialize the mesh, and then click **OK**.

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box by clicking on the corresponding icon in the Main toolbar.

2 On the **General** page, type `range(0,0.005,0.02)` in the **Times** edit field. This provides the solution at 5 equally spaced time steps from 0 to 20 ms or every 5 ms. The tolerances for the time-dependent solver control the actual time stepping.

3 Type `1e-6` in the **Absolute tolerance** edit field and `1e-5` in the **Relative tolerance** edit field. It is important that the absolute tolerance is smaller than the typical displacements by at least an order of magnitude.

4 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

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

2 On the **General** page, select the **Deformed shape** check box to plot using a deformed shape.

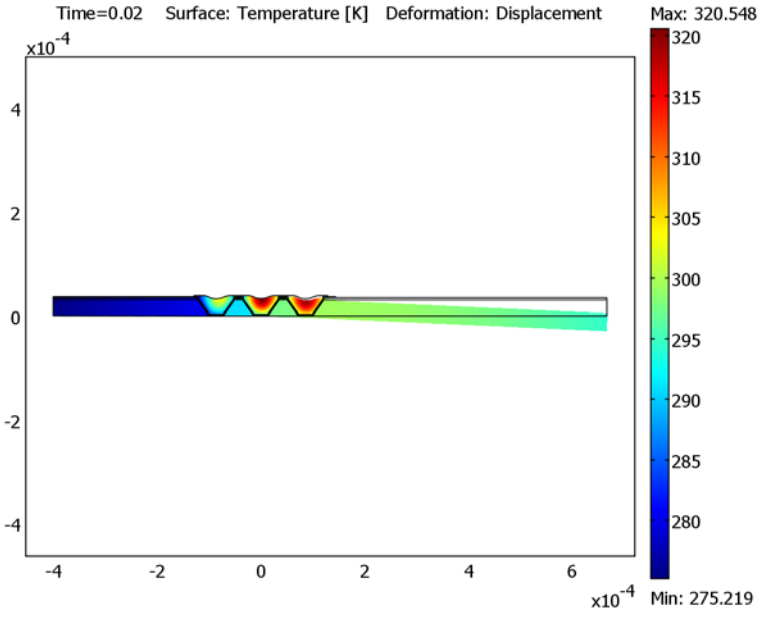
3 Click the **Deform** tab.

4 On the **Subdomain Data** tab in the **Deformation data** area, select **Plane Strain (pn)>Displacement** in the **Predefined quantities** list.

5 To get the following plot, clear the **Auto** check box for automatic scaling of the deformed shape. Then type `1` in the **Scale factor** edit field.

6 Click **OK**.

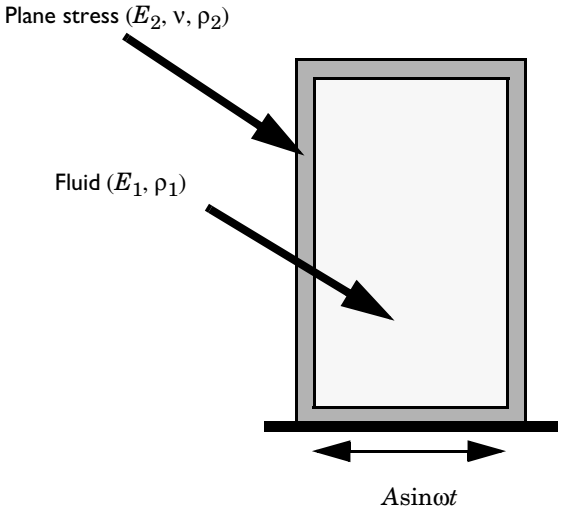
7 To get an animation of the results, click the **Animate** button in the Plot toolbar.



Vibrations in Milk Containers

Introduction

This example illustrates a multiphysics application that involves a fluid-structure interaction. It simulates a filled milk container on a conveyor belt that starts moving. The methodology presented here defines two subproblems, one for the container walls and another for the fluid. The two problems merge into one using special interface conditions that impose continuous normal displacements and normal forces across the interface boundary.



Model Definition

With all variables having a harmonic time dependence, you solve for only one complex amplitude.

DOMAIN EQUATIONS

In the container walls, use Navier's equation for plane stress to find the displacements u and v:

$$\begin{cases} -\rho_2\omega^2 u + \dfrac{E_2}{1-\nu^2}(u_x + \nu v_y)_x + \dfrac{E_2}{2(1+\nu)}(u_y + v_x)_y = 0 \\ -\rho_2\omega^2 v + \dfrac{E_2}{1-\nu^2}(v_y + \nu u_x)_y + \dfrac{E_2}{2(1+\nu)}(u_y + v_x)_x = 0 \end{cases}$$

where ρ_2 is density, E_2 is the elasticity modulus (Young's modulus), and ν is Poisson's ratio.

For the fluid assume irrotational flow. Thus you can give the displacements with the gradient of a displacement potential G:

$$U = G_x,\ V = G_y$$

and the equation for sound waves becomes

$$\rho_1\omega^2 G + E_1\Delta G = 0$$

where E_1 is the elasticity modulus for the fluid, and ρ_1 the fluid density.

INTERFACE CONDITIONS

At the interface, the normal displacements should be continuous, so

$$\mathbf{n} \cdot E_1\nabla G - E_1\mathbf{n} \cdot \begin{bmatrix} u \\ v \end{bmatrix} = 0$$

where $\mathbf{n}$ is the outward-pointing normal. Pressure in the gas, p, follows the relationship

$$p = \rho_1\omega G,$$

and force continuity across the interface gives

$$\mathbf{n} \cdot \underline{\sigma} + \rho_1\omega^2 G\mathbf{n} = 0$$

where $\mathbf{n}$ is the inward-pointing normal.

Modeling in COMSOL Multiphysics

This model uses an equation-based approach, where the modeling of both the Navier's equation and the equation for the sound waves uses PDE modes for PDEs in coefficient form. The Navier's equation is active in the wall only, and the equation for

the sound waves is active in the fluid domain only. For the coupling, you use the equation system view to define the fluid-structure interaction at the boundaries between the two domains.

Results

The solution shows the deformations that occur in the container. Figure 10-12 shows the deformations (scaled) for a container filled with milk. A second analysis provides the deformations for a container filled with gas (see Figure 10-13).

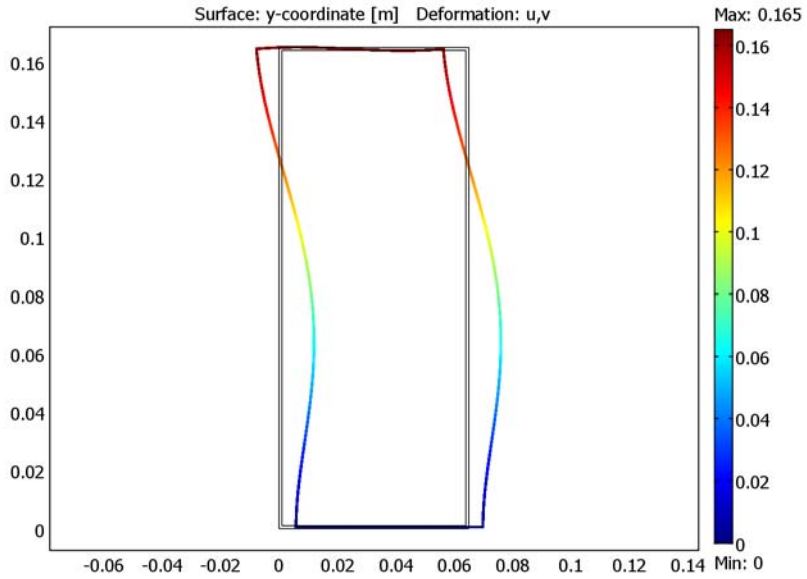


Figure 10-12: The deformation (exaggerated) of the container filled with milk.

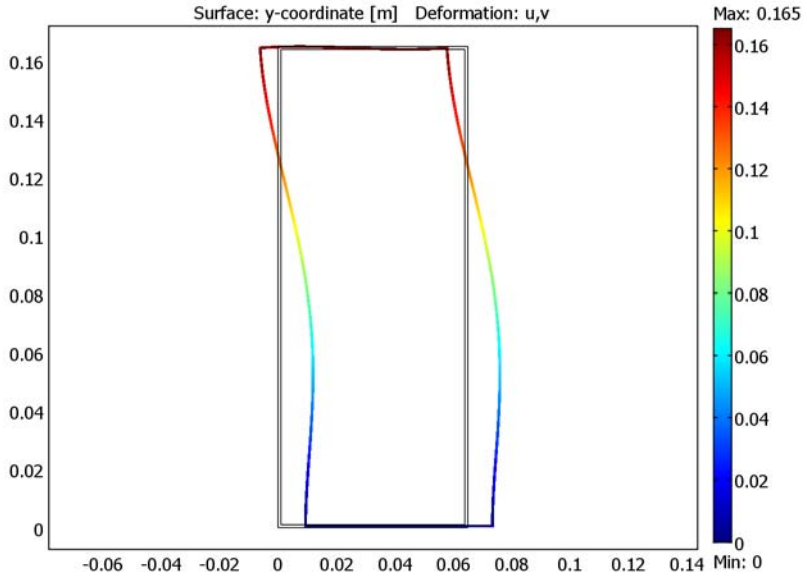


Figure 10-13: The deformation (exaggerated) of the container filled with gas.

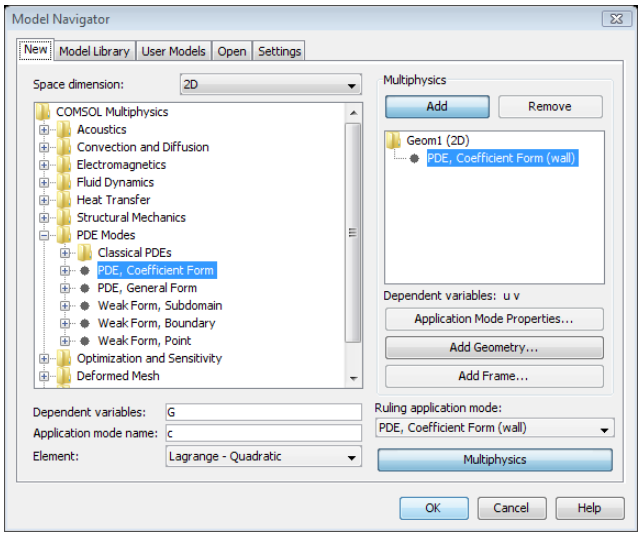
Model Library path: `COMSOL_Multiphysics/Multiphysics/milk_container`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, click the **Multiphysics** button.
2. Select the first application mode from the table below in the **COMSOL Multiphysics>PDE Modes** section and rename it by typing the name in the **Application mode name** edit field.
3. Define the dependent variables by typing the variable names in the table below in the **Dependent variables** edit field.

4 Click the **Add** button.



5 Add the second application mode following the same procedure and then click **OK**.

APPLICATION MODE	APPLICATION MODE NAME	DEPENDENT VARIABLES	ELEMENT TYPE
PDE, coefficient form	`wall`	`u v`	Lagrange - Quadratic
PDE, coefficient form	`fluid`	`G`	Lagrange - Quadratic

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, add the following constants for the material properties and the angular frequency (the constant `w`):

NAME	EXPRESSION
`E1`	`1e10`
`rho1`	`1e3`
`E2`	`1e8`
`rho2`	`1e3`
`nu`	`0.3`
`w`	`2*pi*10`

3 Click **OK**.

GEOMETRY MODELING

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

2 In the **Rectangle** dialog box, specify a rectangle with a lower-left corner at (0.001, 0.001), a width of 0.063, and a height of 0.163.

3 Click **OK** and then click the **Zoom Extents** button.

4 Draw another rectangle using the same method. This rectangle's lower-left corner is at (0, 0), the width is 0.065, and the height is 0.165.

5 Press Ctrl+A to select both objects and then click the **Union** button on the Draw toolbar.

PHYSICS SETTINGS

Boundary Conditions

1 From the **Multiphysics** menu, select the `wall` application mode.

2 From the **Physics** menu, choose **Boundary** settings.

3 In the **Boundary Settings** dialog box, select the **Interior boundaries** check box.

4 Specify the boundary conditions from the table below. Start with Boundary 2. You can the select the **Select by group** check box to set Neumann conditions on the remaining boundaries in one step.

SETTINGS	BOUNDARIES 1,3-8	BOUNDARY 2
Type	Neumann	Dirichlet
h(1,1)		1
h(1,2)		0
h(2,1)		0
h(2,2)		1
r(1)		0.001
r(2)		0

5 Click **OK**.

You do not need to define boundary conditions for the fluid because the fluid domain consists of interior boundaries only.

Subdomain Settings

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

2 In the **Subdomain Settings** dialog box, select Subdomain 2 from the **Subdomain selection** list and then clear the **Active in this domain** check box to deactivate the fluid domain.

3 Select Subdomain 1 and then click the **c**, **a**, and **f** tabs and enter the PDE coefficients for the wall domain according to the following table:

COEFFICIENT	SUBDOMAIN 1
c(1,1)	`E2/(1-nu^2) E2/2/(1+nu)`
c(1,2)	`0 E2/2/(1+nu) E2*nu/(1-nu^2) 0`
c(2,1)	`0 E2*nu/(1-nu^2) E2/2/(1+nu) 0`
c(2,2)	`E2/2/(1+nu) E2/(1-nu^2)`
a(1,1)	`-w^2*rho2`
a(1,2)	0
a(2,1)	0
a(2,2)	`-w^2*rho2`
f(1)	0
f(2)	0

4 Click **OK**.

5 From the **Multiphysics** menu, select the **fluid** application mode.

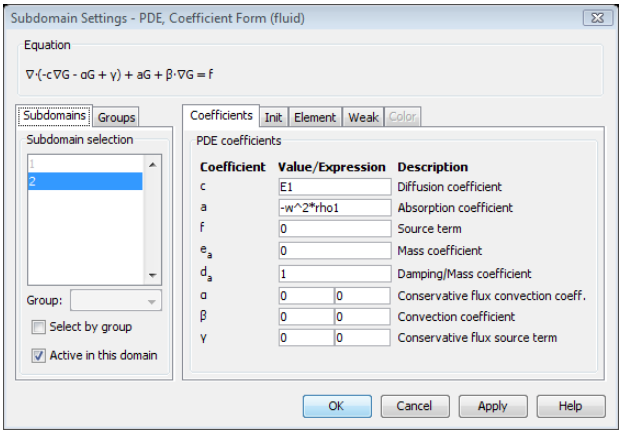
6 From the **Physics** menu, choose **Subdomain Settings**.

7 In the **Subdomain Settings** dialog box, select Subdomain 1 in the **Subdomain selection** list and then clear the **Active in this domain** check box to deactivate the wall domain.

8 Select Subdomain 2 and enter the PDE coefficients for the fluid domain according to the following table:

COEFFICIENT	SUBDOMAIN 2
c	E1
a	`-w^2*rho1`
f	0

9 Click **OK**.



Boundary Conditions—Equation System

To get continuous normal forces and normal displacements on the interior boundaries, use the **Boundary Settings** dialog box for the equation system.

1 On the **Physics** menu, point to **Equation System** and then click **Boundary Settings**.

2 Specify the following components for the q coefficient on Boundaries 4–7 that separate the fluid and the wall:

COMPONENT	BOUNDARY 4	BOUNDARY 5	BOUNDARY 6	BOUNDARY 7
q(1,1)	0	0	0	0
q(1,2)	0	0	0	0
q(1,3)	w*rho1	0	0	-w*rho1
q(2,1)	0	0	0	0
q(2,2)	0	0	0	0
q(2,3)	0	w*rho1	-w*rho1	0
q(3,1)	E1	0	0	-E1
q(3,2)	0	E1	-E1	0
q(3,3)	0	0	0	0

3 Click **OK**.

MESH GENERATION

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

2 Click the **Custom mesh size** button and type `1.7` in the **Element growth rate** edit field.

3 Click **OK**.

4 Click the **Initialize Mesh** button.

COMPUTING THE SOLUTION

For this model, use the stationary solver (the default solver). Click the **Solve** button to solve the problem.

POSTPROCESSING AND VISUALIZATION

1 From the **Postprocessing** menu, choose **Plot Parameters**.

2 In the **Plot type** area on the **General** page, select the **Deformed shape** check box.

3 Click the **Surface** tab.

4 On the **Surface Data** tab, select **Geometry and Mesh>y-coordinate** from the **Predefined quantities** list.

5 Click the **Deform** tab.

6 In the **Deformation data** area, select **PDE, Coefficient Form (wall)>u, v** from the **Predefined quantities** list on the **Subdomain Data** tab to use the x- and y-displacements for the deformed shape.

7 Click **OK**.

SECOND ANALYSIS—USING A GAS-FILLED CONTAINER

To model a container filled with gas instead of milk, update the fluid parameters:

OPTIONS AND SETTINGS

Change the following constants in the **Constants** dialog box:

NAME	EXPRESSION
`E1`	`1e5`
`rho1`	`1`

COMPUTING THE SOLUTION

Solve the problem again with the new material properties for the fluid. You get a similar plot of the solution from the second analysis.

Peristaltic Pump

Introduction

In a peristaltic pump, rotating rollers squeeze a flexible tube. As the pushed-down rollers move along the tube, fluids in the tube follow the motion. The main advantage of the peristaltic pump is that no seals, valves, or other internal parts ever touch the fluid. Due to their cleanliness, peristaltic pumps have found many applications in the pharmaceutical, chemical, and food industries. Besides this, the action of a peristaltic pump is very gentle, which is important if the fluid is easily damaged. Peristaltic pumps are therefore used in medical applications, one of which is moving the blood through the body during open heart surgery. Other pumps would risk destroying the blood cells.

This COMSOL Multiphysics model of a peristaltic pump is a combination of structural mechanics (to model the squeezing of the tube) and fluid dynamics (to compute the fluid's motion); that is, this is an example of fluid-structure interaction, FSI. Because deformations of the tube drive the fluid, you must perform the fluid portion of the simulation in a deforming geometry, one that you can define with COMSOL Multiphysics' Moving Mesh (ALE) application mode.

Model Definition

The model is set up in 2D axial symmetry (Figure 10-14). A vinyl tube 0.1 m long has an inner radius of 1 cm and an outer radius of 1.5 cm; it contains a gas of density $\rho = 1$ kg/m^3 and viscosity $\eta = 3 \cdot 10^{-5}$ Pa·s. A time- and position-dependent force density is applied to the outer wall of the tube, in the radial direction. This force density could have been taken from real data from a peristaltic pump, but for simplicity's sake this example models it with a Gaussian distribution along the length of the tube. The Gaussian distribution has a width of 1 cm and is moving with the constant velocity 0.03 m/s in the positive z direction. To represent the engagement of the roll, the force density, multiplied by a smoothed Heaviside function, kicks in at $t = 0.1$ s and takes the force to its full development at $t = 0.5$ s. Likewise, the disengagement of the roll starts at $t = 1.0$ s and ends at $t = 1.4$ s. The example models the tube's deformation during a full cycle of 1.5 s.

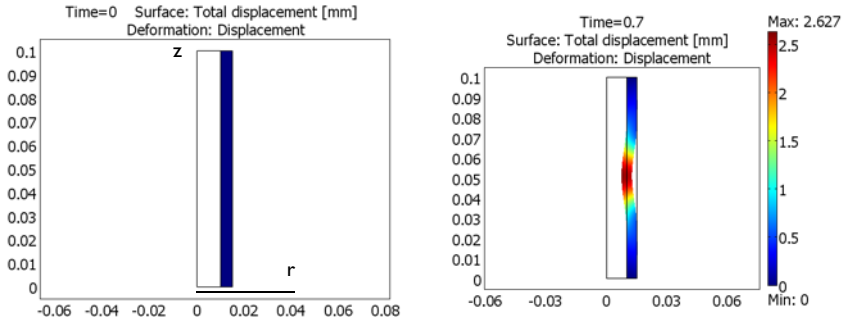


Figure 10-14: The geometry of the peristaltic pump in its initial shape (left) and as it is deforming under the pressure of the roll (right). The tube is rotationally symmetric with respect to the z-axis. The color shows the deformation of the tube material.

DOMAIN EQUATIONS

The structural mechanics computations in this model use a 2D axially symmetric stress-strain formulation. The model uses the assumption that the material is linear and elastic and does not take geometric nonlinearities into account. With the capabilities in the COMSOL Multiphysics Structural Mechanics Module, you can easily extend this model to include large deformations or use a more complicated material model.

The fluid flow is described by the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = 0$$
$$\nabla \cdot \mathbf{u} = 0 \qquad (10\text{-}9)$$

where ρ denotes the density (kg/m^3), $\mathbf{u}$ the velocity (m/s), η the viscosity (Pa·s), and p the pressure (Pa). The equations are set up and solved in axial symmetry on a deformed mesh inside the tube.

Further, you model the motion of the deformed mesh with Winslow smoothing. For more information on this topic, please refer to "The Moving Mesh Application Mode" on page 455 in the *COMSOL Multiphysics Modeling Guide*.

BOUNDARY CONDITIONS

For the structural mechanics computations, the time- and coordinate-dependent load described serves as the boundary condition at the tube's outer surface. The top and bottom ends of the tube are constrained along both coordinate axes, and the inner surface is free. The reaction forces from the fluid on the tube are very small compared

to the force applied by the rollers, so this model does not take them into account. This way you can solve first for the structural mechanics and then for the fluid dynamics, reducing solution time and memory consumption.

The inner surface is free, and the top and bottom ends of the tube are constrained along both coordinate axes.

For the fluid simulation, the boundary condition at the inlet and the outlet assumes that the total stress is zero, that is:

$$\mathbf{n} \cdot [-pI + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] = \mathbf{0} \tag{10-10}$$

Inside the wall of the tube, the moving mesh follows the deformations of the tube. The mesh deformations being the same as the structural deformations is also used as the moving mesh boundary condition where the fluid meets the tube wall. The mesh is fixed to a zero r displacement at the symmetry axis and a zero z displacement at the top and the bottom of the tube.

COMPUTATION OF VOLUMETRIC FLOW RATES AND TOTAL VOLUME OF PUMPED FLUID

The model's dependent variables (those solved for) are the displacements of the tube wall as well as the fluid's velocity $\mathbf{u} = (u, v)$ and pressure p. To get the volumetric flow rate of the fluid $\dot{V}$ in m^3/s and the total volume of pumped fluid, you must perform some additional calculations. To get the volumetric flow rate at any instant t, compute a boundary integral over the pipe's inlet or outlet boundary:

$$\dot{V}_{\mathrm{in}} = -\int_{s_{\mathrm{in}}} 2\pi r(\mathbf{n} \cdot \mathbf{u}) ds$$

$$\dot{V}_{\mathrm{out}} = \int_{s_{\mathrm{out}}} 2\pi r(\mathbf{n} \cdot \mathbf{u}) ds$$

where $\mathbf{n}$ is the outward-pointing unit normal of the boundary, $\mathbf{u}$ equals the velocity vector, and s is the boundary length parameter along which you integrate. In this particular model, the inlet and outlet boundaries are horizontal so $\mathbf{n} \cdot \mathbf{u} = n_x u + n_y v$ simplifies to v or $-v$ depending on the direction of flow.

In a similar manner, you can integrate the total volume of fluid (m^3) contained in the pump as an integral over the fluid domain, A, with the equation

$$V = \int_A 2\pi r dA$$

Note that A is the deformed domain due to the deformation of the wall.

Finally, it is of interest to track how much volume of fluid, $V_{\text{pump}}(t)$ (m^3), that is conveyed out of the outlet during a peristaltic cycle, which is equal to the following time integral:

$$V_{\text{pump}}(t) = \int_0^t \dot{V}_{\text{out}}\, dt' .$$

To compute this integral, specify the corresponding ODE in COMSOL Multiphysics

$$\frac{dV_{\text{pump}}}{dt} = \dot{V}_{\text{out}}$$

with proper initial conditions; the software then integrates this equation.

Results

Figure 10-15 shows three snapshots from the peristaltic pump in action.

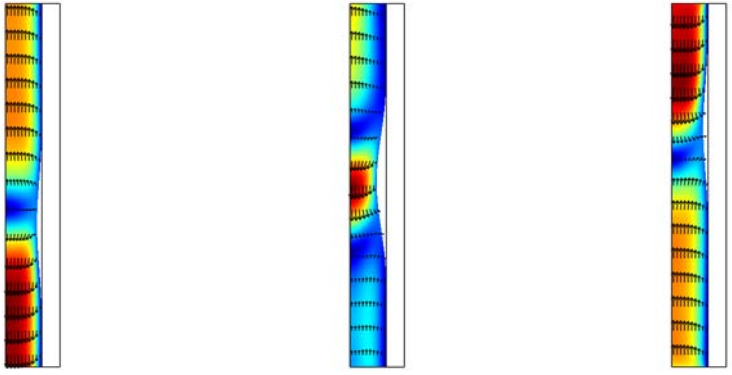


Figure 10-15: Snapshots of the velocity field and the shape of the inside of the tube at $t = 0.3$ s, $t = 0.7$ s, and $t = 1.2$ s. The colors represent the magnitude of the velocity, and the arrows its direction.

Figure 10-16 shows the inner volume of the tube as a function of time. At $t = 0.3$ s, the roll has begun its engagement phase and is increasing its pressure on the tube. As less space is left for the gas, it is streaming out of the tube, through both the inlet and

the outlet. At $t = 0.7$ s, the roll has been fully engaged for a while. As it is moving up the tube, so is the gas, both at the inlet and at the outlet. This is where most of the net flow in the direction from the inlet to the outlet is created. Finally, at $t = 1.2$ s, the engagement process is reversed as the roll is disengaging. Fluid is streaming into the tube from both ends.

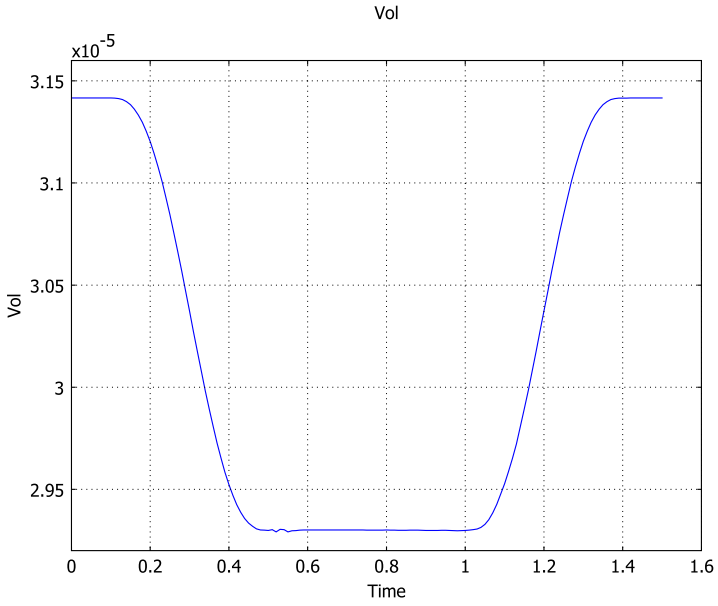


Figure 10-16: The inner volume (m^3) of the tube as a function of time (s).

Figure 10-17 shows the inlet and outlet flows, and it confirms the overall behavior indicated in the velocity snapshots. As the roll is engaged, it squeezes gas out through both the inlet and outlet. When the fully engaged roll moves along the tube, gas flows steadily in through the inlet and out through the outlet. As the roll is disengaging, the gas is being sucked back into the tube. Note that a real peristaltic pump usually removes or minimizes the peaks associated with volume changes with the help of a second roll that engages at the same time as the first roll disengages. This way there are hardly any volume changes, and the fluid flows forward all the time. Also note from Figure 10-17 that by taking the difference of the curves, $\dot{V}_{\text{in}} - \dot{V}_{\text{out}}$ and integrating over time, you generate Figure 10-16.

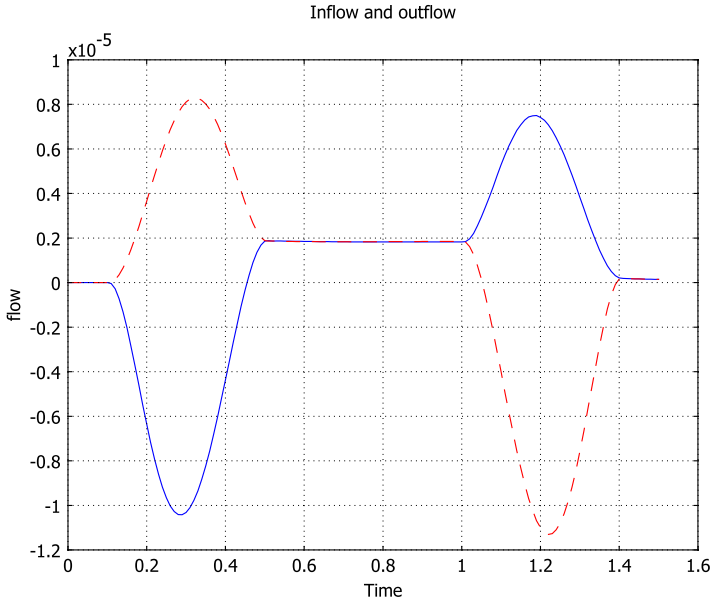


Figure 10-17: Inlet (blue solid line) and outlet (red dashed line) flow in m^3/s as functions of time. Positive values indicate that the gas is flowing in through the inlet and out through the outlet.

Figure 10-18 sums up the process, plotting the accumulated net flow versus time. It is worth noting that although the accumulated flow during the first 0.5 s of the cycle is zero or negative, it is well above zero after the full cycle.

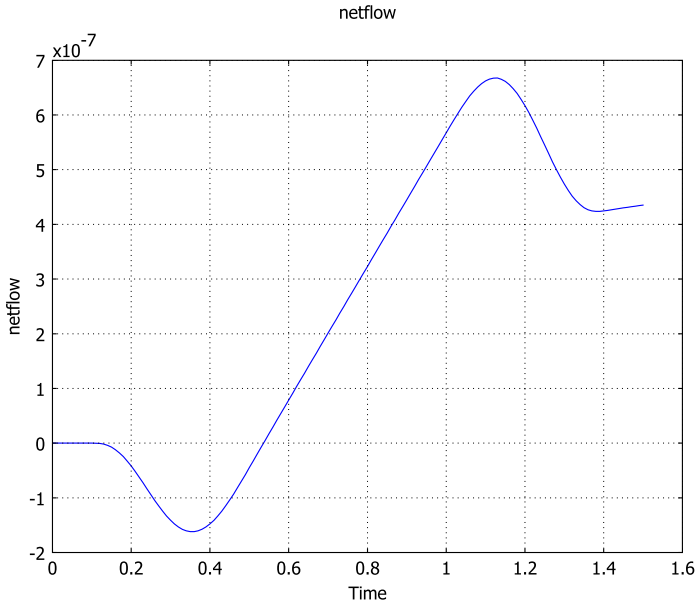


Figure 10-18: Accumulated flow (m^3) through the pump versus time (s).

Modeling in COMSOL Multiphysics

This model is primarily intended to demonstrate the use of the Moving Mesh (ALE) application mode, but it also shows some postprocessing features. It defines integration coupling variables to integrate the total flow rate and to compute the volume inside the tube. An ordinary differential equation calculates the accumulated fluid volume that has passed through the pump at certain points in time. The smooth step function in this model is called `flc2hs` (a C^2-continuous step).

Model Library path: `COMSOL_Multiphysics/Multiphysics/peristaltic_pump`

1 Start COMSOL Multiphysics.

2 In the **Model Navigator,** set the **Space dimension** to **Axial symmetry (2D)** and click the **Multiphysics** button.

3 Select **COMSOL Multiphysics>Structural Mechanics>Axial Symmetry, Stress-Strain>Transient analysis** in the list of application modes and click **Add**.

4 Select **COMSOL Multiphysics>Deformed Mesh>Moving Mesh (ALE)>Transient analysis** and click **Add**.

5 Click the **Application Mode Properties** button and set the **Smoothing method** to **Winslow**. Click **OK**.

6 Select **COMSOL Multiphysics>Fluid Dynamics>Incompressible Navier-Stokes>Transient analysis** and click **Add**.

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

GEOMETRY MODELING

1 Specify two rectangles according to the table below.

NAME	WIDTH	HEIGHT	BASE	R	Z
R1	0.01	0.1	Corner	0	0
R2	5e-3	0.1	Corner	0.01	0

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

OPTIONS AND SETTINGS

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

2 Enter constants according to the following table (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
t_on	0.3[s]	Time when roll is engaged
t_off	1.2[s]	Time when roll is disengaged
dt	0.2[s]	Time to reach full force
z0	0.03[m]	z coordinate where roll starts
v0	0.03[m/s]	Vertical velocity of roll
width	0.01[m]	Width of Gaussian force distribution

NAME	EXPRESSION	DESCRIPTION
Ttot	1.5[s]	Total time for a pump cycle
Lmax	4e6[N/m^2]	Max load

3 From the **Options** menu, choose **Functions**.

4 Define a new function for the Gaussian pulse according to following table; when done, click **OK**.

NAME	ARGUMENTS	EXPRESSION
gauss	x, sigma	1/(sigma*sqrt(2*pi))*exp(-x^2/(2*sigma^2))

5 Go to **Physics>Global Equations** and define an ordinary differential equation (see "Computation of Volumetric Flow Rates and Total Volume of Pumped Fluid" on page 425) with the following settings; when done, click **OK**.

NAME (U)	EQUATION	INIT(U)	INIT (UT)
netflow	netflowt-(inflow+outflow)/(2*Ttot)	0	0

6 Select **Integration Coupling Variables>Boundary Variables** from the **Options** menu and specify the following boundary integration variables for the inflow and outflow, each on a separate row in the table; when done, click **OK**.

SOURCE BOUNDARY	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
2	inflow	2*pi*r*v	4	Selected
3	outflow	2*pi*r*v	4	Selected

7 Select **Integration Coupling Variables>Subdomain Variables** from the **Options** menu and specify the following subdomain integration variable for the volume; when done, click **OK**.

SOURCE SUBDOMAIN	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
1	Vol	2*pi*r	4	Selected

PHYSICS SETTINGS—STRESS-STRAIN

Subdomain Settings

1 In the **Multiphysics** menu, select **Axial Symmetry, Stress-Strain**.

2 From the **Physics** menu, open the **Subdomain Settings** dialog box.

3 Select Subdomain 1 and clear the **Active in this domain** check box.

4 Select Subdomain 2 and click **Load**. Select **Nylon** from the **Basic Material Properties** folder in the **Materials** list. Click **OK**.

5 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

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

6 Apply the following boundary settings.

SETTINGS	BOUNDARIES 5, 6	BOUNDARY 7
Constraint R_R	0	
Constraint R_Z	0	
Load F_R		See below
Load F_Z		0

7 For the F_R load on Boundary 7, enter the following expression:

```
-Lmax*flc2hs((t-t_on)[1/s],dt[1/s])*gauss((z-z0-v0*t)[1/m],
width[1/m])*flc2hs((t_off-t)[1/s],dt[1/s])
```

The purpose of the unit conversions `[1/s]` and `[1/m]` is to make the input to the `flc2hs` and `gauss` functions dimensionless.

8 Click **OK**.

MESH GENERATION

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

2 On the **Global** page, click the **Custom mesh size** button and set the **Maximum element size** to `2e-3`.

3 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1 In the **Solver Manager**, go to the **Solve For** tab and select **Axial Symmetry, Stress-Strain**. Only this application mode and its solution variables **uor** and **w** should be selected. Click **OK** to close the dialog box.

2 In the **Solver Parameters** dialog box, select **Time dependent** from the **Solver** list. Set **Times** to `range(0,0.01,1.5)`, **Relative tolerance** to `0.001` and **Absolute tolerance** to `1e-5`.

3 On the **Time Stepping** tab, set **Time steps taken by solver** to **Strict**.

4 Select **BDF** in the **Method** list.

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the von Mises effective stress distribution.

1. In the **Plot Parameters** dialog box, click the **Deform** tab.
2. Select the **Deformed shape plot** check box and set the **Scale factor** to 1.
3. Use the **Solution at time** list on the **General** tab and click **Apply** to study the stress distribution and the deformation of the tube at a few points in time.

PHYSICS SETTINGS—INCOMPRESSIBLE NAVIER-STOKES

Subdomain Settings

1. In the **Multiphysics** menu, select **Incompressible Navier-Stokes**.
2. Open the **Subdomain Settings** dialog box. Select Subdomain 2 and clear the **Active in this domain** check box.
3. In Subdomain 1, set ρ to `1` (kg/m^3) and η to `3e-5` (Pa·s).
4. Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

1. Open the **Boundary Settings** dialog box from the **Physics** menu.
2. Apply the following boundary conditions; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY4
Type	Symmetry	Open	Open	Inlet
Condition	Axial symmetry	Normal stress	Normal stress	Velocity
u_0				`uaxi_t_axi`
v_0				`wt`
f_0		0	0	

PHYSICS SETTINGS—MOVING MESH

Subdomain Settings

1. In the **Multiphysics** menu, select **Moving Mesh (ALE)**.
2. Open the **Subdomain Settings** dialog box. Keep the default **Free displacement** in Subdomain 1.
3. In Subdomain 2, select **Prescribed displacement**. Enter `uaxi_axi` for **dr** and `w` for **dz**. These are the structural r and z deformations. The reason you cannot use physics-induced displacements here is that `uaxi_axi` is not a solution variable in the Stress-Strain application mode.

4 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

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

2 Apply the following boundary settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3	BOUNDARY 4
Type	Mesh displacement	Mesh displacement	Mesh displacement
dr	0		`uaxi_axi`
dz		0	`w`

COMPUTING THE SOLUTION

1 In the **Solver Manager**, go to the **Initial Value** tab and click the **Store Solution** button. By default, all solutions are selected in the **Store Solution** dialog box. Click **OK** to confirm the selection.

2 In the **Values of variables not solved for and linearization point** area, click the **Stored solution** option button and select **All** in the **Solution at time** list. This makes the solver use the solution for the deformation of the tube when computing the fluid flow.

3 On the **Solve For** page, select all variables except **uor** and **w**. Click **OK**.

4 Open the **Solver Parameters** dialog box, go to the **General** tab. Set the **Absolute tolerance** to `1e-3` and the **Relative tolerance** to `0.01`.

5 On the **Time Stepping** tab, set the **Error estimation strategy** to **Exclude algebraic**.

6 Click **OK**, then click **Solve**.

POSTPROCESSING AND VISUALIZATION

The plot still shows the deformations from the stress-strain computation. To see the velocity field as in Figure 10-15 on page 426, do the following:

1 In the **Plot Parameters** dialog box, go to the **General** page and clear the **Deformed shape** check box.

2 On the **Surface** page, select **Incompressible Navier Stokes (ns)>Velocity field** from the **Predefined quantities** list.

3 On the **Arrow** tab, select **Incompressible Navier Stokes (ns)>Velocity field** from the **Predefined quantities** list. Click the **Color** button and choose a black color; then click **OK**. Select the **Arrow plot** check box and click **Apply**.

4 Once again you can select different times to look at on the **General** page. You see the deformations even though you are not making a deformation plot because the mesh is deformed.

5 To animate the velocity field as a function of time, click the **Animate** tab and then click **Start Animation**. It might take some time for your computer to render the animation.

6 After closing the **Plot Parameters** dialog box, go to **Postprocessing>Domain Plot Parameters**.

7 Use the **Expression** field on the **Point** page to plot, for instance, the expressions `inflow`, `outflow`, `netflow`, or `Vol`. Because these variables are defined with a global destination and do not depend on the location, the coordinates do not matter. To show more than one curve at the same time, select the **Keep current plot** check box on the **General** page.

11

Quantum Mechanics Models

This chapter contains quantum mechanics models that center on solutions of the Schrödinger equation.

Conical Quantum Dots

This model computes the electronic states for a quantum-dot/wetting-layer system. It was inspired largely by the work of Dr. M. Willatzen and Dr. R. Melnik (Ref. 1) as well as B. Lassen.

Introduction

Quantum dots are nanoscale or microscale devices created by confining free electrons in a 3D semiconducting matrix. The tiny islands or droplets of confined "free electrons" (those with no potential energy) present many interesting electronic properties. They are of potential importance for applications in quantum computing, biological labeling, and lasers, to name only a few.

Scientists can create such structures experimentally using the Stranski-Krastanow molecular beam-epitaxy technique. In that way they obtain 3D confinement regions (the quantum dots) by growth of a thin layer of material (the wetting layer) onto a semiconducting matrix. Quantum dots can have many geometries including cylindrical, conical, or pyramidal. This model studies the electronic states of a conical InAs quantum dot grown on a GaAs substrate.

To compute the electronic states taken on by the quantum dot/wetting layer assembly embedded in the GaAs surrounding matrix, you must solve the 1-band Schrödinger equation in the effective mass approximation:

$$-\frac{h^2}{8\pi^2}\left(\nabla\cdot\left(\frac{1}{m_e(r)}\nabla\Psi(r)\right)\right)+V(r)\Psi(r)=E\Psi(r)$$

where h is Planck's constant, Ψ is the eigenwave function, E is the eigenvalue (energy), and m_e is the effective electron mass (to account for screening effects).

Model Definition

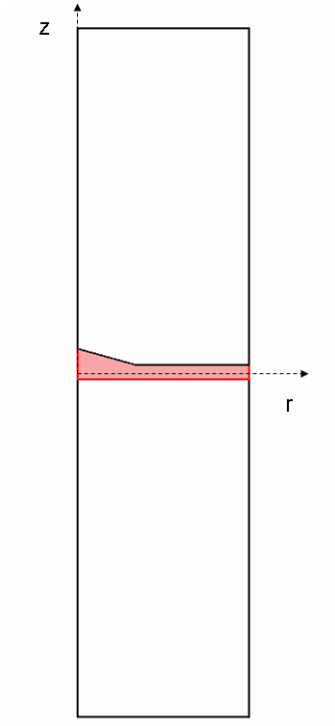
The model works with the 1-particle stationary Schrödinger equation

$$-\nabla\cdot\left(\frac{h^2}{8\pi^2 m}\nabla\Psi\right)+V\Psi=E\Psi$$

It solves this eigenvalue problem for the quantum-dot/wetting-layer system using the following step potential barrier and effective-mass approximations:

- $V = 0$ for the InAs quantum dot/wetting layer and $V = 0.697$ eV for the GaAs substrate.
- $m_e = 0.023m$ for InAs and $m_e = 0.067m$ for GaAs.

Assume the quantum dot has perfect cylindrical symmetry. In that case you can model the overall structure in 2D as shown in the following figure.



2D geometry of a perfectly cylindrical quantum dot and wetting layer.

You can now separate the total wave function Ψ into

$$\Psi = \chi(z, r)\Theta(\varphi)$$

where φ is the azimuthal angle. Then rewrite the Schrödinger equation in cylindrical coordinates as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial\chi}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial\chi}{\partial r}\right)\right]\Theta-\frac{h^2}{8\pi^2}\frac{\chi}{m_e r^2}\frac{d^2\Theta}{d\varphi^2}+V\chi\Theta = E\chi\Theta$$

Dividing this equation by

$$\frac{\chi(z,r)}{m_e r^2}\Theta(\varphi)$$

and rearranging its terms lead to the two independent equations

$$\frac{1}{\Theta}\frac{d^2\Theta}{d\varphi^2} = -l^2 \tag{11-1}$$

and

$$-m_e r^2\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial\chi_l}{\partial z}\right)\frac{1}{\chi_l}+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial\chi_l}{\partial r}\right)\frac{1}{\chi_l}\right]+m_e r^2[V-E] = -\frac{h^2}{8\pi}l^2 \tag{11-2}$$

Equation 11-1 has obvious solutions of the form

$$\Theta = \exp[il\varphi]$$

where the periodicity condition $\Theta(\varphi+2\pi) = \Theta(\varphi)$ implies that l, the principal quantum number, must be an integer. It remains to solve Equation 11-2, which you can rewrite as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial\chi_l}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial\chi_l}{\partial r}\right)\right]+\left(\frac{h^2}{8\pi^2 m_e}\frac{l^2}{r^2}+V\right)\chi_l = E_l\chi_l, \qquad l\in\mathbf{Z}$$

Note that this is an instance of a PDE on coefficient form,

$$\nabla\cdot(-c\nabla u-\alpha u+\gamma)+au+\beta\cdot\nabla u = d_a\lambda u$$

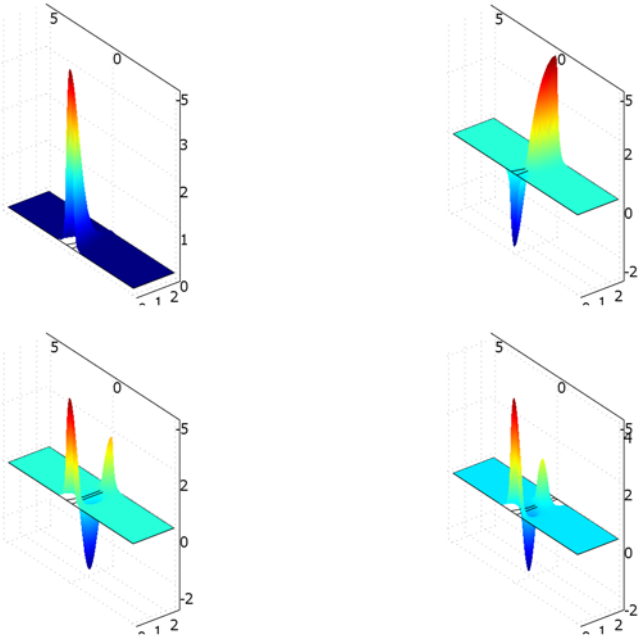
where the nonzero coefficients are

$$c = \frac{h^2}{8\pi^2 m_e}, \qquad a = \frac{h^2}{8\pi^2 m_e}\frac{l^2}{r^2}+V, \qquad \beta_r = -\frac{h^2}{8\pi^2 m_e}\frac{1}{r}, \qquad d_a = 1$$

and $\lambda = E_l$.

Results

This exercise models the eigenvalues for the four lowest electronic energy levels for the principal quantum number $l = 0$. The following plots show the eigenwave functions for those four states.



The four lowest electronic-energy levels for the case l = 0.

Modeling in COMSOL Multiphysics

To solve this problem, use the PDE, Coefficient Form version of the PDE modes in the Model Navigator. The model solves for an eigenvalue/eigenfunction, for which you must input appropriate physical data and constants.

Reference

1. R. Melnik and M. Willatzen, "Band structure of conical quantum dots with wetting layers," *Nanotechnology*, vol. 15, pp. 1–8, 2004.

Model Library path: `COMSOL_Multiphysics/Quantum_Mechanics/conical_quantum_dot`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**. In the **Space dimension** list select **2D**.

2 Click the **Multiphysics** button.

3 In the **Multiphysics** area, click the **Add Geometry** button.

4 In the **Add Geometry** dialog box, specify the **Dependent variables** `r z phi`. Click **OK**.

5 In the list of application modes select **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form>Eigenvalue analysis**.

6 Verify in the **Element** list that **Lagrange - Quadratic** is selected.

7 Click **OK**.

OPTIONS AND SETTINGS

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

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

NAME	EXPRESSION	DESCRIPTION
m	5.68e-12	Electron mass (eV/(m/s)^2)
hbar	6.58e-16	Planck's constant/(2*pi) (eV*s)
V_In	0	Potential barrier, InAs (eV)
V_Ga	0.697	Potential barrier, GaAs (eV)
c_In	hbar^2/(2*0.023*m)	PDE c coefficient, InAs
c_Ga	hbar^2/(2*0.067*m)	PDE c coefficient, GaAs
l	0	Principal quantum number

By defining a constant for the principal quantum number, you can readily modify the model to compute the solutions corresponding to nonzero l-values.

GEOMETRY MODELING

1 From the **Draw** menu select **Specify Objects>Rectangle**.

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

SIZE		POSITION	
Width	25	Base	Center
Height	100	x	12.5
		y	0

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

4 From the **Draw** menu select **Specify Objects>Rectangle**.

5 Enter the following settings; when done, click **OK**.

SIZE		POSITION	
Width	25	Base	Center
Height	2	x	12.5
		y	0

6 From the **Draw** menu select **Specify Objects>Line**.

7 Enter the following settings; when done, click **OK** to create the triangle CO1.

PROPERTY	VALUE/EXPRESSION
Coordinates, r	0 12 0
Coordinates, z	0 0 3.6
Style	Closed polyline (solid)

8 On the Draw toolbar click the **Create Composite Object** button. Select the objects R2 and CO1. Clear the **Keep interior boundaries** check box. Click **OK**.

9 On the Draw toolbar click the **Create Composite Object** button. Select the objects R1 and CO2. Make sure the **Keep interior boundaries** check box is selected, then click **OK**.

10 On the Draw toolbar click the **Scale** button, then, in the **Scale factor** area, enter a scale factor of 1e-9 for both the **r** and **z** axes. Click **OK**.

11 Click the **Zoom Extents** button.

Subdomain Settings

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

2 Enter the PDE coefficients from this table; when done, click **OK**.

SETTINGS	SUBDOMAINS 1, 3	SUBDOMAIN 2
c	c_Ga	c_In
a	c_Ga*(l/r)^2+V_Ga	c_In*(l/r)^2+V_In
β	-c_Ga/r, 0	-c_In/r, 0

Boundary Conditions

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

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

SETTINGS	BOUNDARIES 2, 9	ALL OTHER BOUNDARIES
Type	Dirichlet	Neumann
q	0	0
g	0	0
h	1	
r	0	

MESH GENERATION

From the **Mesh** menu select **Initialize Mesh**.

COMPUTING THE SOLUTION

1 From the **Solve** menu select **Solver Parameters**.

2 On the **General** page, type 4 in the **Desired number of eigenvalues** edit field.

3 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

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

2 On the **General** page find the **Solution to use** area, then go to the **Eigenvalue** list and select the desired eigenvalue (keep in mind that these solutions are valid for $l = 0$).

3 Click **Apply**.

4 On the **Surface** page, click the **Height Data** tab and select the **Height data** check box.

5 Click **Apply**, then click **OK**.

The Schrödinger Equation for the Hydrogen Atom

Introduction

This example shows how to compute energy levels and electron orbits for the hydrogen atom. It models the atom as a 1-particle system using the stationary Schrödinger equation.

$$-\nabla\cdot\left(\frac{h^2}{8\mu\pi^2}\nabla\Psi\right)+V\Psi=E\Psi$$

The equation parameters are:

- h ($6.626\cdot10^{-34}$ Js) is Planck's constant.
- μ is the reduced mass
- V is the potential energy.
- E is the unknown energy eigenvalue.
- Ψ is the quantum mechanical wave function.

Model Definition

The quantity $|\Psi|^2$ corresponds to the probability density function of the electron's position. In this example,

$$\mu=\frac{Mm_e}{M+m_e}\approx m_e$$

where M equals the mass of the nucleus and m_e represents the mass of an electron ($9.1094\cdot10^{-31}$ kg). The hydrogen nucleus consists of a single proton (more than 1,800 times heavier than the electron), so the approximation of μ is valid. Thus you can treat the problem as a one-particle system.

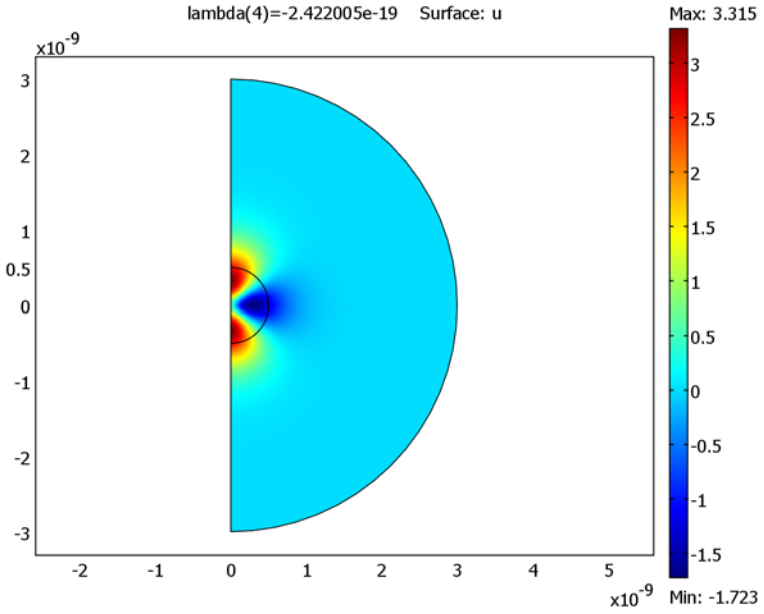
The system's potential energy is

$$V=-\frac{e^2}{4\pi\varepsilon_0 r}$$

where e equals the electron charge (1.602e-19 C), ε_0 represents electric capacitivity in a vacuum (8.854e-12 F/m), and r gives the distance from the center of the atom.

Results

The solution provides a number of the lowest eigenvalues.



Three quantum numbers (n, l, m) characterize the eigenstates of a hydrogen atom:

- n is the principal quantum number.
- l is the angular quantum number.
- m is the magnetic quantum number that appears in the equations above.

These quantum numbers are not independent but have the following mutual relationships:

$$n = 1, 2, 3, \ldots$$
$$0 \le l \le n - 1$$
$$-l \le m \le l.$$

An analytical expression exists for the energy eigenvalues in terms of the quantum number n

$$E_n = -\frac{h^2}{8\pi^2 \mu a_0^2 n^2}$$

where

$$a_0 = \frac{h^2 \varepsilon_0}{\pi \mu e^2}. \tag{11-3}$$

This expression is called the Bohr radius and has an approximate value of $3 \cdot 10^{-11}$ m.

The first three energy eigenvalues, according to the above expression with $\mu \approx m_e$, are:

- $E_1 \approx -2.180 \cdot 10^{-18}$ J
- $E_2 \approx -5.450 \cdot 10^{-19}$ J
- $E_3 \approx -2.422 \cdot 10^{-19}$ J

Comparing these numbers with the computed eigenvalues, you can see a 2-fold degeneracy for $n = 2$ and a 3-fold degeneracy for $n = 3$. This degeneracy corresponds to the following quantum triplets (2,0,0), (2,1,0) and (3,0,0), (3,1,0), (3,2,0). The computed values are separated due to the approximate numerical solution.

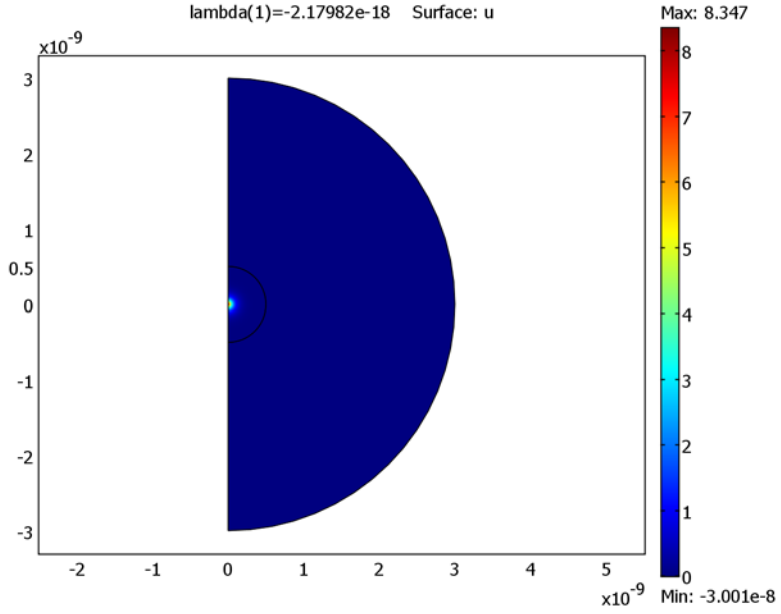
By refining the mesh and solving again, the results are more accurate. The states with $l = 0$ correspond to spherically symmetric solutions, while states with $l = 1$ or 2 correspond to states with one or two radial node surfaces. The 0 energy level corresponds to the energy of a free electron no longer bounded to the nucleus. Energy levels closer to 0 correspond to excited states.

The wave function by itself has no direct physical interpretation. Another quantity to plot is $|u|^2$, which is proportional to the probability density (unnormalized) function $|\Psi|^2$ for the electron position after integration about the z-axis. The plot shows the unnormalized probability density function.

You can now solve the problem for a different integer value of m as well as with a different eigenvalue search range. Remember that high energy levels correspond to large radial components in the solution, so you may have to enlarge the geometry to produce correct results. Also, try to solve the problem using an asymmetric domain.

To determine the ground state energy, use the adaptive solver. Using as many elements as before, the software now adapts the mesh to the first eigenfunction in an attempt to equidistribute the error. This yields an approximation of the ground state energy with

a relative error less than 1e-5, about two orders of magnitude better than the error in the solution using the initial mesh.



Modeling in COMSOL Multiphysics

To solve this problem in COMSOL Multiphysics, reduce the dimension of the problem from three to two by using cylindrical coordinates (ρ, φ, z). The Schrödinger equation transforms into

$$-\frac{h^2}{8\mu\pi^2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+V\Psi = E\Psi$$

and you can write the potential energy as

$$V(\rho,z) = -\frac{e^2}{4\pi\varepsilon_0\sqrt{(\rho^2+z^2)}}.$$

Consider the wave function Ψ as the product of two functions, one with an angular dependence and the other with a radial and z-coordinate dependence,

$$\Psi = \Psi_1(\varphi)\Psi_2(\rho,z)$$

Substituting this expression into the equation gives

$$-\frac{h^2}{8\mu\pi^2}\left(\Psi_1\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi_2}{\partial\rho}\right)+\Psi_2\frac{1}{\rho^2}\frac{\partial^2\Psi_1}{\partial\varphi^2}+\Psi_1\frac{\partial^2\Psi_2}{\partial z^2}\right)+V\Psi_1\Psi_2=E\Psi_1\Psi_2$$

Multiplying by $(8\mu\pi^2/h^2)\rho^2/(\Psi_1\Psi_2)$ and rearranging terms results in

$$-\left(\frac{\rho}{\Psi_2}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi_2}{\partial\rho}\right)+\frac{\rho}{\Psi_2}\frac{\partial}{\partial z}\left(\rho\frac{\partial\Psi_2}{\partial z}\right)\right)+C\rho^2V-C\rho^2E=\frac{1}{\Psi_1}\frac{\partial^2\Psi_1}{\partial\varphi^2},$$

where $C=8\mu\pi^2/h^2$, or equivalently

$$-\left(\frac{\rho}{\Psi_2}(\nabla\cdot(\rho\nabla\Psi_2))\right)+C\rho^2V(\rho,z)-C\rho^2E=\frac{1}{\Psi_1}\frac{\partial^2\Psi_1}{\partial\varphi^2}$$

The left side is independent of φ, and the right side is independent of z and ρ, so the equation is equal to a constant, which you can call $-m^2$. Thus you can split the equation into two parts:

$$-\left(\frac{\rho}{\Psi_2}(\nabla\cdot(\rho\nabla\Psi_2))\right)+C\rho^2V(\rho,z)-C\rho^2E=-m^2$$

and

$$\frac{1}{\Psi_1}\frac{\partial^2\Psi_1}{\partial\varphi^2}=-m^2$$

The equation for Ψ_1 gives the solution

$$\Psi_1=A\sin(m\varphi)+B\cos(m\varphi),$$

where A and B are arbitrary real constants, and $m=0,\pm1,\pm2,\ldots$ due to the periodic boundary condition $\Psi_1(0)=\Psi_2(2\pi k)$, k = any integer.

Using the equation for Ψ_2 with m included and multiplying by Ψ_2/ρ, you arrive at

$$-(\nabla\cdot(\rho\nabla\Psi_2))+\left(C\rho V(\rho,z)+\frac{m^2}{\rho}\right)\Psi_2=C\rho E\Psi_2.$$

The equation now exists in a form that you can immediately transfer into COMSOL Multiphysics. The coordinate variables x and y replace ρ and z, and Ψ_2 becomes u.

COMSOL Multiphysics describes the coefficient form eigenvalue PDE as

$$-\nabla \cdot (c\nabla u + \alpha u) + \beta \nabla u + au = d_a \lambda u \, .$$

For this problem, use the following coefficient values:

$$\begin{cases} c = x \\ a = -C\dfrac{xe^2}{4\pi\varepsilon_0\sqrt{x^2+y^2}} + \dfrac{m^2}{x} \\ d_a = Cx \end{cases}$$

Set all other coefficient values to 0.

The geometry consists of two concentric semicircular solids. The circles have centers at (0, 0) with radii of $3 \cdot 10^{-9}$ m and $5 \cdot 10^{-10}$ m. Remove the portions to the left of the y-axis by subtracting a rectangular solid with corners at $(-1 \cdot 10^{-9}, -1 \cdot 10^{-9})$ and $(0, 1 \cdot 10^{-9})$, to avoid negative x-values, because the use of cylindrical coordinates makes ρ positive.

The boundary conditions are as follows:

- The cylinder axis $x = 0$ is not a boundary in the original problem, but here it becomes one. You must give the artificial boundary condition $\mathbf{n} \cdot (c\nabla u) = 0$. Because $c = 0$ on the cylinder axis, you should not view this boundary condition as a Neumann condition that imposes a constraint. Rather it indicates the absence of constraints.
- On the outer circular boundary, the Dirichlet condition $u = 0$ applies.

The Dirichlet condition corresponds to a zero probability for the electron to be outside the specified domain. This means that the probability of finding the electron inside the domain is 1. It is important to have this approximation in mind when solving for higher-energy eigenvalues because the solution of the physical problem might fall outside the domain, and no eigenvalues are found for the discretized problem. Ideally the domain is infinite and higher-energy eigenvalues correspond to the electron being further away from the nucleus.

Model Library path: `COMSOL_Multiphysics/Quantum_Mechanics/hydrogen_atom`

MODEL NAVIGATOR

1 Select **2D** from the **Space dimension** list.

2 In the list of application modes, open **COMSOL Multiphysics>PDE Modes** and then **PDE, Coefficient Form**.

3 Select **Eigenvalue analysis**. Make sure that **Lagrange - Quadratic** elements are selected in the **Element** list.

4 Click **OK**.

OPTIONS AND SETTINGS

1 Open the **Axes/Grid Settings** dialog box from the **Options** menu.

2 Set axis and grid values:

AXIS		GRID	
x min	-4.5e-9	x spacing	1e-9
x max	4.5e-9	Extra x	
y min	-3.1e-9	y spacing	1e-9
y max	3.1e-9	Extra y	5e-10

3 Open the **Constants** dialog box from the **Options** menu.

4 Enter the following constants and expressions:

NAME	EXPRESSION
me	9.10939e-31
e	1.6021773e-19
hp	6.626076e-34
e0	8.8541878e-12
C	(8*me*pi^2)/hp^2
m	0

These names correspond to the constants m_e, e, h, ε_0, C, and the quantum number m. First set m equal to 0 to catch the ground state energy among the energy eigenvalues.

GEOMETRY MODELING

1 Draw a circle centered at (0, 0) with a radius of $3 \cdot 10^{-9}$.

2 Draw a circle centered at (0, 0) with a radius of $0.5 \cdot 10^{-9}$. Use the tick mark at $y = 0.5 \cdot 10^{-9}$ to assist in placing the radius correctly.

3 Draw a rectangle from $(-3 \cdot 10^{-9}, -3 \cdot 10^{-9})$ to $(0, 3 \cdot 10^{-9})$.

4 From the **Draw** menu, choose **Create Composite Object**.

5 Enter `(C1+C2)-R1` in the **Set formula** edit field.

6 Click **OK**.

PHYSICS SETTINGS

Boundary Conditions

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

2 Enter boundary coefficients as indicated in the table below:

SETTINGS	BOUNDARIES 1–3	BOUNDARIES 4, 7
Type	Neumann	Dirichlet
q	0	0
g	0	0
h		1
r		0

Subdomain Settings

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

2 Enter the following PDE coefficients.

COEFFICIENT	ALL SUBDOMAINS
c	x
a	`-C*(x*e^2)/(4*pi*e0*sqrt(x^2+y^2))+(m^2)/x`
d_a	C*x

MESH GENERATION

Use a finer mesh in the inner circular domain, because the solution shows greater variations in the center region than in the outer regions for low-energy eigenvalues.

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

2 Click the **Custom mesh size** button and type `1.1` in the **Element growth rate** edit field.

3 Click the **Subdomain** tab.

4 Select Subdomain 2 and enter `0.05e-9` in the **Maximum element size** edit field. This ensures that Subdomain 2 (the inner domain) has a finer mesh than the outer subdomain.

5 Click the **Remesh** button.

6 Click **OK**.

COMPUTING THE SOLUTION

1 Open the **Solver Parameters** dialog box from the **Solve** menu.

2 On the **General** page, type `10` in the **Desired number of eigenvalues** edit field.

3 Type `-2e-18` in the **Search for eigenvalues around** edit field.

4 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the lowest energy eigenvalue, or ground state, of approximately $-2 \cdot 10^{-18}$ J.

1 Open the **Plot Parameters** dialog box from the **Postprocessing** menu.

2 Plot some of the eigenfunctions by selecting the corresponding eigenvalue from the **Eigenvalue** list on the **General** page.

3 Click the **Surface** tab.

4 On the **Surface Data** tab, type `abs(u)^2` in the **Expression** edit field.

5 Click **OK** to plot the probability density function.

Finally, try to determine the ground state energy accurately by enabling the adaptive solver. Use approximately as many elements as before, but the solver now adapts the mesh for the first eigenvalue in an attempt to equidistribute the error.

MESH GENERATION

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

2 On the **General** page, click the **Custom mesh size** button and type `1.5` in the **Element growth rate** edit field.

3 Click the **Subdomain** tab and clear the entry in the **Maximum element size** edit field for Subdomain 2.

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

COMPUTING THE SOLUTION

Search for a single eigenvalue using the approximate ground state energy `-2e-18` as shift. This ensures that the eigenvalue solver finds the lowest state.

1. Open the **Solver Parameters** dialog box.
2. On the **General** page, select the **Adaptive mesh refinement** check box.
3. Type `1` in the **Desired number of eigenvalues** edit field.
4. Click the **Adaptive** tab.
5. Type `2500` in the **Maximum number of elements** edit field.
6. Type `10` in the **Maximum number of refinements** edit field.
7. Click **OK**.
8. Click the **Solve** button on the Main toolbar.

12

Semiconductor Device Models

Semiconductor device modeling involve diffusion processes for hole and electron concentrations as well as electric potential distribution. Thermal effects are also a factor. Semiconductor models often include multiphysics couplings and have highly nonlinear material properties, making them difficult to solve.

Distributed SPICE Model of an Integrated Bipolar Transistor

Introduction

Integrated semiconductor devices are used in almost all electrical equipment, and the bipolar junction transistor (BJT) is still a very important device although the MOS technology has taken over a large part of the market. Especially in technologies with new types of semiconductors the bipolar transistor can be the best choice for optimum performance. The BJT consists of three semiconductor layers of alternating dopant type (N-type and P-type) forming an NPN or a PNP structure. These structures can control a large current using a much smaller current.

This particular example describes a high-voltage NPN BJT fabricated from a semiconductor called silicon carbide (SiC). This semiconductor device combines high voltage properties (> 1000 V) and fast switching (> 1 MHz), which is impossible to achieve with comparable silicon devices. The applications for the device are in the drive electronics of electric motors and switched voltage supplies. A higher frequency decreases the size of the passive devices, like inductors and capacitors.

Due to the complicated system of PDEs necessary to calculate the behavior of a semiconductor device, 3D simulations are rather impractical. As a result, most such simulations are performed in 2D, and much effort is put into finding symmetries and removing inactive areas. However, several design considerations need a calculation including the full layout of the device, especially in cases where significant voltage drops from high currents are expected in the metal layers. Further simplifications are therefore necessary, and a powerful approach for BJT structures is to use distributed SPICE expressions on a 2D top view layout of the device.

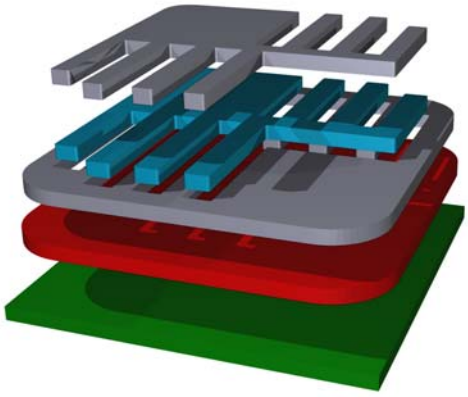


Figure 12-1: 3D view over the layers included in the model. The actual simulation is in 2D, using the top view of this figure.

Model Definition

The potential in each layer obeys the equation

$$\nabla \cdot \left(\frac{W_n}{\rho_n} \nabla V_n \right) = \sum_{m \neq n} J_{n \to m}$$

where W_n is the layer thickness, ρ_n the layer resistivity, and V_n the potential of layer n. The right side is just the sum of all currents going from layer n to layer m. These currents are calculated using SPICE expressions, which is a function on the layer potentials at each point (see Table 12-1 on page 458).

The boundary condition for all boundaries sets the outward current flow to zero.

The electrical connection to the BJT is modeled through point conditions to the base metal and the emitter metal layers. The entire collector layer is connected to a fixed applied voltage through a distributed resistance (models a backside contact). The point conditions can either model a probe tip in on-chip measurements or a bond wire in a packaged device. The emitter point condition is just a constraint to zero volts for the dependent variable of this layer. The base contact condition can either be a constraint on the applied voltage, or a constant current condition. For the latter condition the model uses a point source.

Table 12-1 presents the different SPICE devices along with the expression for each device. Because the devices are distributed, the unit is per area where applicable.

TABLE 12-1: SPICE DEVICES IN THE MODEL

SPICE MODEL	EXPRESSION
Resistor	$J_{n\to m} = (V_n - V_m)/R_{nm}$
Capacitor (trans)	$J_{n\to m} = C_{nm}\frac{d}{dt}(V_n - V_m)$
Capacitor (ac)	$J_{n\to m} = j\omega C_{nm}(V_n - V_m)$
BJT	$J_{b\to e} = \frac{I_{be1}}{B_F} + I_{be2}$ $J_{b\to c} = I_{bc2}$ $J_{c\to e} = \frac{I_{be1}}{K_{qb}}$

Note the following about the expressions above:

- The subscripts n and m denote one of the subscripts e, b, c, or m, depending on the layer the expression refers to.
- The current always has a counterpart representing the flow in the opposite direction.

$$J_{n\to m} = -J_{m\to n}$$

The variables not defined yet are SPICE parameters, which you define as constants in the COMSOL Multiphysics model. The SPICE expressions come from the Gummel-Poon model of the bipolar transistor with a few simplifications (Ref. 1). Because the distributed SPICE model is a transistor with no lateral extension, all parameters referring to lateral losses are ignored (the top view geometry takes the lateral part into account). The voltage dependence on junction capacitance is ignored along with some time constants, because the model is already quite complex. The parameter values are fitted to measurements and device simulations on a silicon carbide BJT fabricated at KTH (The Royal Institute of Technology), Stockholm, Sweden.

Results and Discussion

Figure 12-2 shows the base and collector currents as a function of time when the base is ramped from 2 V to 4 V in 100 ns at a constant collector voltage of 15 V. The figure

reveals that the transistor has no problem to follow the ramp, and only a small overshoot in the base current can be detected after 100 ns.

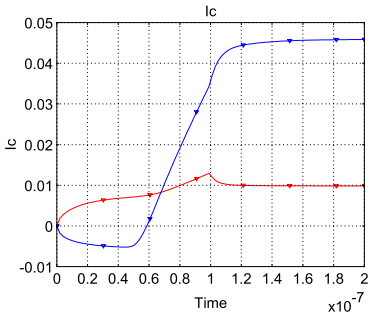


Figure 12-2: Turn on in 100 ns, where the red curve is the base current and the blue curve is the collector current.

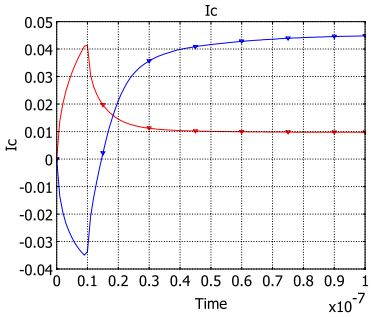


Figure 12-3: Turn on in 10 ns, and now the transistor cannot follow the ramp.

When the rise time is decreased to 10 ns the BJT runs into problems, and Figure 12-3 shows that the actual turn on time is about 30 ns. If faster ramps are required the simulation results have the information about the details on the limiting factors, but in some cases an harmonic simulation is easier to interpret. The plot in Figure 12-4 shows the harmonic component of the collector current density, taken from a harmonic simulation performed at a bias point of 10 mA base current, 15 V collector voltage, and at a 100 MHz frequency. This result shows a significant density beneath the base pad, which does not take part in the current amplification. An improved design would be to use a second metal layer for the pads, resulting in a more efficiently used device area.

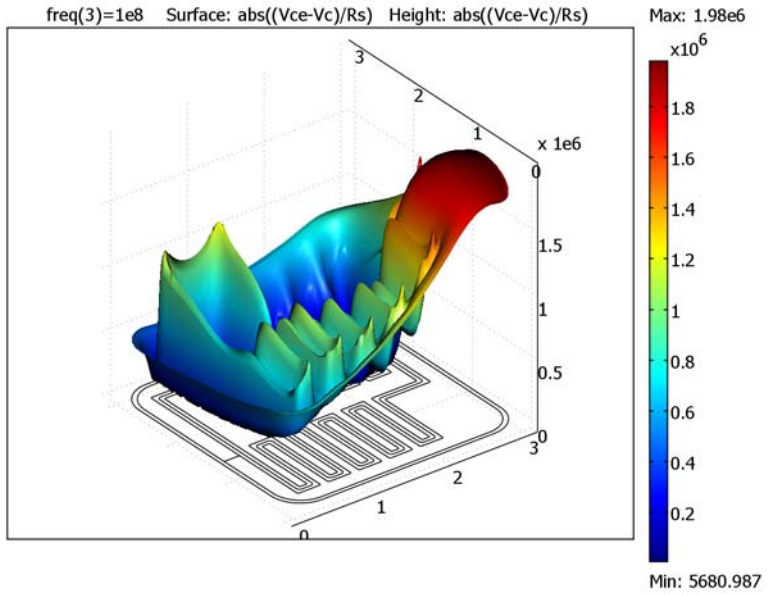


Figure 12-4: The harmonic part of the collector current density at 100 MHz.

These results only qualitatively estimate the switch speed of the device. In an experimental setup, other parasitic elements influence the result (for example, probes, package, and cables). The approximation on the capacitances also affects the result.

Modeling in COMSOL Multiphysics

Use four PDE, General Form application modes—one for each layer—to group the voltages. Within each application mode there are two dependent variables, one for the DC voltage and one for the AC voltage (complex valued).

To model the point current source, use a test function and the weak form settings.

Reference

1. H. K. Gummel and H.C. Poon, "An Integral Charge Control Model of Bipolar Transistors," *The Bell System Technical Journal*, vol. 49, pp. 827–852, 1970.

Model Library path: `COMSOL_Multiphysics/Semiconductor_Devices/bipolar_transistor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Click the **Multiphysics** button in the **Model Navigator**.
2. Select **2D** from the **Space dimension** list.
3. Select the **COMSOL Multiphysics>PDE Modes>PDE, General Form** application mode. In the **Dependent variables** edit field, enter the names of the variables: `Vm_dc Vm_ac`. Enter `metal` as the application mode name, and select the **Lagrange - Linear** element. Click the **Add** button to add the mode to the model.
4. Add the second application mode of the same type and with the same element. Use the variable names: `Ve_dc Ve_ac`. Enter `emitter` as the application mode name.
5. Add the third application mode of the same type and with the same element. Use the variable names: `Vb_dc Vb_ac`. Enter `base` as the application mode name.
6. And finally, add the fourth application mode of the same type and with the same element. Use the variable names: `Vc_dc Vc_ac`. Enter `collector` as the application mode name.
7. Click **OK**.

OPTIONS AND SETTINGS

1. In the **Constants** dialog box, enter the following variable names and expressions. The variable `t` does not affect the time-dependent simulation, because the model uses the internal time variable.

NAME	EXPRESSION	DESCRIPTION
`Vbe`	`2.0`	Applied base-emitter voltage (V)
`Vbe_on`	`4.0`	Final voltage in transient simulations (V)
`t_rise`	`10e-9`	Rise time to reach Vbe_on (s)
`Vce`	`15`	Applied collector-emitter voltage (V)
`Vac`	`1`	Applied AC voltage (V)
`Ib_a`	`0.0`	Base current forced into base contact (A)

NAME	EXPRESSION	DESCRIPTION
Vt	0.0259	Thermal voltage
freq	10e6	Frequency (Hz)
omega	2*pi*freq	Angular frequency (rad/s)
Wb	0.3e-6	Thickness of base layer (m)
We	0.5e-6	Thickness of emitter layer (m)
Ws	0.5e-6	Thickness of sub-collector layer (m)
Wm	0.2e-6	Thickness of metal layer (m)
rhoB0	4.54e-3	Max resistivity of base layer (Ω·m)
rhoBm	0.783e-3	Min resistivity of base layer (Ω·m)
rhoE	0.293e-3	Resistivity of emitter layer (Ω·m)
rhoS	0.290e-3	Resistivity of sub-collector layer (Ω·m)
rhoM	1e-6	Resistivity of metal layer (Ω·m)
Cbe	3.29e-3	Base-emitter capacitance (F/m^2)
Cbc	3.38e-3	Base-collector capacitance (F/m^2)
Rbm	1e-9	Resistance between metal and base layer ($\Omega \cdot m^2$)
Rem	1e-10	Resistance between metal and emitter layer ($\Omega \cdot m^2$)
Rs	7e-8	Resistance between the collector layer and the backside ($\Omega \cdot m^2$)
Nf	1.0	Base-emitter ideality factor
Ne	1.2	Base-emitter second ideality factor
Nc	1.0	Base-collector ideality factor
Nk	0.867	Beta roll-off power factor
Vaf	979	Forward Early voltage (V)
Bf	27.0	Forward current gain
Is	9.37e-42	Base-emitter saturation current (A/m^2)
Isc	1.91e-42	Base-collector saturation current (A/m^2)
Ise	9.7e-35	Base-emitter second saturation current (A/m^2)
Ikf	2.98e7	Beta roll-off current (A/m^2)
t	0.0	Time for stationary solutions

2 In the **Scalar Expressions** dialog box, enter the following expressions.

NAME	EXPRESSION	DESCRIPTION
Ibc2	Isc*exp((Vb-Vc)/(Nc*Vt))	Base-collector current ($A \cdot m^2$)
Kq1	1/(1-(Vb-Vc)/Vaf)	Voltage dependent factor

NAME	EXPRESSION	DESCRIPTION
Kq2	Ibe1/Ikf	Current dependent factor
Kqb	Kq1/2*(1+(1+4*Kq2)^Nk)	Current and voltage dependent factor
rhoB	rhoBm+(rhoB0-rhoBm)/Kqb	Current dependent base resistivity ($\Omega \cdot m^2$)
Vbe_t	Vbe+(t/t_rise*(t<t_rise)+(t>=t_rise))*(Vbe_on-Vbe)	Ramping of Vbe to final voltage (V)
Vm	Vm_ac+Vm_dc	Total metal layer potential (V)
Vmx	Vm_acx+Vm_dcx	X-derivative of layer potential (V/m)
Vmy	Vm_acy+Vm_dcy	Y-derivative of layer potential (V/m)
Ve	Ve_ac+Ve_dc	Total emitter layer potential (V)
Vex	Ve_acx+Ve_dcx	X-derivative of layer potential (V/m)
Vey	Ve_acy+Ve_dcy	Y-derivative of layer potential (V/m)
Vb	Vb_ac+Vb_dc	Total base layer potential (V)
Vbx	Vb_acx+Vb_dcx	X-derivative of layer potential (V/m)
Vby	Vb_acy+Vb_dcy	Y-derivative of layer potential (V/m)
Vc	Vc_ac+Vc_dc	Total collector layer potential (V)
Vcx	Vc_acx+Vc_dcx	X-derivative of layer potential (V/m)
Vcy	Vc_acy+Vc_dcy	Y-derivative of layer potential (V/m)
Jbc_ac	j*omega*Cbc*(Vb_ac-Vc_ac)	

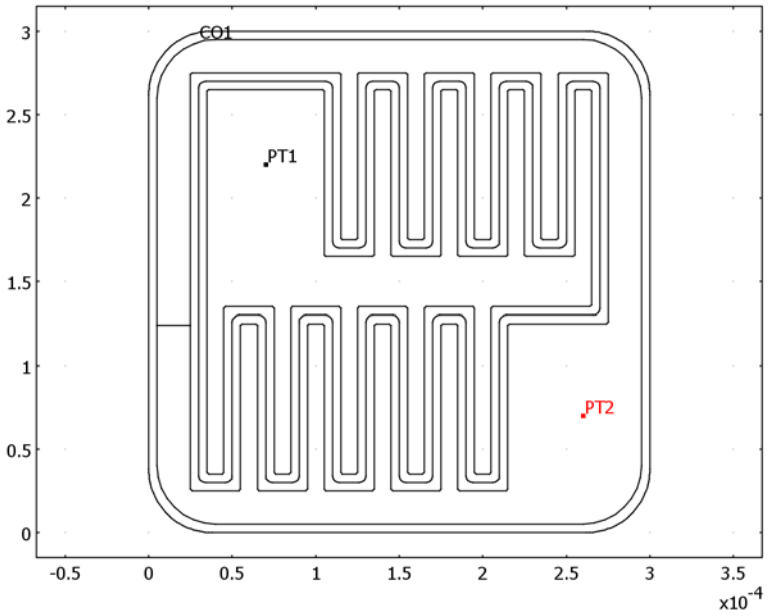
GEOMETRY MODELING

The geometry is constructed from a layout drawing in the GDS file format, which is the most common format used in the fabrication process of reticles for lithography equipment. The file format can be converted to a DXF file and imported to COMSOL Multiphysics. The spatial unit in the GDS file are given in nanometers (nm). Because the length unit in COMSOL Multiphysics is meters and not nanometers, you must scale the geometry.

1. In the **File** menu, select **Import** and choose **CAD Data From File**. Click **Browse** and select the file `bipolar_transistor.dxf`, which you find in the `models/COMSOL_Multiphysics/Semiconductor_Devices` folder. Click **Import**.
2. Click the **Coerce to Solid** button on the Draw toolbar to make it a solid geometry.
3. On the **Draw** menu, point to **Modify**, and then click **Scale**. In the **x** and **y** scale factor edit fields, type the value `1e-9`. Click **OK**.
4. Click the **Zoom Extents** button on the Main toolbar.

5 Choose **Draw>Specify Objects>Point**. In the **Point** dialog box, type `70e-6` in the **x** edit field and `220e-6` in the **y** edit field in the **Coordinates** area. Click **OK**. This defines the point PT1 at the location of the emitter.

6 Choose **Draw>Specify Objects>Point**. In the **Point** dialog box, type `260e-6` in the **x** edit field and `70e-6` in the **y** edit field in the **Coordinates** area. Click **OK**. This defines the point PT2 at the location of the base.



PHYSICS SETTINGS

To simplify the expressions in the subdomains and in the postprocessing, do the following steps:

1 In the **Subdomain Expressions** dialog box, type the following expressions for the given subdomains.

NAME	EXPRESSION	SUBDOMAIN	DESCRIPTION
`Ibe1`	`Is*exp((Vb-Ve)/(Nf*Vt))`	4, 5	`Base-emitter current`
`Ibe2`	`Ise*exp((Vb-Ve)/(Ne*Vt))`	4, 5	`2nd base-emitter current`
`Jbe_ac`	`j*omega*Cbe*(Vb_ac-Ve_ac)`	4, 5	`Harmonic base-emitter current`

2 Select Subdomains 1–3, and the enter `0` in all three edit fields in the **Expression** columns to make all expression variables equal to zero in those subdomains.

3 In the **Subdomain Integration Variables** dialog box, type the expressions given in the table below.

NAME	EXPRESSION	SUBDOMAIN	DESCRIPTION
Ib	(Vm-Vb)/Rbm	2	Base current
Ic	(Vce-Vc)/Rs	all	Collector current
Ie	(Vm-Ve)/Rem	5	Emitter current

Boundary Conditions

All boundaries should be of Neumann type with all parameters set to zero.

1 Select the **PDE, General Form (metal)** application mode from the **Multiphysics** menu.

2 Open the **Boundary Settings** dialog box.

3 Select all boundaries and select the **Neumann boundary condition**.

4 Select each of the other modes from the **Multiphysics** menu and do the same operations there.

Subdomain Settings (Point Settings, Edge Settings)

There are five subdomains with somewhat different settings.

1 Select the **PDE, General Form (metal)** application mode from the **Multiphysics** menu.

2 Open the **Subdomain Settings** dialog box.

3 Select Subdomains 1, 3, and 4 and then clear the **Active in this domain** check box.

4 Enter the expressions for the Γ, F, and d_a coefficients according to the three tables below and click **OK**.

SETTINGS	SUBDOMAINS 2, 5	
Γ_1	Wm/rhoM*Vmx	Wm/rhoM*Vmy
Γ_2	Wm/rhoM*Vmx	Wm/rhoM*Vmy

SETTINGS	SUBDOMAIN 2	SUBDOMAIN 5
F_1	(Vm-Vb)/Rbm	(Vm-Ve)/Rem
F_2	(Vm-Vb)/Rbm	(Vm-Ve)/Rem

SETTINGS	SUBDOMAINS 2, 5	
$d_{a,1}$	0	0
$d_{a,2}$	0	0

5 Select the **PDE, General Form (emitter)** application mode from the **Multiphysics** menu.

6 Open the **Subdomain Settings** dialog box, select Subdomains 1–3 and clear the **Active in this domain** check box.

7 Enter the expressions for the other subdomains according to the tables below and click **OK**.

SETTINGS	SUBDOMAINS 4, 5	
Γ_1	`We/rhoE*Vex`	`We/rhoE*Vey`
Γ_2	`We/rhoE*Vex`	`We/rhoE*Vey`

SETTINGS	SUBDOMAIN 4	SUBDOMAIN 5
F_1	`-(Ibe1/Bf+Ibe2+Ibe1/Kqb)`	`(Ve-Vm)/Rem-(Ibe1/Bf +Ibe2+Ibe1/Kqb)`
F_2	`-(Ibe1/Bf+Ibe2+Ibe1/Kqb) -Jbe_ac`	`(Ve-Vm)/Rem-(Ibe1/Bf +Ibe2+Ibe1/Kqb)-Jbe_ac`

SETTINGS	SUBDOMAINS 4, 5	
$d_{a,1}$	`-Cbe`	0
$d_{a,2}$	0	0

8 Select the **PDE, General Form (base)** application mode from the **Multiphysics** menu.

9 Open the **Subdomain Settings** dialog box. Enter the expressions for the subdomains according to the tables below, and click **OK**.

SETTINGS	ALL SUBDOMAINS	
Γ_1	`Wb/rhoB*Vbx`	`Wb/rhoB*Vby`
Γ_2	`Wb/rhoB*Vbx`	`Wb/rhoB*Vby`

SETTINGS	SUBDOMAINS 1, 3	SUBDOMAIN 2	SUBDOMAINS 4, 5
F_1	`Ibc2`	`Ibc2+(Vb-Vm)/Rbm`	`Ibc2+Ibe1/Bf+Ibe2`
F_2	`Ibc2+Jbc_ac`	`Ibc2+(Vb-Vm)/Rbm+Jbc_ac`	`Ibc2+Ibe1/Bf+Ibe2+ Jbe_ac+Jbc_ac`

SETTINGS	SUBDOMAINS 1–3		SUBDOMAINS 4, 5	
$d_{a,1}$	-Cbc	0	-Cbe-Cbc	0
$d_{a,2}$	0	0	0	0

10 Select the **PDE, General Form (collector)** application mode from the **Multiphysics** menu.

11 Open the **Subdomain Settings** dialog box. Enter the expressions for the subdomains according to the tables below, and click **OK**.

SETTINGS	ALL SUBDOMAINS	
Γ_1	Ws/rhoS*Vcx	Ws/rhoS*Vcy
Γ_2	Ws/rhoS*Vcx	Ws/rhoS*Vcy

SETTINGS	SUBDOMAINS 1–3	SUBDOMAINS 4,5
F_1	-Ibc2+(Vc-Vce)/Rs	-Ibc2+(Vc-Vce)/Rs+Ibe1/Kqb
F_2	-Ibc2+(Vc-Vce)/Rs-Jbc_ac	-Ibc2+(Vc-Vce)/Rs+Ibe1/Kqb -Jbc_ac

SETTINGS	ALL SUBDOMAINS	
$d_{a,1}$	-Cbc	0
$d_{a,2}$	0	0

You must also specify the settings at the two points representing the probe or bond wire connections.

1 Select the **PDE, General Form (metal)** application mode from the **Multiphysics** menu.

2 Open the **Point Settings** dialog box.

3 Enter the point expressions (weak form terms and constraints) according to the following table:

SETTINGS	POINT 133	POINT 413
weak	0 0	-Ib_a*Vm_dc_test 0
constr	Vm_dc Vm_ac	(Vbe_t-Vm_dc)*(Ib_a=0) Vac-Vm_ac

Finally add some cross time-derivative terms, which you cannot specify from the **Subdomain Settings** dialog box. Use the equation-system settings for this.

1 Open the **Subdomain Settings - Equation System** dialog box by selecting **Physics>Equation System>Subdomain Settings**.

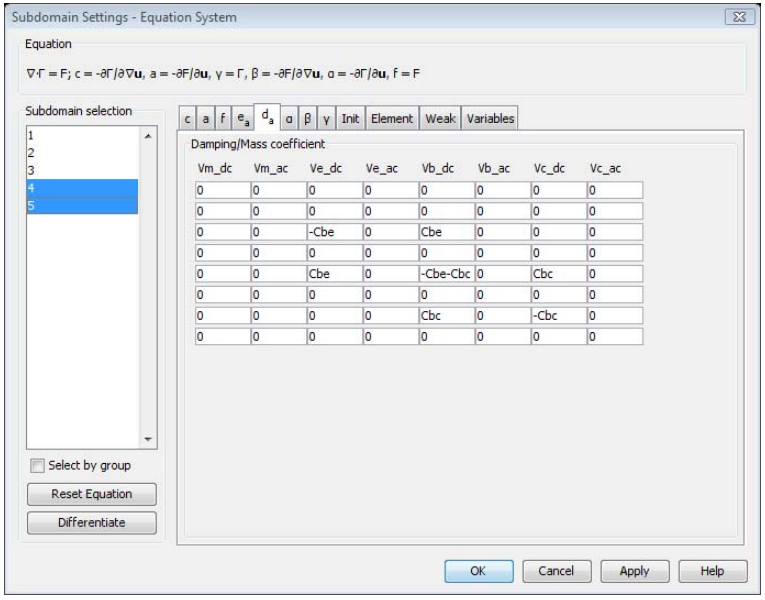
2 Click the $\mathbf{d}_a$ tab and select Subdomains 1–3. Enter the fields specified in the table below. Leave all other existing expressions as is.

ROW NUMBER	COLUMN NUMBER	EXPRESSION
5	7	Cbc
7	5	Cbc

3 Select Subdomains 4 and 5 and fill in the fields specified below.

ROW NUMBER	COLUMN NUMBER	EXPRESSION
3	5	Cbe
5	3	Cbe
5	7	Cbc
7	5	Cbc

4 Click **OK**. Now the settings in this dialog box determine the subdomain settings, which means that the software ignores all changes in the **Subdomain Settings** dialog box from now on. COMSOL Multiphysics indicates this with a padlock symbol next to all subdomain numbers. By clicking the **Reset Equation** button in the **Subdomain Settings - Equation System** dialog box, you set all parameters according to the **Subdomain Settings** dialog box and it is possible to do changes there again.



Initial Conditions

To speed up the DC simulation, the initial conditions of the metal, base, and collector layer can be set equal to the constant variables, `Vbe` and `Vce`. Due to the changes in the **Subdomain Settings - Equation System** dialog box, you must specify all the initial conditions there.

1. Open the **Subdomain Settings - Equation System** dialog box, and click the **Init** tab.
2. Select Subdomain 2 and type `Vbe` in the **Vm_dc(t_0)** edit field.
3. Select all subdomains and type `Vbe` in the **Vb_dc(t_0)** edit field and `Vce` in the **Vc_dc(t_0)** edit field.
4. Click **OK**.

MESH GENERATION

Due to the small features in the defined geometry, it is possible to make the mesh coarser than the default.

1. In the **Mesh** menu, open the **Free Mesh Parameters** dialog box.
2. Select the **Coarser** predefined mesh size.
3. Click the **Boundary** tab, select all boundaries that is part of the finger structure of the emitter and base, and enter `4e-6` in the **Maximum element size** edit field.
4. Click the **Remesh** button.
5. Click **OK**.

COMPUTING THE SOLUTION (TIME-DEPENDENT)

This sequence first finds the initial solution and then continues with the time-dependent simulation.

1. Open the **Solver Manager** dialog box.
2. Click the **Initial value expression** button in the **Initial value** area.
3. Click the **Solve For** tab and expand all modes. Select all DC variables (ending with `_dc`). This makes the solver leave the AC application mode variables unchanged. Click **OK**.
4. Click the **Solve** button on the Main toolbar.
5. When the solution has been found, open the **Solver Manager** dialog box again.
6. Click the **Initial Value** tab. Click the **Store Solution** button, and then click the **Stored solution** button in the **Initial value** area to use the stored solution as the initial value. Click **OK**.

7 Open the **Solver Parameters** dialog box, and select the **Time dependent** solver. In the **Times** edit field, type `0 1e-6`. To avoid large time steps, type `1e-3` in the **Relative tolerance** edit field and `5e-4` in the **Absolute tolerance** edit field.

8 Click the **Time Stepping** tab, and select **Time steps from solver** from the **Times to store in output** list.

9 Click **OK**, then click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION (TIME-DEPENDENT)

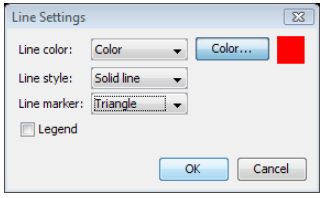
Use the defined coupling variables to plot the base and collector currents versus time:

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

2 Under the **General** tab select **Point plot**. In the **Solutions to use** area, select **Interpolated times** from the **Select via** list. In the **Times** edit field, type `range(0,1e-9,1e-7)`.

3 Click the **Point** tab and type `Ib` in the **Expression** edit field. Select Point 413 (for example by clicking on the point in the middle of the base pad).

4 Click the **Line Settings** button. In the **Line Settings** dialog box, select **Color** from the **Line color** list, and select **Triangle** from the **Line marker** list. Click the **Color** button and select red from the palette. Click **OK**.

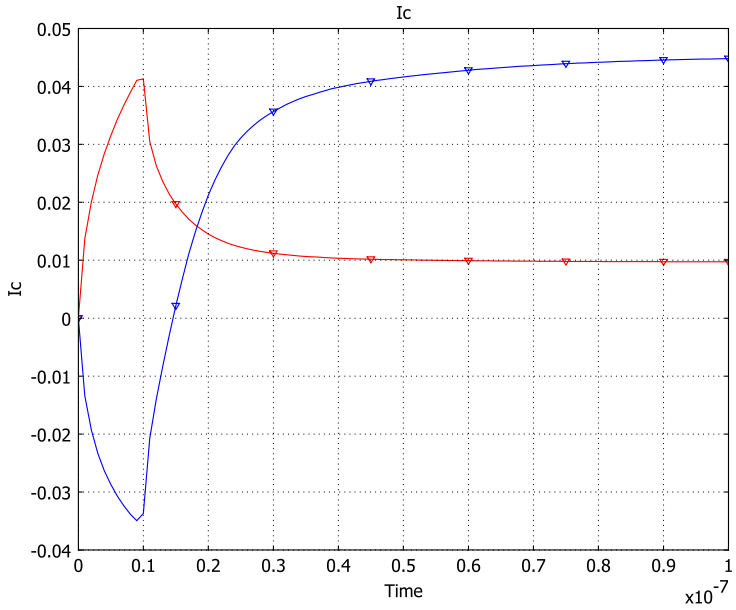


5 In the **Domain Plot Parameters** dialog box, click **Apply** to view the base current.

6 Click the **General** tab and select the **Keep current plot** check box.

7 Go back to the **Point** page and type `Ic` in the expression edit field.

8 Change the color to blue and click the **OK** button. You now get the figure below, which shows how the currents behave during turn on.



COMPUTING THE SOLUTION (TIME-HARMONIC)

This sequence first finds a stationary solution for a base current of 10 mA and then uses this solution as the linearization point for the time-harmonic simulation:

1 Open the **Constants** dialog box from the **Options** menu. Change the variable `Vbe` to `2.5`. Click **OK**. This gives a better initial condition for the constant current solution.

2 Open the **Solver Parameters** dialog box. Select the **Parametric** in the **Solver** list.

3 Type `Ib_a` in the **Parameter names** edit field and `1e-2` in the **Parameter values** edit field. Click **OK**.

4 Open the **Solver Manager** dialog box and select the **Initial value expression** option in the **Initial value** area. Click **OK**.

5 Click the **Solve** button.

6 When the analysis has finished, open the **Solver Manager** dialog box again.

7 Click the **Store Solution** button, and select the solution for the value of 0.01 in the **Parameter value** list. Click **OK**. In the **Values of variables not solved for and linearization point** area, click the **Stored solution** option button.

8 Under the **Solve For** tab, expand all modes, deselect all dc variables and select all ac variables (ending with `_ac`). Click **OK**.

9 Open the **Solver Parameters** dialog box, and select **Parametric** in the **Solver** list.

10 Enter `freq` in the **Parameter names** edit field, and enter the values `1e6 1e7 1e8` in the **Parameter values** edit field.

11 Click the **Stationary** tab. Select **Linear** in the **Linearity** list to ensure that the parametric sweep uses the linear solver.

12 Click **OK**.

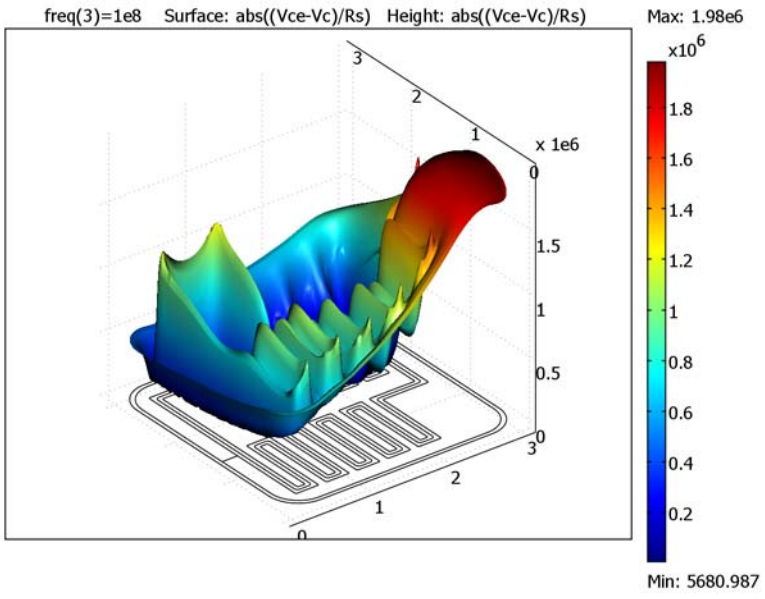
13 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION (TIME-HARMONIC)

1 Open the **Plot Parameters** dialog box.

2 Click the **Surface** tab and make sure that the **Surface plot** and (on the **Height Data** page) **Height data** check boxes are selected. Type `abs((Vce-Vc)/Rs)` in the **Expression** edit fields on the **Surface Data** and **Height Data** pages. Click **OK**.

3 Click the **Headlight** button on the Camera toolbar to the left to make the plot look nicer. The plot should now look like the following figure. Notice the high collector current density under the base pad.

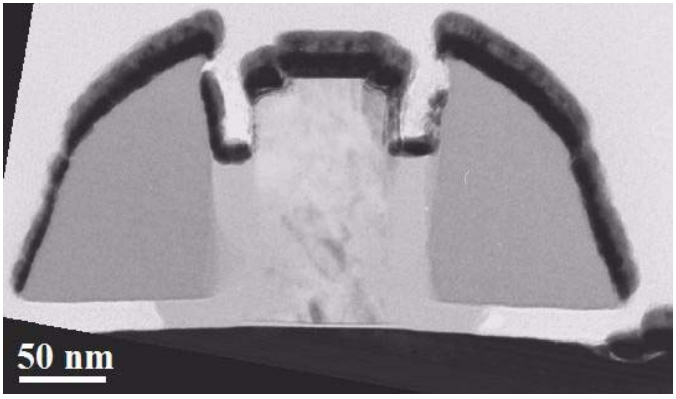


DC Characteristics of a MOS Transistor (MOSFET)

This model calculates the DC characteristics of a MOS (metal-oxide semiconductor) transistor using standard semiconductor physics. In normal operation, a system turns on a MOS transistor by applying a voltage to the gate electrode. When the voltage on the drain increases, the drain current also increases until it reaches saturation. The saturation current depends on the gate voltage.

Introduction

The MOSFET (metal oxide semiconductor field-effect transistor) is by far the most common semiconductor device, and the primary building block in all commercial processors, memories, and digital integrated circuits. During the past decades this device has experienced tremendous development, and today it is being manufactured with feature sizes of 90 nm and smaller.



Cross-section TEM (transmission electron microscope) image of a 70-nm MOSFET fabricated in the clean room at the Royal Institute of Technology in Kista, Sweden (a project of P.-E. Hellström and others).

This model shows the basic functionality of a MOS transistor, where the gate voltage controls the drain-source resistance and thus the drain current. At a certain gate voltage, V_{GS}, and at low drain voltages, the drain current is almost linearly dependent

on the drain voltage. When the drain voltage increases, the drain current saturates. The level of saturation depends on the gate voltage.

The gate voltage also influences the coefficient describing the linear dependence between the gate voltage and gate current at low drain voltages. This coefficient is generally known as the On resistance (R_{on}). In digital devices the transistor operates as a switch, making R_{on} an important parameter influencing the transistor's power loss and driving ability. Its ability to drive an output is of special importance. This characteristic is described by the *fanout*, the number of outputs that a device can drive. In high-speed systems, parasitic effects make the situation more complicated.

Model Definition

DEVICE GEOMETRY

The structure in Figure 12-5 is a cross section of a simplified MOS transistor. The electric field in the gate influences the low-doped p-type silicon; specifically, at a certain gate voltage a thin layer of it, close to the silicon-oxide surface, turns into an n-type material. This process, called inversion, creates a conducting channel between the highly doped n-type source and the drain regions. With this channel present, a voltage across the source and the drain drives a drain current. This model uses the following dimensions: a gate length of 0.2 μm, a gate oxide thickness of 5 nm, and a source-drain junction depth of 0.1 μm.

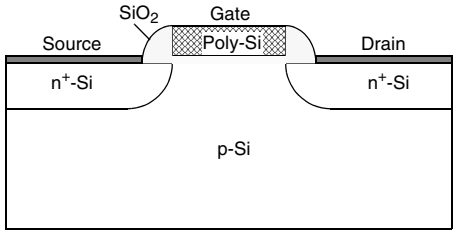


Figure 12-5: The model geometry. The simulation replaces the contacts with boundary conditions.

DOMAIN EQUATIONS

This example models a MOS transistor using the standard drift-diffusion approximation coupled with Poisson's equation. With the aid of some generally accepted simplifications—such as neglecting magnetic fields, assuming a constant density of states in both the valence and the conductance bands, and assuming a

Boltzmann distribution of the carriers—it is possible to derive these equations from Maxwell's equations and Boltzmann transport theory.

The model in this example formulates the problem using three dependent variables: ψ (the electrostatic potential), n, and p. The three basic semiconductor equations are

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi) &= q(p - n + N) \\ -\nabla \cdot \mathbf{J}_\mathrm{n} &= -qR_\mathrm{SRH} \\ -\nabla \cdot \mathbf{J}_\mathrm{p} &= qR_\mathrm{SRH} \end{aligned}$$

where p and n are the hole and electron concentrations, respectively, and N represents the fixed charge associated with ionized donors.

You can express the electron and hole current densities, $\mathbf{J}_\mathrm{n}$ and $\mathbf{J}_\mathrm{p}$, with a drift term and a diffusion term

$$\begin{aligned} \mathbf{J}_\mathrm{n} &= -qn\mu_\mathrm{n}\nabla\psi + qD_\mathrm{n}\nabla n \\ \mathbf{J}_\mathrm{p} &= -qp\mu_\mathrm{p}\nabla\psi - qD_\mathrm{p}\nabla p \end{aligned}$$

where μ_n and μ_p are the carrier mobilities, and D_n and D_p are the carrier diffusivities.

Another term, R_SRH, represents the *Shockley-Read-Hall recombination*, which is a general recombination process using traps constituting energy levels in a semiconductor's forbidden band gap. In the recombination equation

$$R_\mathrm{SRH} = \frac{np - n_i^2}{\tau_\mathrm{p}(n + n_1) + \tau_\mathrm{n}(p + p_1)}$$

n_i is the intrinsic carrier concentration, τ_n and τ_p are the carrier lifetimes, and n_1 and p_1 are parameters related to the trap energy level. If that level is located in the middle of the band gap (which this model assumes), then n_1 and p_1 equal the intrinsic carrier concentration, n_i.

BOUNDARY CONDITIONS

For boundaries in contact with an insulator or far away from the active device area, you can use the symmetry or zero charge (flux) boundary condition for the electrostatic (diffusion) problem. At boundaries in contact with a metal, the electrostatic potential is fixed. Assuming infinite recombination velocity at the contact, the mass action law

$$n_i^{\,2} = np$$

is valid. Using this law along with the assumption that there is no charge at the contact, it is possible to calculate the carrier concentrations. The applied voltage equals the Fermi level in the semiconductor at the contact, so the electrostatic potential at the contact is the applied voltage plus the potential difference between the Fermi level and the electrostatic reference level:

$$\psi = V_a - \chi_{Si} - \frac{E_G}{2} + \frac{kT}{q}\ln\left(\frac{\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}}{n_i}\right)$$

$$n = \frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

$$p = -\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

where V_a is the applied voltage. In this model the reference potential is the vacuum level. This is often a good choice when several materials with different affinities or work functions are present. As a result, the electrostatic potential is continuous across all material interfaces. This reference level also finds use in heterojunction device simulations. The band diagram in Figure 12-6 shows how this model represents the metal-oxide semiconductor material system.

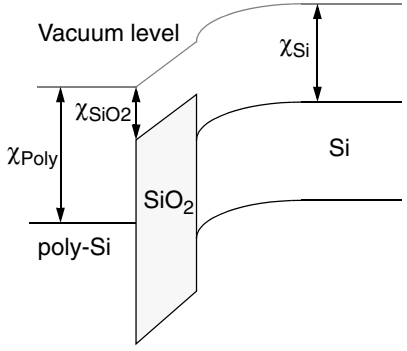


Figure 12-6: A band diagram of the MOS material system. The necessary parameters to align the materials are the affinities of the oxide and semiconductor, plus the work function of the polysilicon gate, which this model assumes has the same properties as aluminum.

The material parameters in the MOS transistor are:

NOTATION	VARIABLE	VALUE
n_i(Si)	ni_Si	$1.46 \cdot 10^{10}$ cm^{-3} (T = 300K)
ε_r(Si)	epsilonr_Si	11.8
ε_r(SiO2)	epsilonr_Si	4.2
μ_n(Si)	mun	1000 cm^2/Vs (low concentration)
μ_p(Si)	mup	500 cm^2/Vs (low concentration)
$D_n = \mu_n(\text{Si})\, kT/q$	Dn	20.7 cm^2/s
$D_p = \mu_p(\text{Si}) kT/q$	Dp	5.17 cm^2/s
τ_n	taun	~0.1 µs
τ_p	taup	~0.1 µs
E_G(Si)	Eg_Si	1.08 eV
χ_{Si}	X_Si	4.0 eV
χ_{SiO2}	X_SiO2	0.3 eV
χ_{poly}	X_poly	4.2 eV

INITIAL-VALUE CALCULATION

The rapid changes and large dynamics of the solution variables in the PDEs require a special technique to calculate the initial value. This model solves an extra electrostatics application mode separately to get the initial value for the other application modes. This extra application mode also solves Poisson's equation but with the difference that it replaces the carrier concentrations with the formulas

$$n = n_i e^{\frac{q\psi + \chi_{Si} + \frac{E_G}{2}}{kT}}$$

$$p = n_i e^{-\frac{q\psi + \chi_{Si} + \frac{E_G}{2}}{kT}}$$

This step produces the exact solution for the full system when all applied voltages are zero. You perform the steps to get the initial condition with the solver sequence functionality in the **Solver Manager** dialog box.

Results and Discussion

The system's nonlinear behavior makes it necessary to use the parametric solver to reach the desired voltage for each contact. This example first raises the gate voltage to 0.8 V and then sweeps the drain voltage to 1 V. Including the first initial-value calculation, three solution steps are necessary, and by defining a solver sequence you can execute all of them with one click on the **Solve** button. The result from the last step appears in Figure 12-7.

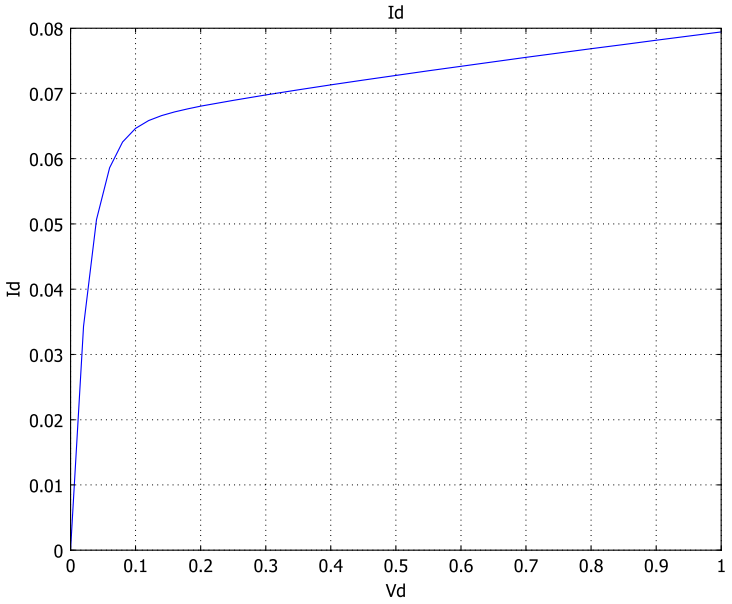


Figure 12-7: Drain current as a function of drain voltage for V_{GS} *= 0.8 V. Note that* R_{on} *is 1/(slope of the curve) at the point where* V_{DS} *= 0, which falls at the far left of the curve.*

A surface plot is useful to view the shape of the solution variables. Figure 12-8 shows the electrostatic potential at the final bias condition. The large negative shift for the potential is due to the vacuum reference potential.

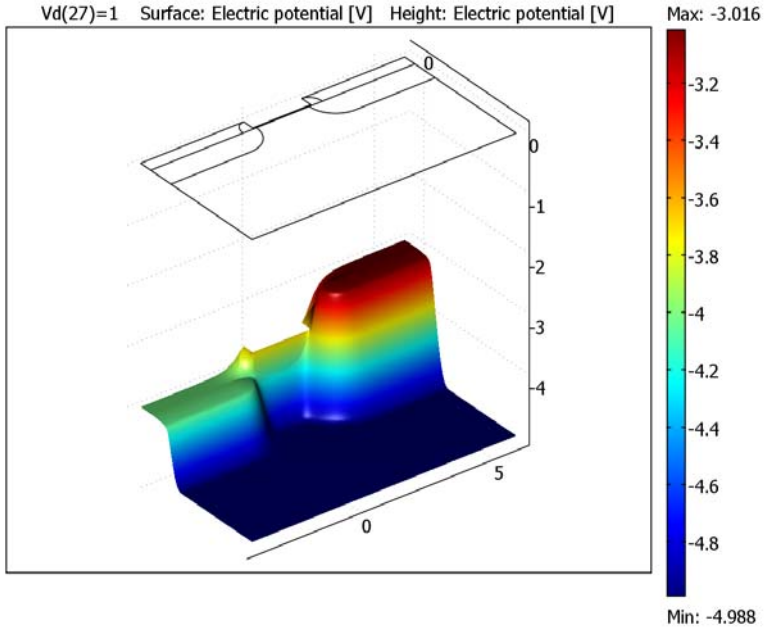


Figure 12-8: Surface plot of the electrostatic potential inside the MOSFET.

The conducting channel at the oxide-semiconductor interface becomes visible in a logarithmic surface plot of the electron concentration (Figure 12-9).

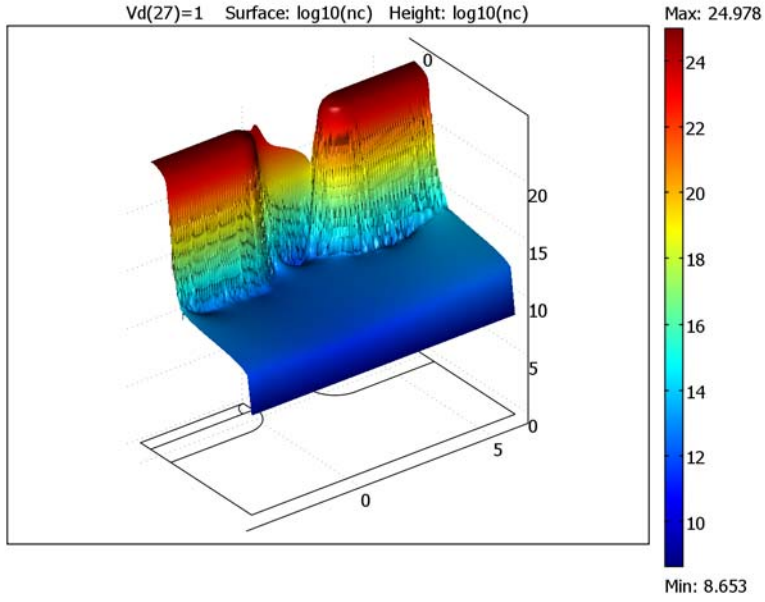


Figure 12-9: The channel close to the interface becomes visible in an electron-concentration plot. Notice the sharp drop in the channel concentration close to the drain contact, which is responsible for the saturation of the drain current.

Model Library path: `COMSOL_Multiphysics/Semiconductor_Devices/mos_transistor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** from the **Space dimension** list.
2. Click the **Multiphysics** button.
3. Select the application mode **COMSOL Multiphysics>Electromagnetics>Electrostatics**.
4. Enter `phi0` in the **Dependent variables** edit field, and enter `init` in the **Application mode name** edit field.

5 Click **Add**.

6 Enter `phi` in the **Dependent variables** edit field.

7 Click **Add**.

8 Select the application mode **COMSOL Multiphysics>Convection and Diffusion> Convection and Diffusion>Steady-state analysis**.

9 Enter `nc` in the **Dependent variables** edit field, and enter `cde` in the **Application mode name** edit field.

10 Click **Add**.

11 Click the **Application Mode Properties** button, select **Conservative** from the **Equation form** list and **On** from the **Weak constraints** list. Click **OK**.

12 Enter `pc` in the **Dependent variables** edit field, and enter `cdh` in the **Application mode name** edit field.

13 Click **Add**.

14 Click the **Application Mode Properties** button, select **Conservative** from the **Equation form** list and **On** from the **Weak constraints** list. Click **OK**.

15 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, define the following constants with names, expressions, and descriptions (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
q	1.602e-19[C]	Elementary charge
T0	300[K]	Lattice temperature
k	1.38e-23[J/K]	Boltzmann's constant
epsilonr_si	11.8	Rel. permittivity for Si
epsilonr_sio2	4.2	Rel. permittivity for SiO2
ni	1.5e10[1/cm^3]	Intrinsic carrier concentration for Si
mun_si	1000[cm^2/(V*s)]	Electron mobility for Si
mup_si	500[cm^2/(V*s)]	Hole mobility for Si
X_si	4.0[V]	Electron affinity for Si
X_sio2	0.3[V]	Electron affinity for SiO2
X_poly	4.5[V]	Work function for poly-Si

NAME	EXPRESSION	DESCRIPTION
Eg_si	1.08[V]	Band gap of Si
taun	0.1[um]	Electron carrier life time
taup	0.1[um]	Hole carrier life time
Vt	k*T0/q	Thermal voltage
x1	-0.1[um]	Help coordinate
x2	0.2[um]	Help coordinate
yj	0.1[um]	Junction depth
NDimpl	1e19[1/cm^3]	Peak concentration of implanted profile
NAsub	5e17[1/cm^3]	Substrate doping
ch	yj/sqrt(log(NDimpl/NAsub))	Characteristic length of implanted region
Vg	0.8[V]	Gate voltage
Vd	0[V]	Drain voltage

3 Click **OK**.

4 From the **Options** menu, choose **Functions**.

5 In the **Functions** dialog box, click the **New** button.

6 In the **New Function** dialog box, type `flgauss` in the **Function name** edit field. Click **OK** to create the new function.

7 Type `x, y, x1, y1, ch` in the **Arguments** edit field, and type the following in the **Expression** edit field: `(exp(-((y-y1)/ch)^2)*(y<y1)+(y>=y1))* (exp(-((x-x1)/ch)^2)*(x>x1)+(x<=x1))`.

8 In the **Derivatives** area, click the **Manual** button and type `d(flgauss(x,y,x1,y1,ch),x),d(flgauss(x,y,x1,y1,ch),y),0,0,0` in the corresponding edit field. The operator `d` provides differentiation of the `flgauss` function with respect to `x` and `y`. The derivatives of `flgauss` with respect to `x1`, `y1`, and `ch` are all equal to 0.

9 Click **OK**.

GEOMETRY MODELING

1 Draw rectangles with the properties according to the following table.

NAME	WIDTH	HEIGHT	CORNER	DESCRIPTION
R1	1e-6	5e-7	(-4e-7,-5e-7)	Substrate

NAME	WIDTH	HEIGHT	CORNER	DESCRIPTION
R2	2.2e-7	5e-9	(-1e-8,0)	Gate oxide
R3	3.9e-7	5e-8	(-4e-7,0)	Air region

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

3 Click the **2nd Degree Bézier Curve** button and draw an arc from (–1e–7, –1e–7), with control point (0, –1e–7), ending it at (0, 0).

4 Continue the arc with straight lines by clicking the **Line** button and then click the coordinate sequence (–4e–7, 0) and (–4e–7, –1e–7). Close to a solid by clicking the right mouse button.

Drawing a curve at coordinates with many decimals or using an expression can be difficult, and you might be forced to specify extra grid points. Here is an alternative approach. First draw a curve with a similar shape as the final curve, using the existing grid points. Then alter the properties of the curve segments with the **Object Properties** dialog box. Do the following to draw the small spacer regions on the sides of the poly-gate:

5 Click the **2nd Degree Bézier Curve** button and draw an arc from (–1e–7, 0), with control point (–1e–7, 1e–7), ending it at (0, 1e–7).

6 Continue the arc with straight lines by clicking the **Line** button and then click the coordinate sequence (0, 0) and (–1e–7, 0). Close to a solid by clicking the right mouse button.

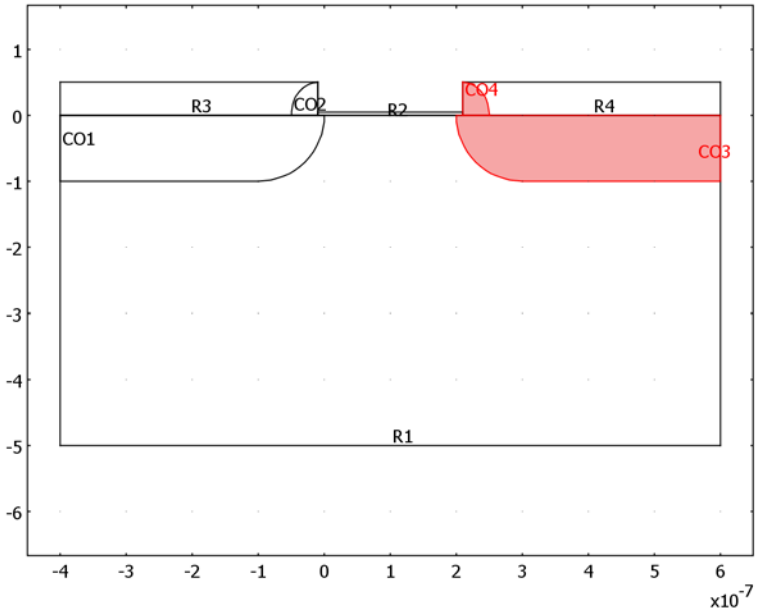
7 From the **Draw** menu, choose **Object Properties**.

8 In the **Object Properties** dialog box, change the properties for each curve segment according the table below.

CURVE NUMBER	POINT NUMBER (ROW IN TABLE)	X	Y	WEIGHT
1	1	-5e-8	0	1
	2	-1e-8	0	1
2	1	-1e-8	0	1
	2	-1e-8	5e-8	1
3	1	-5e-8	0	1
	2	-5e-8	5e-8	1/sqrt(2)
	3	-1e-8	5e-8	1

9 Select the objects CO1, CO2, and R3, then click the **Mirror** button on the Draw toolbar.

10 In the **Mirror** dialog box, enter `1e-7` in the **x** edit field at the **Point on line** row. Leave all other fields at their default values and click **OK**. The geometry should look like the figure below.



PHYSICS SETTINGS

Expression Variables

1 From the **Options** menu, choose **Expressions>Scalar Expressions**.

2 In the **Scalar Expressions** dialog box, define the following variables with names and expressions, and descriptions (the **Description** field is optional):

NAME	EXPRESSION	DESCRIPTION
Dn	Vt*mun	Electron diffusivity
Dp	Vt*mup	Hole diffusivity
n0	ni*exp((phi0+X_si+ 0.5*Eg_si)/Vt)	Electron concentration in thermal equilibrium
p0	ni*exp(-(phi0+X_si+ 0.5*Eg_si)/Vt)	Hole concentration in thermal equilibrium
R_srh	(nc*pc-ni^2)/(taun*(pc+ni)+ taup*(nc+ni))	Shockley-Reed-Hall recombination term

NAME	EXPRESSION	DESCRIPTION
phi_init	Vt*(-log(p_init/ni)*(Ndoping<0)+log(n_init/ni)*(Ndoping>=0))-X_si-0.5*Eg_si	Initial guess for phi0
n_init	(abs(Ndoping)/2+sqrt(Ndoping^2/4+ni^2))*(Ndoping>=0)+ni^2/(abs(Ndoping)/2+sqrt(Ndoping^2/4+ni^2))*(Ndoping<0)	Electron concentration at thermal equilibrium and charge neutrality
p_init	(abs(Ndoping)/2+sqrt(Ndoping^2/4+ni^2))*(Ndoping<0)+ni^2/(abs(Ndoping)/2+sqrt(Ndoping^2/4+ni^2))*(Ndoping>=0)	Hole concentration at thermal equilibrium and charge neutrality
Ndoping	NDimpl*flgauss(x,y,x1,0,ch)-NAsub+NDimpl*flgauss(x2-x,y,x1,0,ch)	Doping concentration

3 Click **OK**.

Subdomain Variables

1 From the **Options** menu, choose **Expressions>Subdomain Expressions**.

2 In the **Subdomain Expressions** dialog box, define the following variables:

VARIABLE	SUBDOMAINS 1, 2, 6	SUBDOMAINS 4, 5, 7	ALL OTHER SUBDOMAINS
epsilonr	epsilonr_si	epsilonr_sio2	1
mun	mun_si		
mup	mup_si		

3 Click **OK**.

Boundary Variables

1 From the **Options** menu, choose **Expressions>Boundary Expressions**.

2 In the **Boundary Expressions** dialog box, define the following variables with names and expressions:

VARIABLE	BOUNDARIES 6, 19	ALL OTHER BOUNDARIES
Jn	-q*lm3	
Jp	q*lm4	

3 Click **OK**.

Integration Coupling Variables

The drain current `Id` is defined as an integral of the normal current density along the drain contact. This can be implemented by using an integration coupling variable:

1 From the **Options** menu, select **Integration Coupling Variables>Boundary Variables**.

2 In the **Boundary Integration Variables** dialog box, select Boundary 19 and then type `Id` in the **Name** column, and type `Jn+Jp` in the **Expression** column. Click **OK**.

Subdomain Settings

1 On the **Multiphysics** menu, select the **Electrostatics (init)** application mode.

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

3 In the **Subdomain Settings** dialog box, enter the following settings:

SETTINGS	SUBDOMAINS 1, 2, 6	ALL OTHER SUBDOMAINS
ε_r	`epsilonr`	`epsilonr`
ρ	`q*(p0-n0+Ndoping)`	`0`

4 Click the **Init** tab, and enter the following initial value:

SETTING	ALL SUBDOMAINS
phi0(t_0)	`phi_init`

5 Click **OK**.

6 On the **Multiphysics** menu, select the **Electrostatics (es)** application mode.

7 Open the **Subdomain Settings** dialog box and enter the following settings:

SETTINGS	SUBDOMAINS 1, 2, 6	ALL OTHER SUBDOMAIN
ε_r	`epsilonr`	`epsilonr`
ρ	`q*(pc-nc+Ndoping)`	`0`

8 Click the **Init** tab, and enter the following initial value:

SETTING	ALL SUBDOMAINS
phi(t_0)	`phi0`

9 Click **OK**.

10 On the **Multiphysics** menu, select the **Convection and Diffusion (cde)** application mode.

11 Open the **Subdomain Settings** dialog box, select Subdomains 3–5, 7, and 8, and clear the **Active in this subdomain** check box. Then enter the following settings for the other subdomains:

SETTINGS	SUBDOMAINS 1, 2, 6
D (isotropic)	Dn
R	-R_srh
u	mun*phix
v	mun*phiy

12 Click the **Init** tab and enter the following initial value:

SETTING	SUBDOMAINS 1, 2, 6
$nc(t_0)$	n0

13 Click **OK**.

14 On the **Multiphysics** menu, select the **Convection and Diffusion (cdh)** application mode.

15 Open the **Subdomain Settings** dialog box, select Subdomains 3–5, 7, and 8, and clear the **Active in this subdomain** check box. Then enter the following settings for the other subdomains:

SETTINGS	SUBDOMAINS 1, 2, 6
D (isotropic)	Dp
R	-R_srh
u	-mup*phix
v	-mup*phiy

16 Click the **Init** tab, and enter the following initial value:

SETTING	SUBDOMAIN 1, 2, 6
$pc(t_0)$	p0

17 Click **OK**.

Boundary Conditions

1 On the **Multiphysics** menu, select the **Electrostatics (init)** application mode.

2 From the **Physics** menu, select **Boundary Settings**. Select the **Interior boundaries** check box.

3 In the **Boundary Settings** dialog box, enter the following settings:

SETTINGS	BOUNDARIES 2, 6, 19	BOUNDARIES 11, 12, 17	BOUNDARIES 1, 3, 5, 7, 18, 21–23
Boundary condition	Electric potential	Electric potential	Zero charge/Symmetry
V_0	`phi_init`	`Vg-X_poly`	

4 Click **OK**.

5 On the **Multiphysics** menu, select the **Electrostatics (es)** application mode.

6 Open the **Boundary Settings** dialog box, select the **Interior boundaries** check box, and enter the following settings:

SETTINGS	BOUNDARIES 2, 6	BOUNDARY 19	BOUNDARIES 11, 12, 17	BOUNDARIES 1, 3, 5, 7, 18, 21–23
Boundary condition	Electric potential	Electric potential	Electric potential	Zero charge/ Symmetry
V_0	`phi_init`	`phi_init+Vd`	`Vg-X_poly`	

7 Click **OK**.

8 On the **Multiphysics** menu, select the **Convection and Diffusion (cde)** application mode.

9 Open the **Boundary Settings** dialog box and enter the following settings:

SETTINGS	BOUNDARIES 2, 6, 19	ALL OTHER BOUNDARIES
Boundary condition	Concentration	Insulation/Symmetry
nc_0	`n_init`	

10 Click **OK**.

11 On the **Multiphysics** menu, select the **Convection and Diffusion (cdh)** application mode.

12 Open the **Boundary Settings** dialog box and enter the following settings:

SETTINGS	BOUNDARIES 2, 6, 19	ALL OTHER BOUNDARIES
Boundary condition	Concentration	Insulation/Symmetry
pc_0	`p_init`	

13 Click **OK**.

MESH GENERATION

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

2 Click the **Custom mesh size** button and enter `0.2` in the **Mesh curvature factor** edit field. This gives a slightly higher resolution of the curvature than the default setting.

3 Click the **Subdomain** tab.

4 Select Subdomains 2 and 6 and type `1e-8` in the **Maximum element size** edit field.

5 Click the **Boundary** tab.

6 Select Boundaries 4, 20, 24, and 26 and type `5e-9` in the **Maximum element size** edit field.

7 Select Boundary 13 and type `2e-9` in the **Maximum element size** edit field.

8 Click the **Remesh** button and then click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu, choose **Solver Manager**.

2 In the **Solver Manager** dialog box, click the **Solve For** tab.

3 In the **Solve for variables** tree, select only the **Electrostatics (init)** node.

4 Go to the **Sequence** page and click the **Store Current Settings** button.

5 In the **Store Solver Settings** dialog box, enter the **Name** `init` and then click **OK**.

6 Leaving the **Solver Manager** dialog box open, choose **Solve>Solver Parameters**.

7 In the **Solver Parameters** dialog box, change the **Solver** to **Parametric**.

8 In the **Parameters** area on the **General** page on the right, type `Vd` in the **Parameter names** edit field and `range(0,0.02,0.2) range(0.25,0.05,1)` in the **Parameter values** edit field.

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

10 Return to the **Solver Manager** dialog box and click the **Initial Value** tab.

11 In the **Values of variable not solved for and linearization point** area, click the **Current solution** button.

12 On the **Solve For** page, clear the **Electrostatics (init)** node and select the three other nodes, that is, **Electrostatics (es)**, **Convection and Diffusion (cde)**, and **Convection and Diffusion (cdh)**.

13 On the **Sequence** page, click the **Store Current Settings** button.

14 In the **Store Solver Settings** dialog box, enter the **Name** `parametric` and then click **OK**.

15 In the **Stored solver settings** area, select both **Init** and **Parametric** and then click the **>** button to add them to the **Solver sequence** list.

16 Select the **Solve using solver sequence** check box, then click **OK** to close the **Solver Manager** dialog box.

17 Click the **Solve** button on the Main toolbar to start the simulation. Note that the solver sequence overrides all other settings in the **Solver Parameters** and **Solver Manager** dialog boxes.

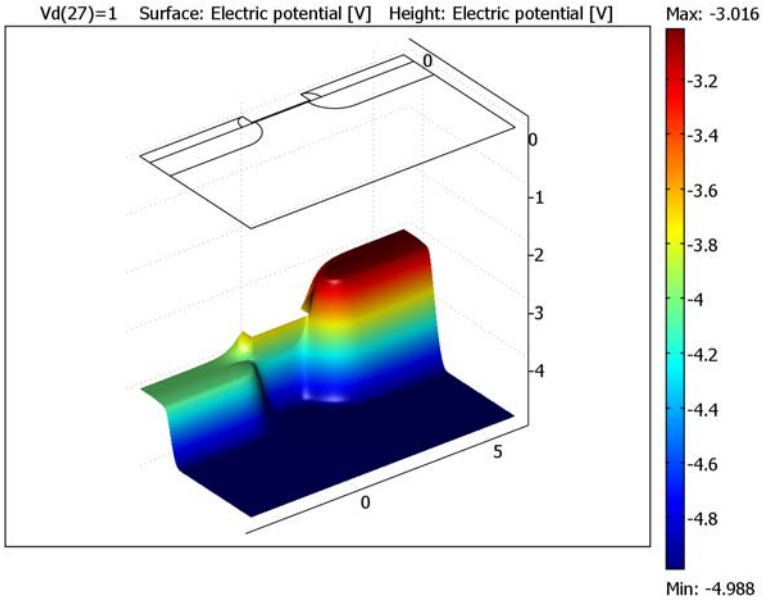
POSTPROCESSING AND VISUALIZATION

1 Open the **Plot Parameters** dialog box.

2 Click the **Surface** tab.

3 On the **Surface** page, enter `phi` in the **Expression** edit fields on both the **Surface Data** page and the **Height Data** page. Remember to select the **Height data** check box on the **Height Data** page.

4 Click **OK** to get the plot in the following figure. Also click the **Headlight** button on the Camera toolbar.

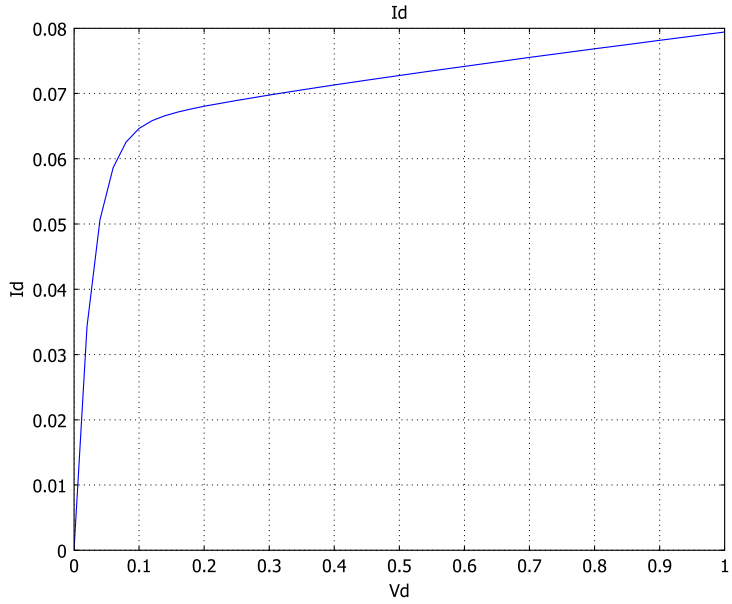


5 To plot the drain characteristics open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.

6 Click the **Point plot** button to select that plot type and make sure that all parameter values are selected in the **Solutions to use** list.

7 On the **Point** page, type `Id` in the **Expression** edit field in the **y-axis data** area.

8 Select Vertex 1, then click **OK**. In a separate window you should see the plot below.



Semiconductor Diode[1]

Introduction

A ***semiconductor diode*** consists of two regions with different doping: a p-type region with a dominant concentration of holes, and an n-type region with a dominant concentration of electrons. The ***anode*** contact ties to the p-type region, and the ***cathode*** connects to the n-type region. Impurities that the manufacturing process adds to the semiconductor material determine each region's doping type. Scientists typically denote the dopant concentration with N. A negative value indicates acceptor atoms (p-type material), and a positive value indicates donor atoms (n-type material).

It is possible to derive a semiconductor model from Maxwell's equations and Boltzmann transport theory with the aid of some generally accepted simplifications such as assuming the absence of magnetic fields and the constant density of states. The model presented here formulates the problem using three dependent variables: ψ, n, and p. Even in this model's simplest form, strong nonlinear dependencies are present. The three basic semiconductor equations appear below (Ref. 1).

$$-\nabla \cdot (\varepsilon \nabla \psi) = q(p - n + N)$$
$$-\nabla \cdot \mathbf{J}_\mathrm{n} = -qR_\mathrm{SRH}$$
$$-\nabla \cdot \mathbf{J}_\mathrm{p} = qR_\mathrm{SRH}$$

These equations contain the following variables:

- ψ indicates electrostatic potential
- q equals the elementary charge
- p and n are the hole and electron concentrations, respectively
- N represents the fixed charge associated with ionized donors

You can express the electron and hole current densities, $\mathbf{J}_\mathrm{n}$ and $\mathbf{J}_\mathrm{p}$, in terms of ψ, n and p:

$$\mathbf{J}_\mathrm{n} = -qn\mu_\mathrm{n}\nabla\psi + qD_\mathrm{n}\nabla n$$
$$\mathbf{J}_\mathrm{p} = -qp\mu_\mathrm{p}\nabla\psi - qD_\mathrm{p}\nabla p$$

where μ_n and μ_p are the carrier mobilities, and D_n and D_p are the carrier diffusivities.

1. Model provided by Erik Danielsson, Royal Institute of Technology, Stockholm.

The term R_{SRH} represents the *Shockley-Read-Hall recombination*, which is a general recombination process using traps in the forbidden band gap of the semiconductor.

$$R_{\text{SRH}} = \frac{np - n_i^2}{\tau_{\text{p}}(n + n_1) + \tau_{\text{n}}(p + p_1)}$$

Here n_i is the intrinsic carrier concentration, τ_{n} and τ_{p} are the carrier lifetimes, and n_1 and p_1 are parameters related to the trap energy level. If the trap level is located at the middle of the band gap (which the model assumes), then n_1 and p_1 equal n_i.

BOUNDARY CONDITIONS

For boundaries in contact with an insulator, you can use symmetric boundary conditions. For boundaries far away from the active device area, the electric field and carrier currents have zero normal component. You can describe both of these types with Neumann boundary conditions

$$\begin{aligned} \mathbf{n} \cdot \nabla\psi &= 0 \\ \mathbf{n} \cdot \mathbf{J}_{\text{n}} &= 0 \\ \mathbf{n} \cdot \mathbf{J}_{\text{p}} &= 0 \end{aligned}$$

At boundaries in contact with a metal, the electrostatic potential is fixed. If you assume infinite recombination velocity at the contact, the mass action law is valid:

$$n_i^{\,2} = np.$$

It is now possible to calculate the carrier concentrations using this law along with the dopant concentration N and the assumption that there is no charge at the contact. The applied voltage equals the Fermi level in the semiconductor at the contact, so the electrostatic potential at the contact is the applied voltage plus the energy difference between the Fermi level and the reference level used for the electrostatic potential. The energy difference has a logarithmic dependence of the carrier concentrations. The boundary conditions are

$$\psi = V_a + \frac{kT}{q}\ln\left(\frac{\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}}{n_i}\right)$$

$$n = \frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

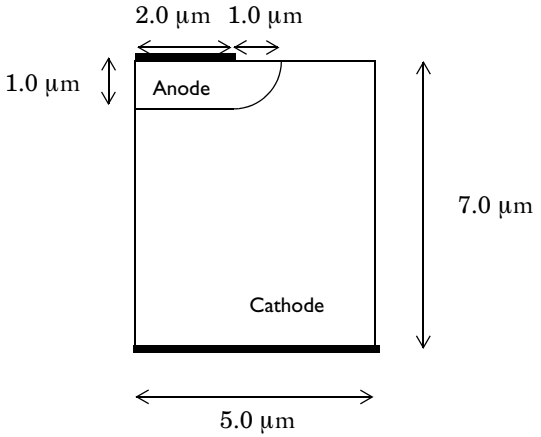
$$p = -\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

where V_a is the applied voltage. This is the simplest type of electrical contact. It is also possible to define a specific contact metal (some examples being aluminum or titanium) and to specify the current at the contact instead of the voltage.

Model Definition

DIODE GEOMETRY

The diode's geometry appears below.



Thicker lines indicate electrical contacts. This example applies a potential V_a to the anode, and the cathode is grounded.

Use the following notation for the dimensions of the device.

VARIABLE	VALUE
y_l	$7 \cdot 10^{-6}$ m
x_l	$5 \cdot 10^{-6}$ m
ju	$1 \cdot 10^{-6}$ m
ac	$2 \cdot 10^{-6}$ m

MESHING

The large dynamic range of the carrier concentrations makes the numerical simulation of the semiconductor equations a difficult task, especially because the entire range changes in the vicinity of the junction. Therefore you must select the mesh quite carefully, otherwise the solution process might not converge or could give inaccurate results. Thus, this example places a subdomain boundary at the junction to establish high accuracy. You must make the mesh denser around the junction and at the cathode and anode. Use the adaptive solver to obtain additional accuracy.

MATERIAL PROPERTIES

The most common material used for semiconductor devices is silicon, and the following table summarizes some key material properties used in this model.

NOTATION	VARIABLE	VALUE
n_i	ni	$1.46 \cdot 10^{10}$ cm^{-3} (T = 300K)
ε_r	epsilonr	11.8
μ_n	mun	800 cm^2/Vs (low conc.)
μ_p	mup	200 cm^2/Vs (low conc.)
$D_n = \mu_n kT/q$	Dn	20.7 cm^2/s
$D_p = \mu_p kT/q$	Dp	5.17 cm^2/s
τ_n	taun	~0.1 µs
τ_p	taup	~0.1 µs

Mobilities and diffusivities often depend on N, but this effect is relatively small in the diode structure. The carrier lifetime can vary from a few picoseconds up to several microseconds and depends on parameters such as doping, temperature, and recombination centers.

DOPANT CONCENTRATION FUNCTION

The p-type doping of the diode can be accomplished by implantation or diffusion of acceptor atoms. The resulting profile from these two steps is often approximated with a gauss function. In addition, the transition between the n-type doped substrate and the lower doped n-type epitaxial layer can also be approximated with a Gauss function, because the dopants diffuse from the highly doped substrate during the high temperature step of the epitaxial growth. The final expression for the diode doping is

$$N = N_{D\mathrm{n}} + N_{D\mathrm{nmax}} G(x, -y, \infty, y_1) - N_{A\mathrm{pmax}} G(x, y, x_1, 0)$$

where $N_{D\mathrm{n}}$ is the doping of the epitaxial layer, $N_{D\mathrm{nmax}}$ the doping of the substrate, and $N_{A\mathrm{pmax}}$ the peak of the implantation of diffusion profile. G is the Gauss function defined by

$$G(x, y, x_1, y_1) = \begin{cases} e^{-\frac{(x-x_1)^2}{ch^2}} e^{-\frac{(y-y_1)^2}{ch^2}} & x > x_1 \; y > y_1 \\ e^{-\frac{(x-x_1)^2}{ch^2}} & x > x_1 \; y \le y_1 \\ e^{-\frac{(y-y_1)^2}{ch^2}} & x \le x_1 \; y > y_1 \\ 1 & x \le x_1 \; y \le y_1 \end{cases}$$

The following constants are used in the expression for N:

NOTATION	VARIABLE	VALUE
$N_{D\mathrm{n}}$	NDn	10^{15} cm^{-3}
$N_{D\mathrm{nmax}}$	NDnmax	10^{17} cm^{-3}
$N_{A\mathrm{pmax}}$	NApmax	10^{17} cm^{-3}
x_1	ac	2 μm
y_1	y1	7 μm
ch	ch	calculated from ju

BOUNDARY CONDITIONS

The contact boundary conditions are

$$\psi = V_a + \frac{kT}{q}\ln\left(\frac{\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}}{n_i}\right)$$

$$n = \frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

$$p = -\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

To compute an accurate value of the current you can use weak constraints for the contact boundary conditions. To implement the weak boundary conditions on n and p you need to introduce Lagrange multipliers lm_2 and lm_3 on the anode and cathode. The variables `lm2` and `lm3` provide a more accurate value than what you obtain by the expression for the current densities. Therefore, the outward normal current densities are `q*lm2` and `-q*lm3`, for electrons and holes, respectively.

PARAMETRIC STUDY

Solving the numerical problem for higher anode voltage is extremely difficult. You must increase the voltage from 0 V in small steps and use the solution from a previous step as the initial condition for the next one. The parametric solver takes care of this automatically. The anode voltage V_a varies from 0 V to 1 V in steps of 0.025 V.

You must also provide the nonlinear solver with an initial guess for the solution corresponding to $V_a = 0$ V that is compatible with the boundary conditions.

$$\psi = \frac{kT}{q}\ln\left(\frac{\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}}{n_i}\right)$$

$$n = \frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

$$p = -\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}$$

The initial guess for lm_2 and lm_3 is zero. Because the problem is nonlinear, you should convert it to general form to get a correct Jacobian and fast convergence.

COMSOL Multiphysics lets you scale the degrees of freedoms by setting reference values for the degrees of freedom. The relative tolerance in the nonlinear solver is by

default 10^{-6}. The absolute tolerance is the scaling times the relative tolerance. The solver disregards errors that are below the absolute tolerance. In this case the absolute tolerance for the variables ψ, u, and v is 10^{-6}, while the absolute tolerance for lm_2 and lm_3 is 10^{-4}. The absolute tolerance for lm_2 and lm_3 should be at least 10^{-4}, because the round-off errors in the equations induce errors of this magnitude in lm_2 and lm_3. For this problem, the parameter step length control works best if you use the highly nonlinear option.

Results

When no bias is applied, the hole concentration is at thermal equilibrium. With 0.5 V forward bias, the holes from the p-type region flow into and through the low doped n-type region without significant recombination (see Figure 12-10). As a result, the hole concentration increases several orders of magnitude in the n-type region.

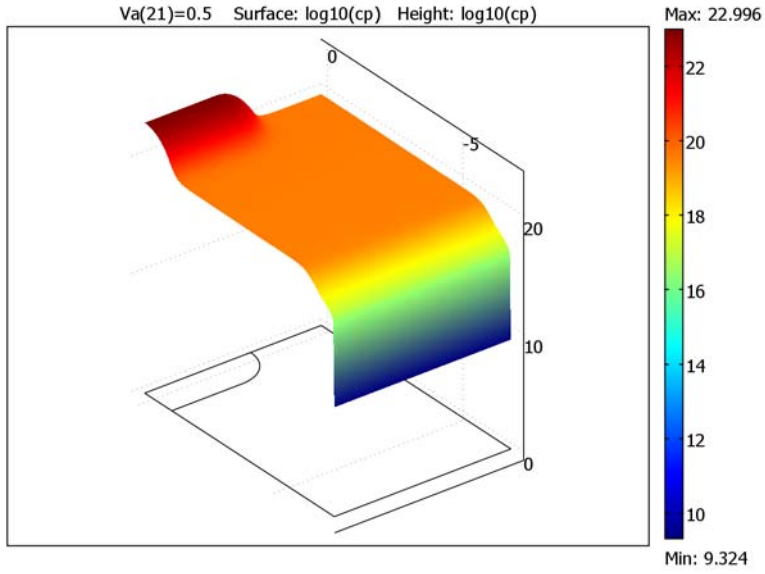


Figure 12-10: The hole concentration at 0.5 V forward bias.

COMPUTING THE IV CHARACTERISTICS

To compute the currents through the anode and cathode you have to integrate the normal component of the current densities

$$\mathbf{n} \cdot \mathbf{J}_\mathrm{n}$$
$$\mathbf{n} \cdot \mathbf{J}_\mathrm{p}$$

which are more accurately available by the Lagrange multipliers lm_2 and lm_3, respectively. The currents through the anode and cathode are

$$I_a = 10^{-6} \int_{\text{anode}} -q(\mathrm{lm}_u - \mathrm{lm}_2)$$

$$I_c = 10^{-6} \int_{\text{cathode}} q(\mathrm{lm}_u - \mathrm{lm}_3)$$

Because the geometry is 2D, the unit A/μm is used for the current. Note that I_a and I_c are vectors with one value for each value of the voltage. The exact agreement of the anode and cathode currents is a consequence of the finite element method. To see this, consider the weak equations

$$0 = \int_\Omega \left(\frac{R_\mathrm{SRH}}{n_i} u_\mathrm{test} + \mathbf{J}_n \cdot \nabla u_\mathrm{test} \right) dA - \int_B \mathrm{lm}_2 \cdot u_\mathrm{test} \; ds$$

$$0 = \int_\Omega \left(\frac{R_\mathrm{SRH}}{n_i} v_\mathrm{test} + \mathbf{J}_p \cdot \nabla v_\mathrm{test} \right) dA - \int_B \mathrm{lm}_3 \cdot v_\mathrm{test} \; ds$$

which are valid for all test functions u_test and v_test in the finite element space. B is the union of the anode and the cathode. Taking $u_\mathrm{test} = v_\mathrm{test} = 1$ and subtraction of these equations gives

$$\int_B (\mathrm{lm}_2 - \mathrm{lm}_3) ds = 0$$

which shows that $I_a = I_c$. The plot in Figure 12-11 shows the current versus the voltage.

Because the current for zero voltage is zero (theoretically), it has been omitted from the plot.

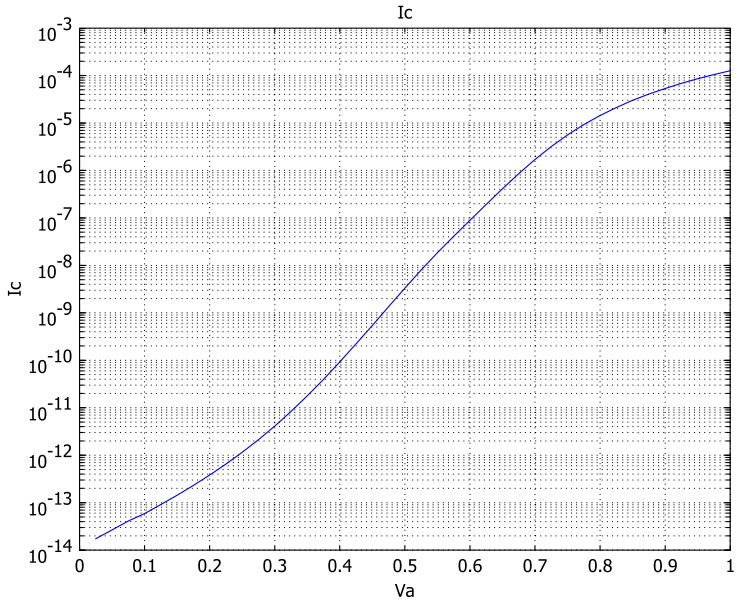


Figure 12-11: The IV characteristics of the semiconductor diode plotted in a logarithmic scale.

One very important parameter in the diode equation is the ideality factor, η.

$$I = I_0\left(e^{\frac{qV}{\eta kT}} - 1\right).$$

The factor η lies between 1 and 2, where $\eta \sim 1$ represents an ideal diode. In a diode with $\eta \sim 2$, the current is recombination/generation controlled (Ref. 1). In the IV-characteristic curve, you can identify two different slopes in the diode's forward bias region. These slopes are dependent on the ideality factor, the first with $\eta = 1.6$ and the second with $\eta = 1.08$. This situation is common for ordinary silicon diodes; at low forward biases the current is almost recombination controlled, and when the bias is increased the current characteristics becomes almost ideal ($\eta \sim 1$).

References

1. S.M. Sze, *Physics of Semiconductor Devices*, John Wiley & Sons, 1981, ISBN 0-471-05661-8.

2. S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer-Verlag, 1984, ISBN 0-387-81800-6.

Model Library path: `COMSOL_Multiphysics/Semiconductor_Devices/semiconductor_diode`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 Click the **Multiphysics** button.

3 In the **COMSOL Multiphysics>Electromagnetics** folder, select **Electrostatics**. Make sure **Lagrange - Quadratic** is selected in the **Element** list.

4 Enter `psi` in the **Dependent variables** edit field.

5 Click **Add**.

6 In the **COMSOL Multiphysics>Convection and Diffusion** folder, select **Convection and Diffusion** and then **Steady-state analysis**. Make sure **Lagrange - Quadratic** is selected in the **Element** list.

7 Enter `cn` in the **Dependent variables** edit field.

8 Click **Add**.

9 Click the **Application Mode Properties** button, select **Conservative** from the **Equation form** list and **On** from the **Weak constraints** list. Click **OK**.

10 In the **COMSOL Multiphysics>Convection and Diffusion** folder, select **Convection and Diffusion** and then **Steady-state analysis**. Make sure **Lagrange - Quadratic** is selected in the **Element** list.

11 Enter `cp` in the **Dependent variables** edit field.

12 Click **Add**.

13 Click the **Application Mode Properties** button. Then select **Conservative** from the **Equation form** list and **On** from the **Weak constraints** list. Click **OK**.

14 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, define the following constants with names and expressions:.

NAME	EXPRESSION	DESCRIPTION
q	1.602e-19[C]	Elementary charge
T	300[K]	Room temperature
k	1.38e-23[J/K]	Boltzmann's constant
epsilonr	11.8	Rel. permittivity for Si
ni	1.46e10[1/cm^3]	Intrinsic concentration for Si
mun	800[cm^2/(V*s)]	Electron mobility for Si
mup	200[cm^2/(V*s)]	Hole mobility for Si
Dn	k*T/q*mun	Electron diffusivity
Dp	k*T/q*mup	Hole diffusivity
taun	0.1[us]	Electron life time
taup	0.1[us]	Hole life time
c	q/(k*T)	Reciprocal thermal voltage
y1	7[um]	Diode dimension
x1	5[um]	Diode dimension
ju	1[um]	Junction depth
ac	2[um]	Anode dimension
NApmax	1e17[1/cm^3]	Maximum p-type doping
NDn	1e15[1/cm^3]	Drift layer n-type doping
NDnmax	1e17[1/cm^3]	Maximum n-type doping
ch	ju/sqrt(log(NApmax/NDn))	Doping fall-off constant

3 From the **Options** menu, choose **Axes/Grid Settings**.

4 Enter the axis and grid settings in the table below. To enter the grid spacing, first clear the **Auto** check box.

AXIS		GRID	
x min	0	x spacing	1e-6
x max	1e-5	Extra x	

AXIS		GRID	
y min	-8e-6	y spacing	1e-6
y max	0	Extra y	

5 Click **OK**.

GEOMETRY MODELING

1 Draw a rectangle from (0, -7e-6) to (5e-6, 0).

2 Turn off the solidify feature by double-clicking the **SOLID** button on the status bar.

3 Click the **Line** button and draw a line from (0, -1e-6) to (2e-6, -1e-6).

4 Click the **2nd Degree Bézier Curve** button and continue with an arc to (3e-6, -1e-6) and finish the arc at (3e-6, 0).

5 Click the **Point** button and add a point at (2e-6, 0).

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

PHYSICS SETTINGS

Expression Variables

1 From the **Options** menu, point to **Expressions**, and then click **Scalar Expressions**.

2 Enter each item in the table below as a single line without the line break.

NAME	EXPRESSION	DESCRIPTION
N	NDn+NDnmax*exp(-((y+y1)/ch)^2)-NApmax*exp(-(y/ch)^2)*((x<ac)+(x>=ac)*exp(-((x-ac)/ch)^2))	Doping concentration
RSRH	(cn*cp-ni^2)/(taup*(cn+ni)+taun*(cp+ni))	Recombination term
psi_init	1/c*(-log(p_init/ni)*(N<0)+log(n_init/ni)*(N>=0))	Charge neutrality voltage
n_init	(abs(N)/2+sqrt(N^2/4+ni^2))*(N>=0)+ni^2/(abs(N)/2+sqrt(N^2/4+ni^2))*(N<0)	Charge neutrality electron concentration
p_init	(abs(N)/2+sqrt(N^2/4+ni^2))*(N<0)+ni^2/(abs(N)/2+sqrt(N^2/4+ni^2))*(N>=0)	Charge neutrality hole concentration

3 Click **OK**. The inconsistent unit warning for the variable RSH is due to the use of mol as unit For the solution variables in the Convection and Diffusion application modes. The convention in Semiconductor physics is to use $1/\mathrm{cm}^3$ for

concentrations, and this is the assumed unit for the solution variables. The units for solution variables cannot be changed by the user.

Integration Coupling Variables

The cathode current `Ic` is defined as an integral of the normal current density along the cathode. This can be implemented by using an integration coupling variable:

1. From the **Options** menu, point to **Integration Coupling Variables** and then click **Boundary Variables**.
2. Select Boundary 2 and then type `Ic` in the **Name** column, `1e-6*q*(lm2-lm3)` in the **Expression** column, and `4` in the **Integration order** column. Click **OK**.

Boundary Conditions

1. On the **Multiphysics** menu, select the **Electrostatics (es)** application mode.
2. Open the **Boundary Settings** dialog box and enter the following settings:

SETTINGS	BOUNDARIES 1, 3, 6, 7, 8	BOUNDARY 2	BOUNDARY 5
Boundary condition	Zero charge/Symmetry	Electric potential	Electric potential
V_0		`psi_init`	`Va+psi_init`

3. On the **Multiphysics** menu, select the **Convection and Diffusion (cd)** application mode.
4. Open the **Boundary Settings** dialog box and enter the following settings:

SETTINGS	BOUNDARIES 1, 3, 6, 7, 8	BOUNDARIES 2, 5
Boundary condition	Insulation/Symmetry	Concentration
cn_0		`n_init`

5. On the **Multiphysics** menu, select the **Convection and Diffusion (cd2)** application mode.
6. Open the **Boundary Settings** dialog box and enter the following settings:

SETTINGS	BOUNDARIES 1, 3, 6, 7, 8	BOUNDARIES 2, 5
Boundary condition	Insulation/Symmetry	Concentration
cp_0		`p_init`

Subdomain Settings

1. On the **Multiphysics** menu, select the **Electrostatics (es)** application mode.

2 Open the **Subdomain Settings** dialog box and enter the following settings:

SETTINGS	SUBDOMAINS 1, 2
ε_r	epsilonr
ρ	q*(N-cn+cp)

3 Click the **Init** tab, and enter the following initial value:

SETTING	SUBDOMAINS 1, 2
psi(t_0)	psi_init

4 On the **Multiphysics** menu, select the **Convection and Diffusion (cd)** application mode.

5 Open the **Subdomain Settings** dialog box and enter the following settings:

SETTINGS	SUBDOMAINS 1, 2
D (isotropic)	Dn
u	mun*psix
v	mun*psiy
R	-RSRH

6 Click the **Init** tab and enter the following initial value:

SETTING	SUBDOMAINS 1, 2
cn(t_0)	n_init

7 On the **Multiphysics** menu, select the **Convection and Diffusion (cd2)** application mode.

8 Open the **Subdomain Settings** dialog box and enter the following settings:

SETTINGS	SUBDOMAINS 1, 2
D (isotropic)	Dp
u	-mup*psix
v	-mup*psiy
R	-RSRH

9 Click the **Init** tab, and enter the following initial value:

SETTINGS	SUBDOMAINS 1, 2
cp(t_0)	p_init

MESH GENERATION

1. From the **Mesh** menu, choose **Free Mesh Parameters**.
2. Click the **Boundary** tab.
3. Select Boundaries 2, 4, 5, and 9 and type `1e-7` in the **Maximum element size** edit field.
4. Click the **Remesh** button and then click **OK**.

COMPUTING THE SOLUTION

1. From the **Solve** menu, choose **Solver Parameters**.
2. In the **Solver** list, select **Parametric**.
3. Type `Va` in the **Parameter names** edit field and `range(0,0.025,1)` in the **Parameter values** edit field.
4. Click the **Stationary** tab. Enter `50` in the **Maximum number of iterations** edit field.
5. Select the **Highly nonlinear problem** check box.
6. Click **OK** and then click the **Solve** button to start the simulation.

POSTPROCESSING AND VISUALIZATION

The plot visualizes the logarithm of the hole concentration for the parameter value, $V_a = 0.5$ V.

1. Open the **Plot Parameters** dialog box from the **Postprocessing** menu.
2. On the **General** page, select **0.5** from the **Parameter value** list.
3. Click the **Surface** tab. Enter the expression `log10(cp)` in the **Expression** edit fields on the **Surface Data** tab and the **Height Data** tab. On the **Height Data** tab, select the **Height data** check box.
4. Click **OK** to get the plot shown in Figure 12-10 on page 498.
5. To plot the IV characteristics open the **Domain Plot Parameters** dialog box from the **Postprocessing** menu.
6. On the General page, click the **Point plot** button and select all parameters except 0 from the **Solutions to use** list.
7. Click the **Title/Axis** button to open the **Title/Axis Settings** dialog box. Select the **Log scale** check box for the secondary axis. Click **OK**.
8. On the **Point** tab, type `Ic` in the **Expression** edit field.
9. Select Vertex 1 and click **OK**. As a separate window you see the plot in Figure 12-11 on page 500.

SPICE Parameter Extraction for a Semiconductor Diode

This model shows how the Optimization application mode can extract SPICE parameters from the model of a semiconductor diode for use in an equivalent circuit.

Note: This model requires the Optimization Lab.

Introduction

In the design of a semiconductor device, it is often desirable to develop a compact model to use when analyzing its behavior in larger systems. SPICE models are compact descriptions of electronic circuits, where a set of SPICE parameters determines the device's behavior in static, transient, and time-harmonic analysis. In developing such a compact model, the extraction of the SPICE parameters usually requires several different characteristics that show how the device behaves for a range of operating conditions. The characteristics can either be the result of measurements or come from simulations of a more-detailed reference model.

This example reviews the development of a compact model for a semiconductor diode. The reference finite-element model is "Semiconductor Diode" on page 492. From this model it is possible to extract the forward characteristics where the diode is biased from 0 V up to 1.5 V. Six SPICE parameters control the forward characteristics of the compact model. This sets a lower limit on the number of reference data required to extract the compact model.

Model Definition

SEMICONDUCTOR MODEL

The previously mentioned example in the Model Library solves for a forward bias of only up to 1 V. This level is not high enough to extract all the needed parameters, especially the resistor parameter, so the characteristics must go a bit further. As a result, the first part of this example solves the semiconductor diode with a bias reaching 1.5 V.

EQUIVALENT DIODE CIRCUIT

A diode is an electrical rectifier that conducts current for positive voltages and insulates for negative voltages. The current-voltage characteristics (or IV characteristics) for an ideal semiconductor diode follow the relationship

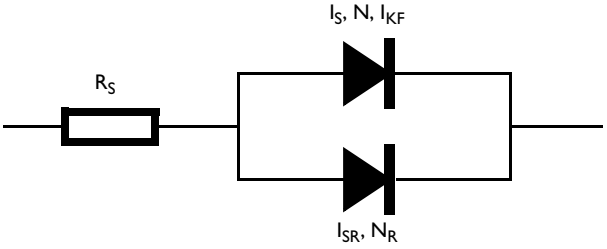
$$I = I_S\left(e^{\frac{V}{V_T}} - 1\right)$$

where V_T is the thermal voltage. The compact model of a real diode actually consists of two ideal diodes in parallel and a resistor in series (see nearby figure). Furthermore, a parameter called the ideality factor, N, is introduced into the ideal diode equation so that

$$I = I_S\left(e^{\frac{V}{NV_T}} - 1\right).$$

One of the ideal diodes also has a parameter for high-level injection, which is a change in its characteristics for high currents.

The following image shows the complete equivalent circuit for a real diode with the SPICE parameters next to each device.



You cannot express the compact model as an explicit relationship between its current and voltage, so to obtain its characteristics, it is necessary to solve an implicit nonlinear problem. An easy way to set up this equivalent circuit is to use the SPICE Circuit Editor available for the AC/DC Module, MEMS Module, and the RF Module. With a simple circuit file, this feature automatically generates ODE expressions that model the equivalent diode circuit. In this case the ODE representation does not involve any time derivatives, so from the mathematical viewpoint you have the special case of static, algebraic equations. A parametric solution of this system of ODEs can give the current

for a predefined list of voltages. The SPICE parameters are given as constants in the equivalent circuit model according to the following table:

PARAMETER	CONSTANT	DESCRIPTION
I_S	`sim_D1_IS`	Saturation current
N	`sim_D1_N`	Ideality factor
I_{KF}	`sim_D1_IKF`	High-injection knee current
I_{SR}	`sim_D1_ISR`	Recombination current
N_R	`sim_D1_NR`	Ideality factor for recombination current
R_S	`sim_D1_RS`	Series resistance

For users that do not have the AC/DC Module, MEMS Module, or RF Module, there is a pre-saved model file where the initial steps before the optimization have been done.

OPTIMIZATION

The Optimization Lab searches for values for the six SPICE parameters shown in the equivalent circuit such that the IV characteristics from the ODE circuit simulations match the IV characteristics extracted from the reference finite-element diode model. This is an optimization problem of six unknowns that enter the objective function in a nonlinear fashion. The initial guess for the parameters is crucial to reduce the search time.

It is also necessary to define a couple of constraints in the search because otherwise the two diodes in parallel become hard to distinguish. These diodes have a physical interpretation, where the upper one controls the main diode characteristics. The ideality factor of the main diode should lie close to one. The lower diode is responsible for the recombination effects in the semiconductor, and that effect shows an ideality factor close to 2. Therefore, a proper constraint is to force the ideality factor N to be less than the ideality factor N_R. A high ideality factor also results in a high saturation current, I_{SR}, so the same constraint can be used for the saturation currents. That is,

$$N < N_R$$
$$I_S < I_{SR}$$

In addition, it is necessary to set lower and upper bounds to all parameters and to use the logarithmic values for the parameters, I_S, I_{SR}, R_S, and I_{KF} because they usually span several orders of magnitude.

To summarize, the optimization problem is

$$
\begin{array}{lll}
\underset{x}{\text{minimize}} & \frac{1}{2}\sum_i F_i(V_i, x)^2 & \text{Objective function} \\
\text{subject to} & I_S \le I_{SR} & \text{Linear constraints} \\
& N \le N_R & \\
& \begin{bmatrix} -20 \\ 1 \\ -20 \\ 1 \\ 2 \\ -7 \end{bmatrix} \le x \le \begin{bmatrix} -10 \\ 2 \\ -10 \\ 2 \\ 6 \\ -4 \end{bmatrix} & \text{Parameter bounds} \\
& I_{\text{cir}} = I_{\text{cir}}[V, x] & \text{Algebraic equations}
\end{array}
$$

where

$$x = (\log(I_S), N, \log(I_{SR}), N_R, \log(R_S), \log(I_{KF}))^T .$$

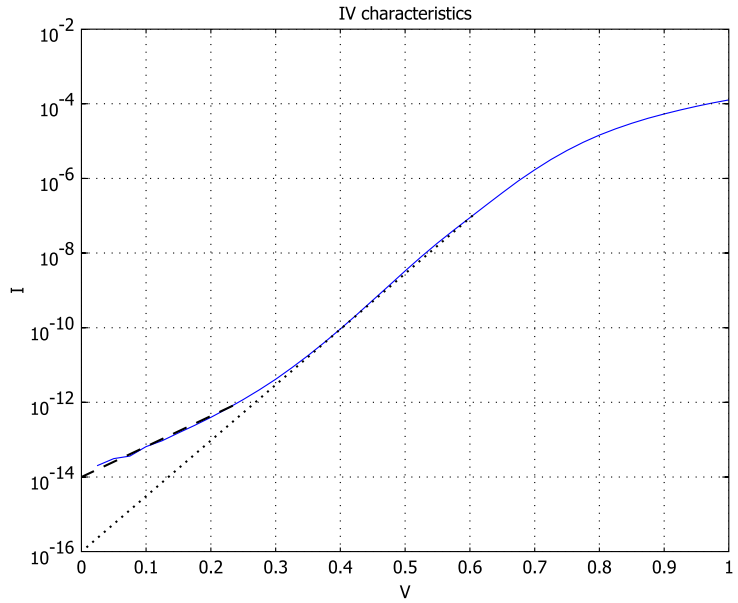
The objective is to determine the SPICE parameters (x) so that the equivalent circuit matches the original diode with respect to the IV characteristics in a least-squares sense. Again, using a logarithmic scale:

$$F_i(x) = \log_{10}(I(V_i)) - \log_{10}(I_{\text{cir}}[V_i, x]) .$$

Because I_{cir} depends implicitly on the SPICE parameters, the system of algebraic equations describing the IV relationship of the equivalent circuit must be solved for each voltage in the range of the characteristic you wish to match. This must be done every time the optimization solver evaluates the objective function with updated SPICE parameters. The function $I(V_i)$ could be directly evaluated from the semiconductor diode example while performing the optimization, but this is a quite time-consuming evaluation. It is much faster to create an interpolation function from the IV-characteristics of the semiconductor diode example.

Initial Guess

The initial guess for the parameter values is very important in order to speed up the search, and in some cases also to get convergence. You can easily extract proper parameter values directly from the IV characteristics of the semiconductor diode. In the following figure you can see some straight lines that represents the diode equations presented earlier, one for each diode in the equivalent circuit.



The intersections between these lines and the y-axis serve as good initial guesses for the parameters I_S and I_{SR}. Next, the ideality factors usually have values close to one and two, so use those values as initial guess. The parameter I_{KF} determines where the curve has its knee for large currents, so the current value where this appears is suitable as an initial guess. The final parameter, R_S, also controls the flat region of the curve, so approximately the maximum voltage divided by the maximum current is a good guess. The initial parameters from this simple analysis are summarized in this table:

PARAMETER	VALUE	INITIAL VALUE IN X	DESCRIPTION
I_S	10^{-16} A/m	-16	Saturation current
N	1	1	Ideality factor
I_{SR}	10^{-14} A/m	-14	Recombination current
N_R	2	2	Ideality factor for recombination current
R_S	10^{4} Ωm	4	Series resistance
I_{KF}	10^{-6} A/m	-6	High injection knee current

The unit for current is A/m because the circuit is compared to a 2D simulation in SI units.

The optimization uses the built-in optimization solver with a gradient based search. Fitting the parameters needs about 30 iterations, which takes a few minutes on a modern PC. The resulting compact model characteristics appear as a green line in the next figure, which plots the IV characteristics from the finite element reference model as a blue line. The agreement is quite good over the entire voltage range up to 1.5 V.

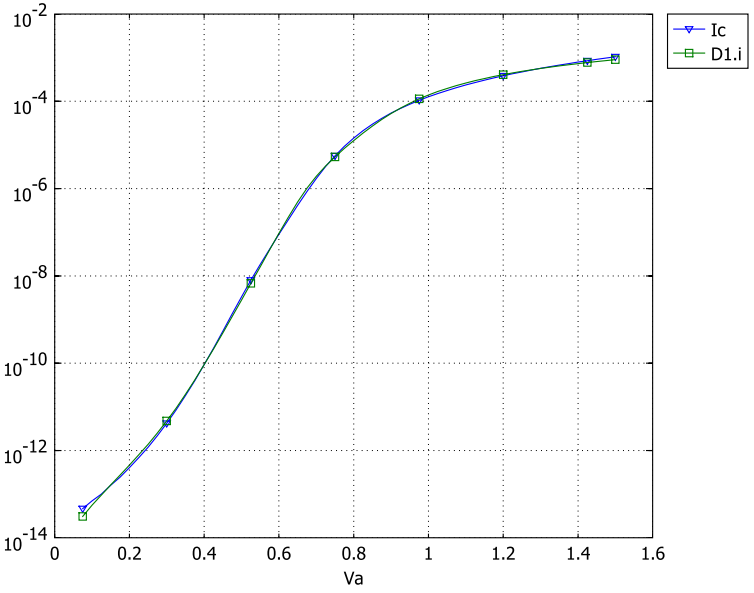


Figure 12-12: The green line with squares show the IV characteristics of the equivalent circuit, the blue line with triangles is that from the COMSOL Multiphysics Model Library model semiconductor_diode.

PARAMETER	OPTIMIZED VALUE	DESCRIPTION
I_S	$4.88 \cdot 10^{-17}$ A/m	Saturation current
N	1.08	Ideality factor
I_{SR}	$8.68 \cdot 10^{-15}$ A/m	Recombination current
N_R	2.00	Ideality factor for recombination current
R_S	$5.21 \cdot 10^{2}$ Ωm	Series resistance
I_{KF}	$1.70 \cdot 10^{-6}$ A/m	High injection knee current

Model Library path: `COMSOL_Multiphysics/Semiconductor_Devices/spice_parameter_extraction_diode`

Model Library path: `COMSOL_Multiphysics/Semiconductor_Devices/spice_parameter_extraction_circuit`

Modeling Using the Graphical User Interface

CREATING THE REFERENCE DATA

First start COMSOL Multiphysics and open the semiconductor diode example and resolve it with a longer sweep.

1. In the **Model Navigator**, click the **Model Library** tab.
2. Browse to the model **COMSOL Multiphysics>Semiconductor Devices>semiconductor diode**.
3. Select it, then click **OK**.

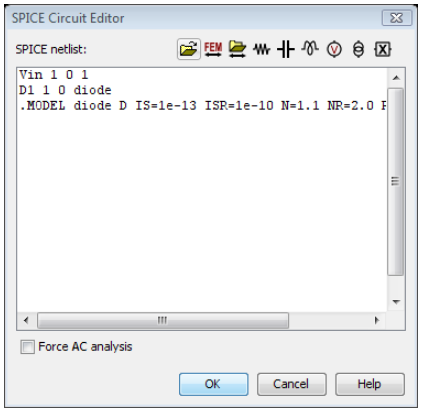
SPICE IMPORT

This section requires that you have the AC/DC Module, MEMS Module, or the RF Module. Users that do not have any such license can skip this section and continue with the section "Loading the Pre-Saved Model File" on page 514.

1. From the **Physics** menu, choose **SPICE Circuit Editor**.
2. You can just type the netlist as it is shown below, or open the saved netlist file called `diode.cir` located in the Model library path for this model. If you choose to open the netlist file, click the **Load Netlist from File** toolbar button. The final netlist is shown below.

```
Vin 1 0 1
D1 1 0 diode
```

```
.MODEL diode D IS=1e-13 ISR=1e-10 N=1.1 NR=2.0 RS=1e1 IKF=1e-5
```



3 Click **OK** to generate the system of global equations.

Skip the next section and continue with the section "Model Navigator".

LOADING THE PRE-SAVED MODEL FILE

This section is intended for users that did not complete the previous sections. If you have completed all those steps, you just skip this section and continue with the next section.

1 From the **File** menu, choose **Open Model Library**.

2 In the **Model Navigator**, open the model **COMSOL Multiphysics>Semiconductor Devices>spice parameter extraction circuit**.

3 Click **OK**.

MODEL NAVIGATOR

1 From the **Multiphysics** menu, choose **Model Navigator**.

2 In the **Model Navigator** dialog box, select the **COMSOL Multiphysics>Optimization and Sensitivity>Optimization** application mode.

3 Click **OK**.

OPTIONS AND SETTINGS

Constants

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

2 In the **Constants** dialog box, delete the following constants.

NAME
sim_D1_IS
sim_D1_N
sim_d1_ISR
sim_D1_NR
sim_D1_RS
sim_d1_IKF

3 The change the expression of the constant `sim_VIN_ARG` to `Va`.

4 Click **OK**.

Global Expressions

1 From the **Options** menu, choose **Expressions>Global Expressions**.

2 In the **Global Expressions** dialog box, define the following variables with names, expressions, and (optionally) descriptions:

NAME	EXPRESSION	DESCRIPTION
sim_D1_IS	10^logIS	Saturation current
sim_d1_ISR	10^logISR	Saturation current (recombination)
sim_D1_RS	10^logRS	Series resistance
sim_d1_IKF	10^logIKF	High-injection current

3 Click **OK**.

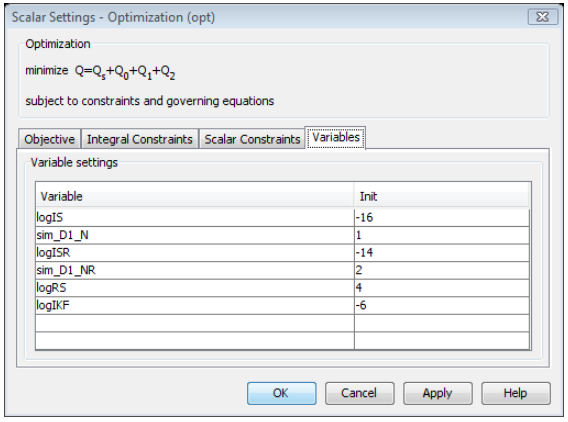
PHYSICS SETTINGS

1 From the **Physics** menu, choose **Scalar Settings**.

2 On the **Variables** page, enter the six parameters according to the following table:

VARIABLE	INIT	DESCRIPTION
logIS	-16	Log of the saturation current
sim_D1_N	1	Ideality factor
logISR	-14	Log of the saturation current (recombination)
sim_D1_NR	2	Ideality factor (recombination)
logRS	4	Log of the series resistance
logIKF	-4	Log of the high-injection current

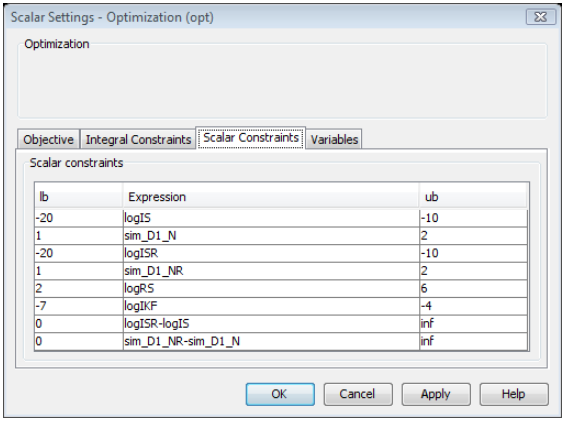
The dialog box should look like the figure below when you are done.



3 On the **Scalar Constraints** page, enter the upper and lower bounds for the parameters plus two linear constraints according to the following table:

LB	EXPRESSION	UB
-20	logIS	-10
1	sim_D1_N	2
-20	logISR	-10
1	sim_D1_NR	2
2	logRS	6
-7	logIKF	-4
0	logISR-logIS	inf
0	NR-N	inf

The dialog box should look like the figure below when you are done.



4 Click the **Objective** tab. In the **Scalar contribution** edit field, type `0.5*(log10(Ic)-log10(sim_D1_i))^2`. The variable `Ic` is the current from the finite element model.

5 Click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu, open the **Solver Parameters** dialog box.

2 Change the value in the edit field **Parameter values** to `range(0.075,0.025,1.5)`.

3 Go to the **Stationary** page and clear the **Highly nonlinear problem** check box.

4 Click **OK**.

5 Click the **Solve** button on the Main toolbar. This solves the semiconductor diode model using the new range of parameters. When it is done, you can continue with the optimization.

6 From the **Solve** menu, open the **Solver Manager** dialog box.

7 In the frame **Values of variables not solved for and Linearization point**, click the **Current solution** button, and choose **All** from the **Parameter value** list.

8 On the **Solve For** page, select the **ODE (OD)** and **Optimization (opt)** items. Make sure that no other items are selected.

9 Click **OK**.

10 From the **Solve** menu, open the **Solver Parameters** dialog box.

11 Select the **Optimization/Sensitivity** check box.

12 On the **Optimization/Sensitivity** page, set the **Analysis** to **Optimization**.

13 Click **OK**.

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

The parameter sweep suffers from some overhead because it needs to analyze the equations from the semiconductor diode problem in each step. It is possible to speed up the simulation by using interpolation functions. First you create an interpolation function holding the IV-characteristics from the diode model. Then you delete the three application modes for that model, and change the objective function so it uses the interpolation function instead of the variable `Ic`. Such an operation reduces the time for the parameter sweep about 8 times.

POSTPROCESSING AND VISUALIZATION

1 From the **Postprocessing** menu, choose **Global Variables Plot**.

2 In the **Global Variables plot** dialog box, type `Ic` in the **Expression** edit field and click the **>** button.

3 From the **Predefined quantities** list, choose **D1.i** and click the **>** button. You should now see the two variables in the **Quantities to plot** list.

4 Click the **Line Settings** button.

5 In the dialog box that appears choose **Cycle** for both the **Line style** list and the **Line marker** list.

6 Select the **Legend** check box and click **OK** to close the **Line Settings** dialog box.

7 Click the **Title/Axis** button. In the dialog box that appears, select the **Log scale** check box for the **Second axis label**.

8 Click **OK**.

9 Click **OK** again to see the plot in Figure 12-12 on page 512.

10 To view the calculated SPICE parameters, choose **Data Display>Global** from the **Postprocessing** menu.

11 From the **Predefined quantities** list, choose **Optimization (opt)>sim_DI_N**.

12 Click **Apply** to see the ideality factor in the message log at the bottom of the main user interface. Do the same for each of the variables **logIS**, **sim_DI_NR**, **logISR**, **logRS**, and **logIKF** to see their values.

13 To see the actual values for the variables in log-scale, just type `10^` in front of the variable name in the **Expression** edit field before you click **Apply**.

13

Structural Mechanics Models

This section contains a modal analysis of a crankshaft based on a NASTRAN mesh; a 3D model of a feeder clamp; a parametric study of the stresses in a pulley; and a model of a communication mast's diagonal mounting. The model of the communication mast is a 3D model that highlights the use of assemblies, interactive meshing, and import of CAD data. There is also a model that performs topology optimization of a loaded knee (the model requires the Optimization Lab). The *COMSOL Multiphysics Modeling Guide* includes two benchmark models using 2D stress analysis. A comprehensive set of solved examples is available in the Model Library that comes with the Structural Mechanics Module.

Eigenvalue Analysis of a Crankshaft

This model describes a modal analysis of a crankshaft. The pistons' reciprocating movement is transferred to the crankshaft through connecting rods by means of crankshaft throws. The forces, torques, and bending moments, which are highly variable both in time and space, subject the crankshaft to very high and complex loading. The crankshaft design must therefore incorporate careful and precise calculations of the vibrational characteristics.

Model Definition

GEOMETRY

The geometry comes from a NASTRAN mesh, which you import into the COMSOL Multiphysics user interface.

MATERIAL PROPERTIES AND BOUNDARY CONDITIONS

The crankshaft geometry is in millimeters, and a suitable unit system for geometries given in millimeters is the MPa system. The crankshaft is made of solid steel, and you give the material properties in the MPa unit system; that is, express the Young's modulus in MPa and the density in t/mm^3.

The boundary conditions are as follows:

- The crankshaft's main bearing surfaces are constrained from moving in the normal directions; that is, the crankshaft is allowed to rotate and slide at the bearing surfaces.
- The axial movement is constrained at the rear axial bearing surface.
- The crankshaft is fixed at the rear surface where the flywheel is mounted.

Results

The analysis provides the 20 first eigenfrequencies, of which several of them show the same modal shapes. This first eigenmode has an eigenfrequency at approximately 5778 Hz and it has a torsional characteristic. There are five additional eigenfrequencies in rather close vicinity to this frequency. Each of them also shows similar torsional characteristics, which suggests that they are all in fact showing the first torsional mode.

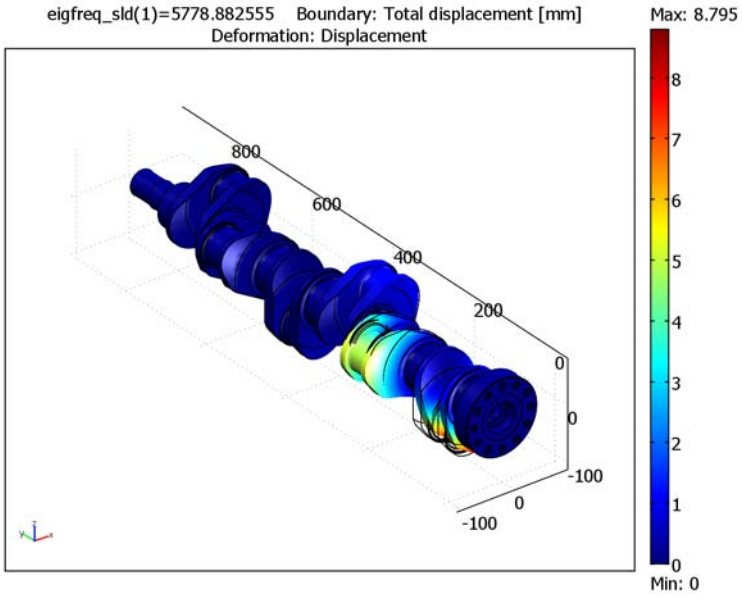


Figure 13-1: The first torsional mode in the crankshaft.

The next distinctly shaped eigenmode has an eigenfrequency at 8132 Hz. It can be characterized as a bending mode in the crankshaft throws. Here there are also five additional eigenfrequencies in rather close vicinity to this frequency. Each of these frequencies shows similar bending shapes as in the previously mentioned eigenmode at 8132 Hz. This suggests that they are all in fact showing the first bending mode in the crankshaft throws.

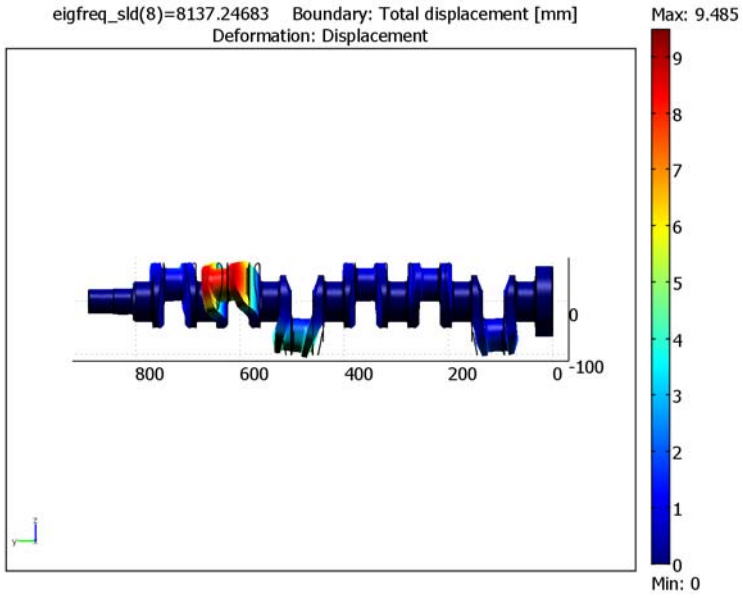


Figure 13-2: The bending mode of the crankshaft throws.

The third distinctly shaped eigenmode has an eigenfrequency at 8891 Hz. This modal shape can be characterized as a twisting mode in the crankshaft throws. There are, in the same manner as earlier, five additional eigenfrequencies in rather close vicinity to this frequency. Each of these frequencies shows similar twisting shapes.

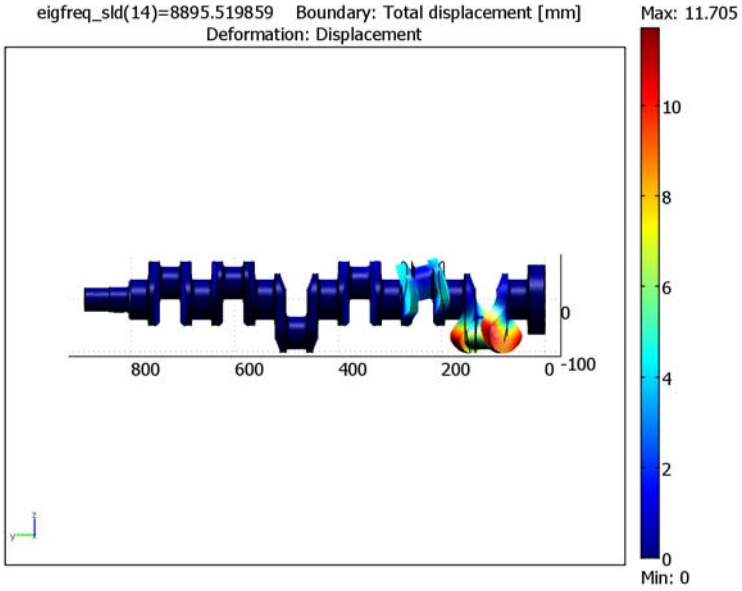


Figure 13-3: The twisting mode of the crankshaft throws.

Model Library path: `COMSOL_Multiphysics/Structural_Mechanics/crankshaft`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, and in the **Space dimension** list select **3D**.

2 In the list of application modes select **COMSOL Multiphysics>Structural Mechanics>Solid, Stress-Strain>Eigenfrequency analysis**.

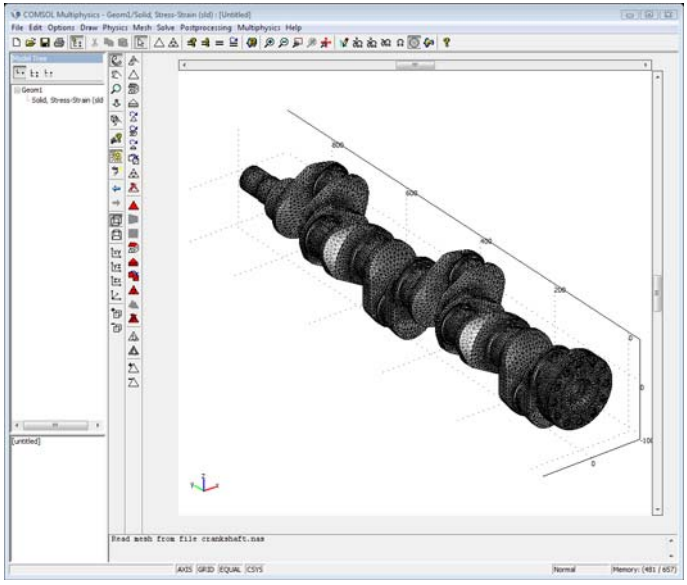
3 Click **OK**.

GEOMETRY MODELING

1 From the **File** menu choose **Import** and then **Mesh From File**.

2 Browse to the NASTRAN mesh file located at `models/COMSOL_Multiphysics/Structural_Mechanics/crankshaft.nas` in the COMSOL installation directory.

3 Click the **Import** button.



PHYSICS SETTINGS

Model Settings

1 From the **Physics** menu choose **Model Settings**.

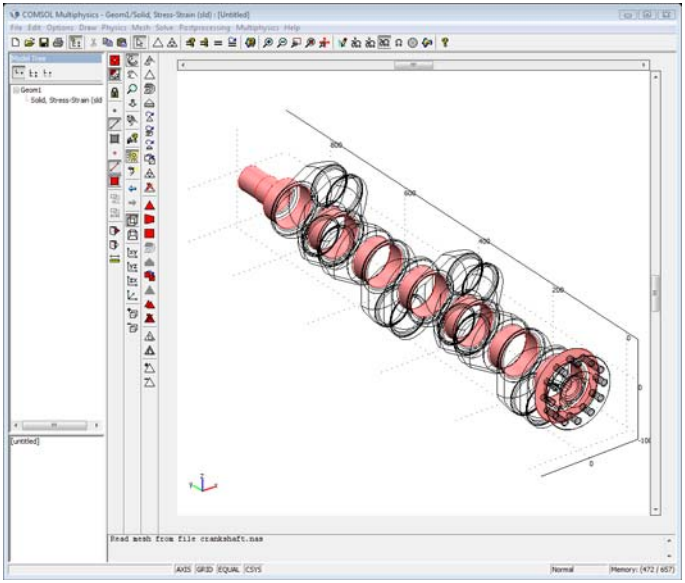
2 In the **Base unit system** list select **MPa**.

3 Click **OK**.

Boundary Conditions

1 From the **Physics** menu choose **Boundary Settings**.

2 In the **Boundary selection** list choose Boundaries 27, 55, 65, and 68–74.



3 Click the **General notation, Hu=R** button, then click the **Edit** button associated with the **H Matrix**. In the matrix position (1, 1) enter nx, in the (1, 2) position enter ny, and in the (1, 3) position enter nz. Click **OK**.

These settings constrain the normal direction movements of the main bearing surfaces.

4 In the **Boundary selection** list choose **26**.

5 Click the **Standard notation** button, then select the $\mathbf{R_x}$, $\mathbf{R_y}$, and $\mathbf{R_z}$ check boxes to fix this surface.

6 Click **OK**.

Subdomain Settings

The crankshaft geometry is in millimeters. This means that you must enter the material properties in the MPa unit system to avoid having to scale the geometry; that is, you specify the Young's modulus in MPa and the density in t/mm^3.

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

2 Select Subdomain 1, then enter the following material properties:

PROPERTY	VALUE
E	2.0e5
ν	0.33
ρ	7850e-12

3 Click the **Element** tab.

4 Select **Lagrange - Linear** in the **Predefined elements** list. The model uses linear elements to conform with the NASTRAN mesh.

5 Click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu choose **Solver Parameters**.

2 In the **General** page go to the **Desired number of eigenfrequencies** edit field and enter 20. Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

COMSOL Multiphysics plots the first eigenmode using a slice plot. To change the plot to show the deformed shape and other eigenmodes, follow these steps:

1 From the **Postprocessing** menu choose **Plot Parameters**.

2 In the **Plot type** area on the **General** page, clear the **Slice** check box, then select the **Boundary** and **Deformed shape** check boxes.

3 Select the second eigenfrequency in the **Eigenfrequency** list and click **Apply** to plot it.

4 Select the last eigenfrequency in the **Eigenfrequency** list and click **OK** to plot the twentieth eigenmode and close the **Plot Parameters** dialog box.

Deformation of a Feeder Clamp

Introduction

This example, from the field of structural mechanics, analyzes the deformation of a feeder clamp under stress. The clamp secures a feeder that carries high-frequency electromagnetic fields, and it's important that it remains as straight as possible.

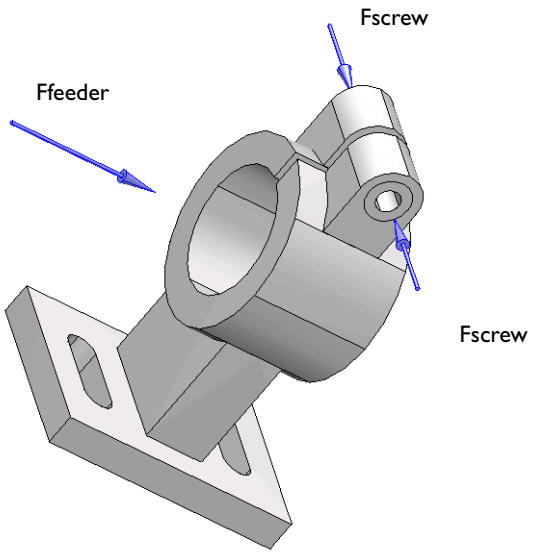
This example analyzes deformations in the clamp with two key questions in mind:

- How much does the force from the feeder incline the clamp? The inclination must be less than 1 degree.
- Does a prestressed screw of a certain type have enough strength to deform the clamp so that it adequately anchors the feeder? The gap must shrink by at least 0.5 mm.

Model Definition

Forces on the clamp include those from the feeder as well as those on the sleeve arising from the clamping screw. In this analysis, the feeder clamp is attached to a wall using only one of its two mounting holes, so that you can better analyze how it performs when poorly secured.

.



LOADING DATA

Assume that an installation technician fastens the feeder into the clamp using a standard metric M3 screw of Class 8.8 (where the first digit stands for a breaking load of 800 N/mm^2, and the second digit indicates a yield strength of 80% of the breaking strength). Prestressing the screw to the yield limit results in a screw force of 4500 N. This model tests if a screw force of 80% of this is adequate. A 7-mm washer distributes the prestressed load evenly onto both sides of the sleeve. The maximum load from the feeder onto the clamp is 1000 N, and is applied evenly throughout the inside of the clamp.

Due to symmetry in both loading and the geometry, you can perform a complete model analysis while looking at only one half of the geometry. For illustrative purposes, though, this example models the entire geometry.

The *z*-deformation for the whole clamp is depicted in Figure 13-4.

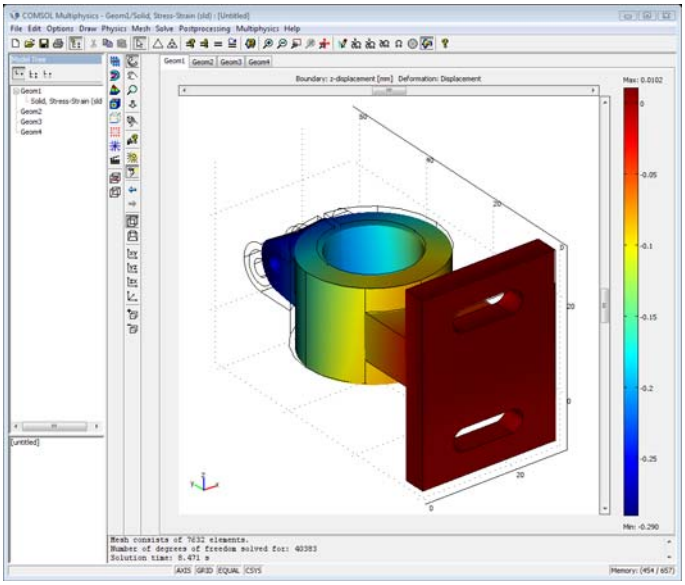


Figure 13-4: z-deformation.

The maximum inclination about the *z*-axis can be derived from the difference between the maximum and the minimum deformation in the *y* direction.The maximum and minimum values can be found from the color legend on the right in Figure 13-5. It can be shown that the sine of the maximum inclination is equal to the difference between the maximum and the minimum *y*-deformation, divided by the width of the clamp in the *z* direction. For small angles, a, this becomes

$$\alpha = \frac{0.094 - (-0.014)}{20} \cdot \frac{180}{\pi}$$

which gives an inclination of 0.31 degrees which is less than the maximum allowed angle of 1 degree.

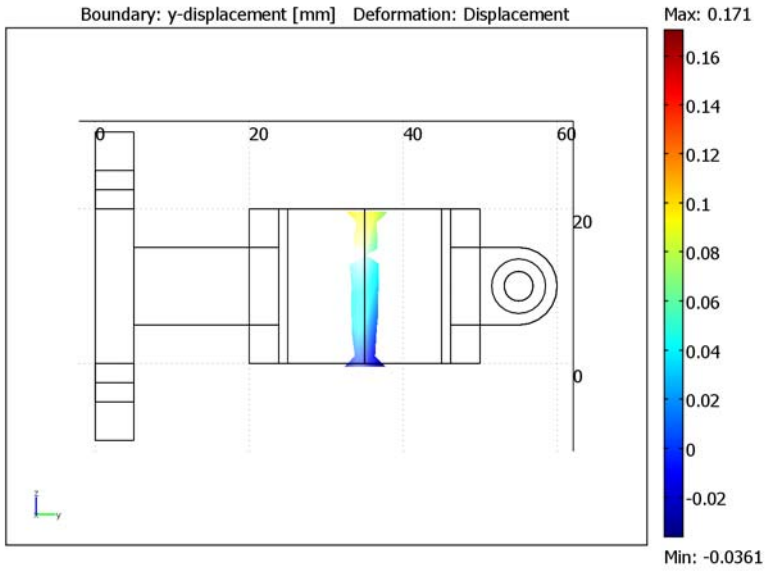


Figure 13-5: Maximum and minimum y-displacement at the center of the clamp cylinder.

To see the maximum displacement in the x direction, you can plot abs(u)> 0.25 mm. Figure 13-6 shows that the deformation in the feeder clamp gap is larger than 0.25 mm on both sides, which is the minimum requirement for being able to fasten the feeder adequately. The boundary conditions in this model are valid only as long as the installation technician does not squeeze the gap in the clamping sleeve completely shut. However, if the gap is squeezed shut, you can be sure that the requirements are fulfilled.

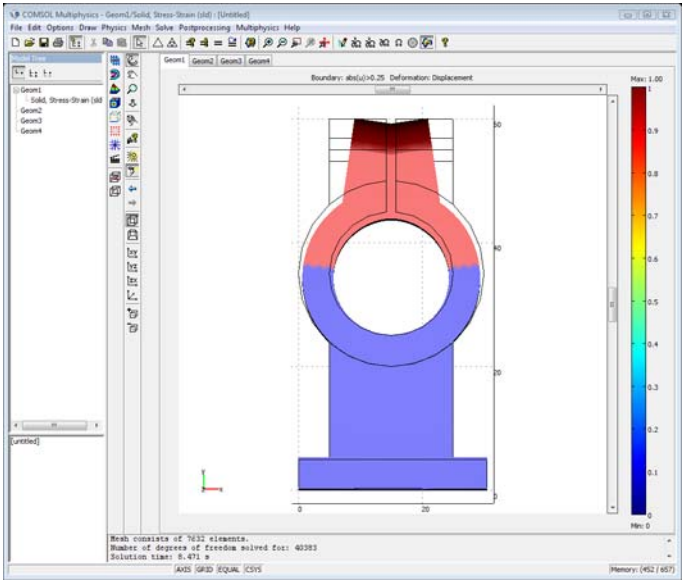


Figure 13-6: Clamp deformation due to the screw force.

Model Library path: `COMSOL_Multiphysics/Structural_Mechanics/feeder_clamp`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

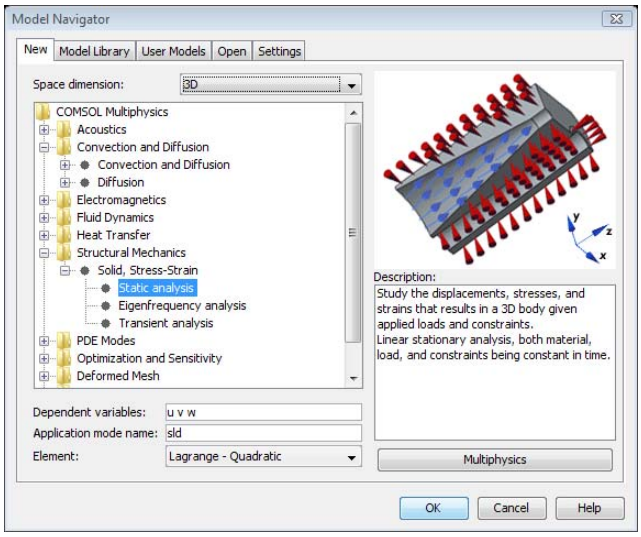
1 Start COMSOL Multiphysics. This invokes the **Model Navigator**.

2 On the **New** page, select **3D** from the **Space dimension** list.

3 Double-click the **COMSOL Multiphysics>Structural Mechanics** folder and select **Solid, Stress-Strain>Static analysis**.

4 Click **OK**.

Notice that this gives you second-order elements, **Lagrange - Quadratic**, by default.



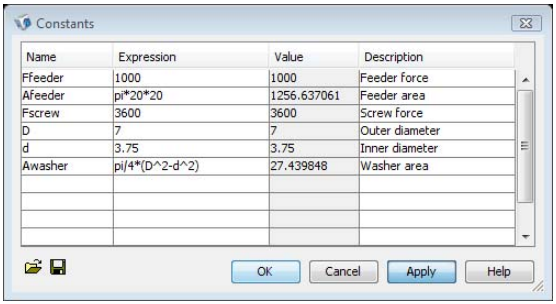
OPTIONS AND SETTINGS

1. Double-click **AXIS** on the status bar to turn off the 3D axis.
2. Choose **Model Settings** from the **Physics** menu and select **MPa** from the **Base unit system** list. Click **OK**.
3. Choose **Constants** from the **Options** menu.
4. Enter the following constant names, expressions, and descriptions (optional):

NAME OF CONSTANT	EXPRESSION	DESCRIPTION
Ffeeder	1000	Feeder force
Afeeder	pi*20*20	Feeder area
Fscrew	3600	Screw force
D	7	Outer diameter
d	3.75	Inner diameter
Awasher	pi/4*(D^2-d^2)	Washer area

To add a constant, enter its name in the **Name** edit field and its corresponding constant value or defining equation in the **Expression** edit field. Adding a description

in the **Description** edit field is optional. After you finish entering constants, click **Apply** to evaluate all the expressions.



5 Click **OK**.

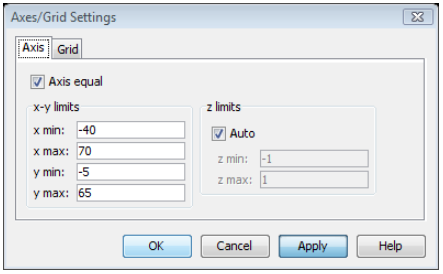
GEOMETRY MODELING

Creating the First Work-Plane Geometry

1 Choose **Work-Plane Settings** from the **Draw** menu and click **OK** in the dialog box to enter the default work plane, which is the *xy*-plane.

2 Choose **Axes/Grid Settings** from the **Options** menu to open the corresponding dialog box.

3 On the **Axis** page, type `-40`, `70`, `-5`, and `65` in the **x min**, **x max**, **y min**, and **y max** edit fields, respectively. Click **Apply** to update the axis settings.



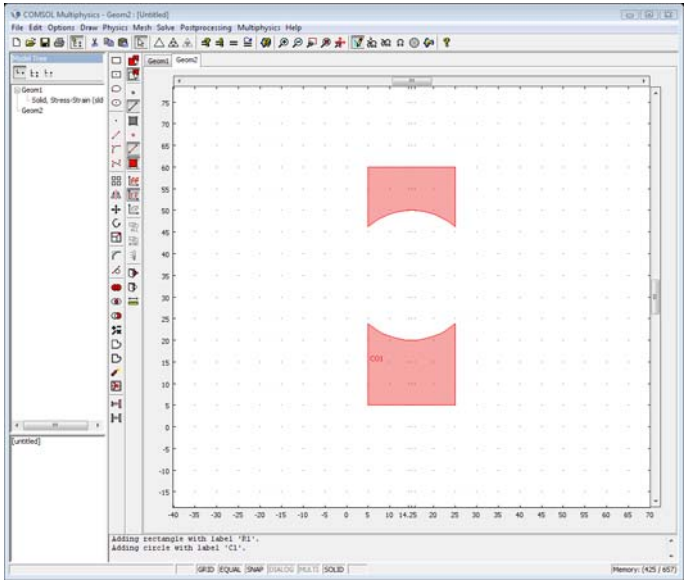
4 Click the **Grid** tab. Clear the **Auto** check box, and type `5` in both the **x spacing** and **y spacing** edit fields. Add extra grid lines at $x = 14.25$ and $x = 15.75$ by entering these values, with a space separating them, in the **Extra x** edit field. Click **OK**.

5 Using the left mouse button, draw a rectangle with corners at (5, 5) and (25, 60). Use the **Rectangle/Square** button on the Draw toolbar.

6 Draw a circle with a radius of 15 by selecting the **Ellipse/Circle (Centered)** toolbar button. Using the right mouse button, place the center of the circle at (15, 35) and drag the mouse until you have the correct radius. During dragging, you can monitor the current value of the radius in the coordinate field to the left in the Status bar.

7 Press Ctrl+A to select both geometry objects.

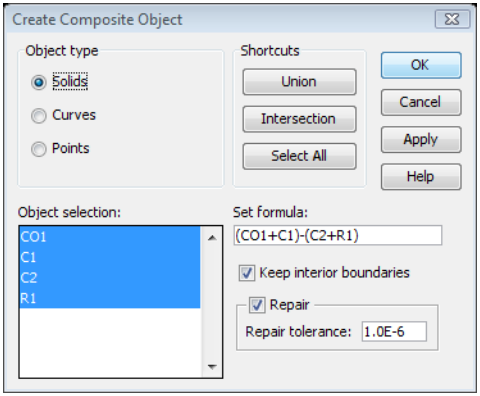
8 Click the **Difference** button on the Draw toolbar to remove the circle from the rectangle.



9 Draw another circle with the same radius at the same position as the deleted one. Then draw yet another circle centered at (15, 35), but give this one a radius of 10. Select the **Ellipse/Circle (Centered)** button on the Draw toolbar and then click-and-drag using the right mouse button to create a circle.

10 Draw a rectangle with corners at (14.25, 40) and (15.75, 60) by choosing the **Rectangle/Square** button and using the extra grid lines.

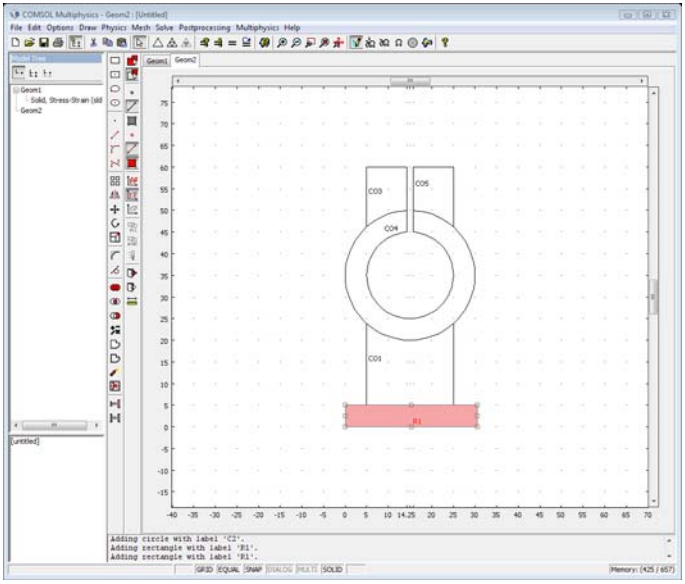
11 Click the **Create Composite Object** button on the Draw toolbar. In the **Set formula** edit field of the dialog box that opens enter the Boolean expression `(CO1+C1)-(C2+R1)`. Click **OK** to create the composite solid object CO2.



I2 If you make a mistake, choose **Undo** from the **Edit** menu to revert to the previous state.

I3 Split the created composite solid object into its constituents. To do so, click the **Split Object** button on the Draw toolbar.

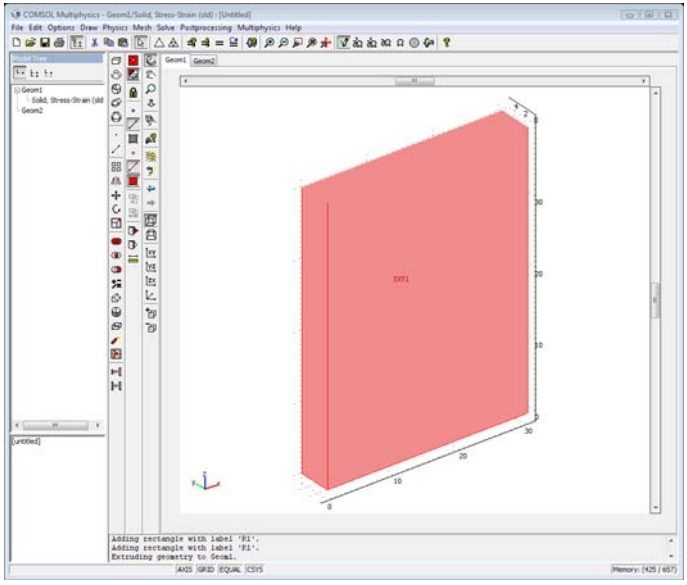
I4 Click the **Rectangle/Square** toolbar button and use the left mouse button to make a rectangle with corners at (0, 0) and (30, 5).



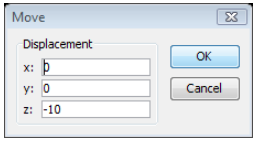
Extruding the 2D Geometry Objects into 3D Solid Objects

1 To extrude the 2D rectangle into a 3D object, choose **Extrude** from the **Draw** menu. This selection opens the **Extrude** dialog box. Make sure that the last created rectangle is selected and enter 40 in the **Distance** edit field before clicking **OK**.

2 The resulting 3D geometry object appears in a 3D view. Click **Zoom Extents** in the main toolbar to view the entire block.



3 Click the **Move** button in the Draw toolbar; in the resulting dialog box first make sure the 3D block is selected. Then enter a z-displacement of −10 and click **OK**.



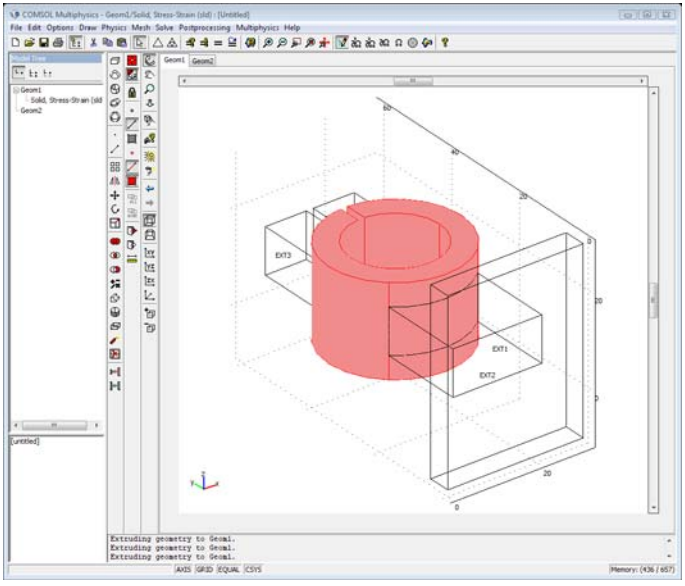
4 Enter the work plane again by selecting **I Geom2 (2D)** from the **Draw** menu. Click the **Projection of All 3D Geometries** button at the lower part of the Draw toolbar.

5 While working in the plane, open the **Extrude** dialog box from the **Draw** menu and select the objects CO1, CO3, and CO5 that came from the first rectangle you created. Enter an extruding distance of 10. Click **OK** to extrude the 2D geometry and enter the 3D view.

6 Make sure that the recently created 3D objects are selected. Click the **Move** button on the Draw toolbar. In the resulting dialog box enter 5 in the **z** edit field and click **OK**.

7 Re-enter the work plane by selecting **I Geom2 (2D)** from the **Draw** menu.

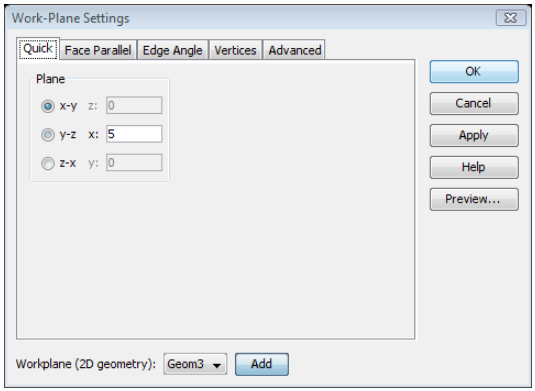
8 Select the circular-shaped solid object, object CO4, and open the **Extrude** dialog box. Enter a distance of 20 and click **OK**. Click **Zoom Extents** in the Main toolbar to see the entire resulting geometry. Click and drag in the figure to rotate the geometry to get the desired view.



Creating a Second Work Plane

1 It is now necessary to add a work plane, so choose **Work-Plane Settings** from the **Draw** menu. In the resulting dialog box, click the **Add** button. The software creates a work

plane and automatically assigns it the name Geom3. Select the **Quick** page. Click the **y-z** button and specify an offset of 5 in the **x** edit field.



2. Click **OK** to enter the work plane environment and then click the **Zoom Extents** button in the work plane. The 3D projection of the geometry onto the work plane is visible if any of the **Projection of All 3D Geometries** or **Project Work-Plane Intersection** buttons are selected at the bottom of the Draw toolbar. You can snap to the projection when drawing.
3. Choose **Axes/Grid Settings** from the **Options** menu. In the resulting dialog box, go to the **Grid** page, uncheck the **Auto** check box and enter a grid spacing of 5 in both the **x spacing** and **y spacing** fields. Add extra grid lines at $x = 56.875$ and $x = 58.5$ by entering these values, separated with a space, in the **Extra x** field. Click **OK** to close the dialog box.
4. Draw a circle with its center at (55, 10) by choosing **Ellipse/Circle (Centered)** and clicking the right mouse button. Drag the cursor from the center to the right and release the button over one of the extra grid lines. Draw another circle centered at the same position, but this time release the mouse button over the other extra grid line. Now you have two circles with radii of 1.875 and 3.5.
5. Press Ctrl+A to select both circles. Click the **Difference** button on the Draw toolbar to subtract the smaller circle from the larger one. The resulting object is given the name CO1.
6. Redraw the smaller of the two circles. The circle is given the name C1 by the software. Additionally draw a new circle with a radius of 5 with the same center coordinates. It will be named C2. Click the **Rectangle/Square** button and use the left mouse button to draw a rectangle with corners at (55, 5) and (60, 15).

7 Open the **Create Composite Object** dialog box by Shift-clicking the associated button on the Draw toolbar. In the **Set formula** edit field type `R1-C2+C1`. Click **OK** to create the composite solid object CO2.

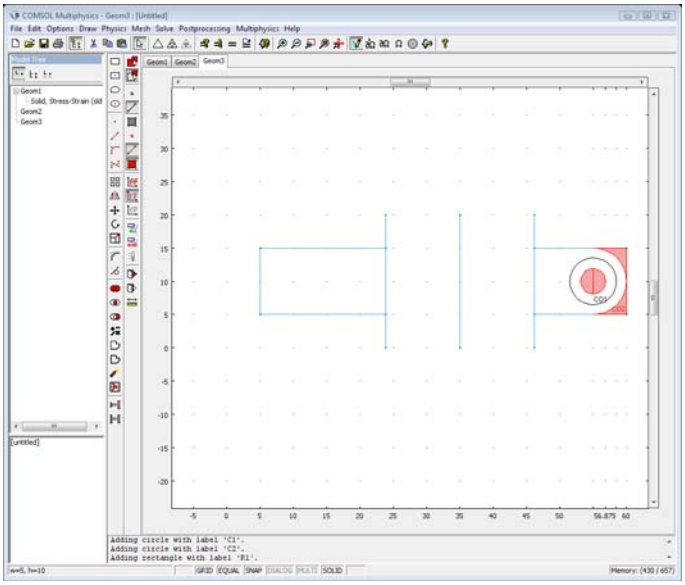


Figure 13-7: Extruding the 2D Geometry Object and Creating 3D Solid Object

1 Choose **Extrude** from the **Draw** menu. In the resulting dialog box make sure the last created object, CO2, is selected. Then enter `9.25` in the **Distance** edit field and click **OK**.

2 In 3D view, click the **Copy** button in the main toolbar and then click the **Paste** button. In the **Displacement** area, enter an *x*-displacement of `10.75` in the **x** edit field, then click **OK**.

3 Return to the work plane by clicking on the **Geom3** tab above the drawing area.

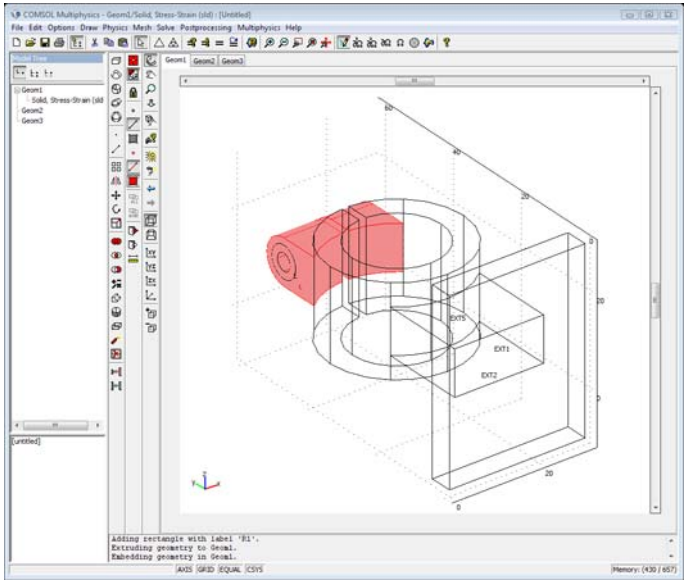
4 To define the area of the washer that distributes pressure from the screw, choose **Embed** from the **Draw** menu. In the resulting dialog box, select CO1 and click **OK**.

5 In 3D view, click the **Copy** button in the main toolbar and then click the **Paste** button. In the **Displacement** area, enter an *x*-displacement of `20` in the **x** edit field, then click **OK**.

6 To round off the top of the clamp and create a hole for the clamping screw, subtract solid object EXT6 and EXT7 from objects EXT3 and EXT4 using the **Create Composite Object** dialog box.

To do so, click the **Create Composite Object** toolbar button to open the dialog box and select the **Solids** option button in the **Object type** frame.

7 Type `(EXT3+EXT4)-EXT6-EXT7` in the **Set formula** edit field. Click **OK**.



8 You can add lighting to the plot by clicking the **Headlight** button in the Camera toolbar.

Creating a Third Work Plane and the Final 3D Solid Model

1 Press Ctrl+A to select all geometry objects, then choose **Work-Plane Settings** from the **Draw** menu.

2 In the dialog box, click the **Add** button to create a new work plane, which automatically gets the name Geom4. On the **Face Parallel** page select the folder/solid object EXT1 and the face number **2** from the list. Click the **Downward normal** button. Click **OK** to enter the new work plane.

3 Select **Axes/Grid Settings** from the **Options** menu. In the resulting dialog box, click the **Grid** tab, clear the **Auto** check box, and enter a grid spacing of `2.5` in both the **x spacing** and **y spacing** fields. Add extra grid lines at $x = 9.5$ and $x = 20.5$ by entering

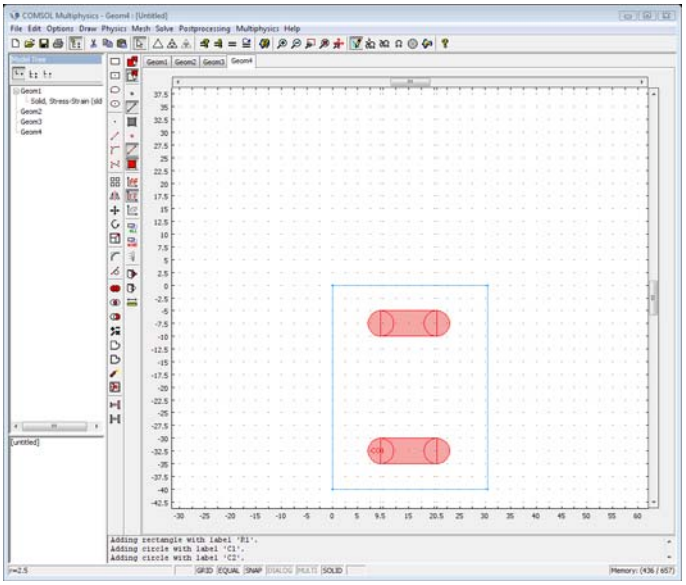
these values, separated by a space, in the **Extra x** edit field. Click **OK** to close the dialog box. Click the **Zoom Extents** button on the Main toolbar.

4. Draw a rectangle with corners at (9.5, –10) and (20.5, –5) using the left mouse button and the **Rectangle/Square** toolbar button.

5. Click the **Ellipse/Circle (Centered)** button, and use the right mouse button to draw a circle centered at (9.5, –7.5) with a radius of 2.5. Draw a similar circle centered at (20.5, –7.5).

6. Press Ctrl+A to select all objects. Click the **Copy** button in the main toolbar, then click the **Paste** button. In the **Displacement** area, enter a *y*-displacement of `-25` in the **y** edit field, then click **OK**.

7. Press Ctrl+A to select all objects and click the **Union** button in the Draw toolbar.



8. Choose **Extrude** from the **Draw** menu. In the dialog box, type `5` in the **Distance** edit field. Click **OK** to enter 3D view.

9. In 3D view, the recently extruded objects are already selected. Holding down the Shift key, click on the block you created first, `EXT1`, using the left mouse button to add it to the selection. Then click the **Difference** toolbar button to create the mounting holes in the clamp.

Boundary Conditions

The boundary conditions consist of loads and constraints. The following tables list the loads (top) and constraints (bottom):

	BOUNDARY 25		BOUNDARY 68		BOUNDARIES 17, 18, 45, 47	
Page	Load		Load		Load	
	F_x	`Fscrew/Awasher`	F_x	`-Fscrew/Awasher`	F_x	0
	F_y	0	F_y	0	F_y	0
	F_z	0	F_z	0	F_z	`-Ffeeder/Afeeder`

	BOUNDARIES 32, 33, 36, 37, 60, 61	
Page	Constraint	
	R_x	0
	R_y	0
	R_z	0

The constraint means that the feeder clamp is fixed (no displacements) at the mount. All other boundaries are free.

In relatively complicated geometries like this it is often convenient to arrange the different boundaries in groups. This allows you to set properties for a group of domains at once. To simplify the specification of the boundary conditions, create five groups:

- `clamp`, containing the four boundaries which constitute the inside surface of the large cylinder. These are the boundaries where the feeder force is applied.
- `mount`, containing the six boundaries where the feeder clamp is attached.
- `washer top`, containing the top boundary where the screw force is applied.
- `washer bottom`, containing the bottom boundary, where the screw force is applied.
- `free`, containing the rest of the boundaries, which are free of loads and constraints.

The following steps describe, in addition to the boundary settings, how to create the boundary domain groups.

1. Open the **Boundary Settings** dialog box by selecting **Boundary Settings** from the **Physics** menu. This dialog box enables you to select boundaries and enter expressions for boundary conditions.
2. To create the boundary groups, click the **Groups** tab. Select the existing group **(unnamed1)**, enter the name `free` in the **Name** edit field, and press Enter.

3 Click the **New** button and enter the name `clamp`, and press Enter. Similarly, add the remaining groups `mount`, `washer top`, and `washer bottom`.

Now enter the boundary conditions for the groups:

GROUP	WASHER TOP		WASHER BOTTOM		CLAMP	
Page	Load		Load		Load	
	F_x	`Fscrew/Awasher`	F_x	`-Fscrew/Awasher`	F_x	0
	F_y	0	F_y	0	F_y	0
	F_z	0	F_z	0	F_z	`-Ffeeder/Afeeder`

GROUP	MOUNT	
Page	Constraint	
	R_x	0
	R_y	0
	R_z	0

The **free** group should have the default settings, so make sure that all loads are zero for this group and that none of the displacement check boxes are selected on the **Constraint** tab.

1 Click the **Boundaries** tab and select Boundary 25, then choose **washer top** from the **Group** list.

2 Select Boundary 68, then choose **washer bottom** from the **Group** list.

3 Select Boundaries 17, 18, 45, and 47, then choose **clamp** from the **Group** list.

4 Select Boundaries 32, 33, 36, 37, 60, and 61, then choose **mount** from the **Group** drop down list.

5 Make sure the remaining boundaries belong to the **free** group.

6 Click **OK** to close the dialog box.

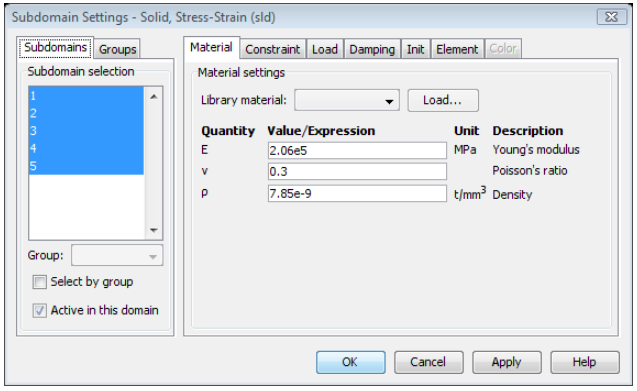
Subdomain Settings

The domain parameters for this model are:

SETTINGS	SUBDOMAINS 1–5
E	`2.06e5`
ν	`0.3`

This example models the geometry in millimeters, which means that for consistency you must specify Young's modulus, E, in N/mm^2.

1. Open the **Subdomain Settings** dialog box by selecting **Subdomain Settings** from the **Physics** menu
2. Select all subdomains by pressing Ctrl+A.
3. Click the **Material** tab.
4. Ignore the value for the density, a parameter that has no effect on the solution in this static simulation.
5. Type `2.06e5` in the **E** edit field.
6. Type `0.3` in the edit field for Poisson's ratio, ν.
7. Click **OK**.



MESH GENERATION

Change the default mesh parameters to distribute the mesh elements in a more reasonable way. The maximal stresses in this model will be found in the sleeve, on the side facing the wall. Therefore, it makes sense to require a finer mesh in the sleeve than in the rest of the geometry. To accomplish this, do the following:

1. Choose **Free Mesh Parameters** from the **Mesh** menu.
2. Select **Coarser** from the **Predefined mesh sizes** list, which saves memory and computation time.
3. To obtain a higher mesh resolution in the sleeve (Subdomain 2), click the **Subdomain** tab, select Subdomain 2, and type `3` in the **Maximum element size** edit field. This imposes an upper bound of 3 mm on the element edge lengths in Subdomain 2.
4. Click the **Remesh** button.

5 Click **OK**.

COMPUTING THE SOLUTION

To start computing the solution, click the **Solve** toolbar button. COMSOL Multiphysics displays the results automatically as a slice plot of the von Mises stress.

POSTPROCESSING AND VISUALIZATION

1 Choose **Plot Parameters** from the **Postprocessing** menu to open the **Plot Parameters** dialog box. On the **General** page, clear the **Slice** check box and then select the **Boundary** and **Deformed shape** check boxes to add the corresponding plot types. The **Geometry edges** plot is on by default.

2 To plot the deformation in the *z* direction, select **z-displacement** in the **Predefined quantities** field on the **Boundary** page.

3 Click **Apply** to display a plot using the new settings (see Figure 13-4).

4 To change the view of the solution plot, work with the buttons in the Camera toolbar.

5 To compute the maximum inclination in the *z* direction, you can derive it from the difference between the maximum and the minimum deformation in the *y* direction. Select **y-displacement** from the **Predefined quantities** list on the **Boundary** page in the **Plot Parameters** dialog box.

6 On the **General** page, select the **Element selection** check box and type `(x==5)&&(y==35)` in the **Logical expression for inclusion** edit field. Select **At least one** from the **Element nodes to fulfill expression** list and click **OK**. This plots the deformation on the inside of the feeder clamp. Click the **Go to YZ View** button to get a better view (see Figure 13-5).

7 To see the maximum displacement in the *x* direction, clear the **Element selection** check box on the **General** page in the **Plot Parameters** dialog box and type `abs(u)>0.25` in the **Expression** edit field on the **Boundary** page. Click **OK**.

To get a better view of the clamping sleeve, zoom in on the top of the clamp; click the **Go to XY View** button and use the **Zoom Window** button in the Main toolbar (see Figure 13-6).

Topology Optimization of a Loaded Knee Structure

Introduction

Imagine that you are designing a light-weight mountain bike frame that should fit in a box of a certain size and it should weigh no more than 8 kg. Given that you know the loads on the bike, you can achieve this by distributing the available material while making sure that the stiffness of the frame is at a maximum. This way you have formulated the topology optimization of the frame as a material distribution problem.

This model demonstrates how you can apply the *SIMP model* (Solid Isotropic Material with Penalization) for structural topology optimization with COMSOL Multiphysics.

Model Definition

The maximum stiffness structural optimization problem is often formulated as the equivalent minimum compliance problem, which can be written as

$$\begin{aligned} &\text{minimize} && c(\rho) = \int_{\Omega} \frac{1}{2}\varepsilon^T \mathbf{D}(\rho)\varepsilon d\Omega \\ &\text{such that} && \int_{\Omega} \varepsilon^T \mathbf{D}\varepsilon d\Omega = \int_{\Omega} \mathbf{f}\mathbf{u} d\Omega + \int_{\Gamma_t} \mathbf{t}\mathbf{u} ds \end{aligned} \tag{13-1}$$

Here Ω denotes the design domain; ε and $\mathbf{u}$ are the strain and displacement vectors; $\mathbf{D}$ refers to the stiffness matrix; $\mathbf{f}$ is an applied body load; and $\mathbf{t}$ is a boundary traction.

In the SIMP model, the stiffness matrix is expressed as

$$\begin{gathered} \mathbf{D}(\rho,\mathbf{x}) = \rho(\mathbf{x})^p \mathbf{D}_0, \\ p > 1, \\ \mathbf{x} \in \Omega \end{gathered} \tag{13-2}$$

In the above equation, $\mathbf{D}_0$ represents the stiffness matrix of a given isotropic material, and p is a penalty parameter. The design variable, $\rho(\mathbf{x})$, which can be interpreted as a generalized material density, is required to satisfy the following constraints:

$$0 \le \int_{\Omega} \rho(\mathbf{x}) d\Omega \le V, \qquad 0 \le \rho(\mathbf{x}) \le 1 \tag{13-3}$$

where V is the material volume available for distribution. A penalty parameter value above 1 assures that density values of 0 (no material) or 1 (material) are favored ahead of the intermediate values.

The model geometry is an L-shaped knee structure, see Figure 13-8 below.

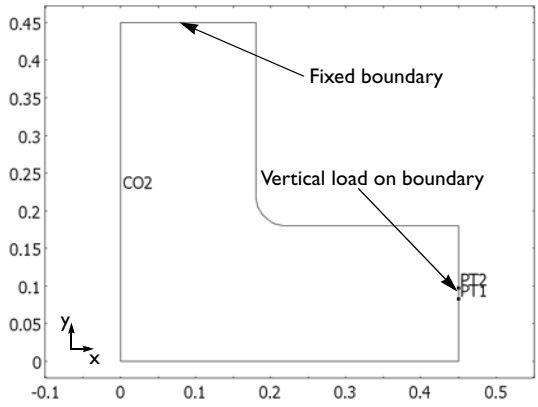


Figure 13-8: Geometry of the structure with loads and constraints.

The structure's uppermost boundary is fixed and you can apply a load in the negative y direction on the boundary shown in the figure above.

The material properties for the base material are Young's modulus, $E_0 = 200$ GPa, and Poisson's ratio, $\nu = 0.33$.

According to Ref. 1, the SIMP model can be considered as a two-phase material model in 2D if the penalty parameter, p, satisfies that

$$p \ge \max\left\{\frac{2}{1-\nu}, \frac{4}{1+\nu}\right\} \tag{13-4}$$

According to Equation 13-4 the smallest admissible p is 3 for $\nu = 0.33$.

THE FINITE ELEMENT MESH

Problems of this type are intrinsically mesh-size dependent. For this model, generate a mesh with the free quad mesher using a maximum element size of 0.007. The final mesh, shown in Figure 13-9, consists of approximately 2800 quadrilateral elements.

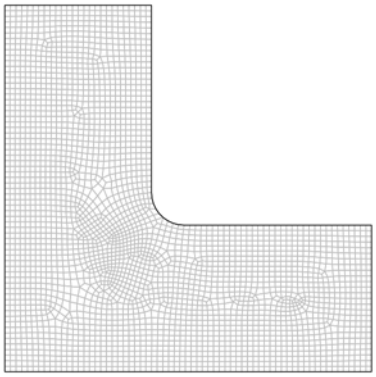


Figure 13-9: Finite element mesh of the structure.

Results and Discussion

Figure 13-10 and Figure 13-11 show the initial and optimal material distributions in the structure, respectively. Black areas represent material and white areas represent void. Unless composite materials are considered, gray areas are unphysical so a useful optimized design should be essentially black and white, like the one in Figure 13-11.

Figure 13-10: Initial distribution of the design variable.

Figure 13-11: Distribution of the design variable after optimization.

As discussed in Ref. 1, SIMP structural topology optimization problems are intrinsically mesh dependent. Because introducing more holes in a structure (without changing the volume) generally increases its efficiency, a finer mesh usually leads to a more detailed structure, approaching a fine-scale microstructure for sufficiently small mesh sizes.

Reference

1. M.P. Bendsøe and O. Sigmund, *Topology Optimization Theory, Methods, and Applications*, Springer, 2004.

Modeling in COMSOL Multiphysics

You can solve this structural optimization model by coupling two application modes:

- The Plane Stress application mode
  - solves for the displacements; corresponds to solving Equation 13-1 (2)
  - use Young's modulus according to Equation 13-2
- The Optimization application mode
  - solves for the design variable by minimizing the internal strain energy, Equation 13-1 (1)
  - define constraints according to Equation 13-3.

The internal strain energy is a predefined variable in COMSOL Multiphysics and is readily available to use as the objective function for the optimization problem. In each iteration, the software calculates a solution for the structural mechanics problem, based upon which the internal strain energy is calculated. The optimization routine then updates the design variable. If the specified convergence criterion is fulfilled, the solution process terminates; otherwise the new design variable value is used in the next calculation of the displacement field.

Model Library path: `COMSOL_Multiphysics/Structural_Mechanics/loaded_knee`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator** begin by clicking the **Multiphysics** button.

2 Select **COMSOL Multiphysics>Structural Mechanics>Plane Stress**, then click **Add**.

3 Select **COMSOL Multiphysics>Optimization and Sensitivity>Optimization**, then click **Add**.

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

GEOMETRY MODELING

1 Create two rectangles according to the following table. For each rectangle, Shift-click the **Rectangle/Square** button on the Draw toolbar; then specify width, height, and corner position; and finally click **OK**.

WIDTH	HEIGHT	CORNER
0.45	0.45	(0, 0)
0.27	0.27	(0.18, 0.18)

2 Click the **Zoom Extents** button to fit the model geometry to the drawing area.

3 Select both squares by pressing Ctrl+A, then click the **Difference** button on the Draw toolbar.

In the following steps you create a fillet at the inner corner of the L-shape.

4 Click the **Fillet/Chamfer** button on the Draw toolbar.

5 Select Vertex 3 and set the **Radius** to 0.04.

6 Click **OK**.

Next draw two points to define the boundary region where you later apply the load on the structure.

7 Draw the first point by shift-clicking the **Point** button and then entering `0.45` and `0.083` in the **x** and **y** edit fields, respectively. Click **OK**.

8 Repeat the previous step to draw the second point at the coordinates (0.45, 0.097).

The geometry should now look like that in Figure 13-8.

OPTIONS AND SETTINGS

Constants

1 From the **Options** menu, open the **Constants** dialog box.

2 Define constants according to the following table:

NAME	EXPRESSION	DESCRIPTION
F_load	700[kN/m]	Applied load
area_frac	0.45	Fraction of area to use for distributing material
p	3	SIMP penalty parameter

3 Click **OK** to close the dialog box.

Expressions

1 Choose **Options>Expressions>Scalar Expressions**.

2 Enter names and expressions according to the following table:

NAME	EXPRESSION	DESCRIPTION
E_SIMP	2e11[Pa]*rho_design^p	Penalized Young's modulus

3 Click **OK**.

Integration Variables

You can calculate the area of the structure and use it in expressions by defining an integration variable.

1 Select **Options>Integration Coupling Variables>Subdomain Variables**.

2 Select Subdomain 1. Type `area_tot` in the **Name** column and `1` in the **Expression** column.

3 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Plane Stress

1. From the **Model Tree** or the **Multiphysics** menu, select the **Plane Stress (ps)** application mode.
2. From the **Physics** menu, open the **Subdomain Settings** dialog box.
3. Select Subdomain 1, and type `E_SIMP` in the **E** edit field.
4. Click **OK**.

Boundary Conditions—Plane Stress

In the next steps, you fix the structure for rigid body translation and rotation by prescribing zero displacements along one of the sides, then apply the load.

1. From the **Physics** menu, open the **Boundary Settings** dialog box.
2. From the **Boundary selection** list, select Boundary 3.
3. Select the $\mathbf{R_x}$ and $\mathbf{R_y}$ check boxes and make sure that zero is specified in the corresponding edit fields.
4. Now select Boundary 7.
5. Switch to the **Load** page, then enter `-F_load` in the $\mathbf{F_y}$ edit field.

   All other boundaries have the default free boundary condition.
6. Click **OK**.

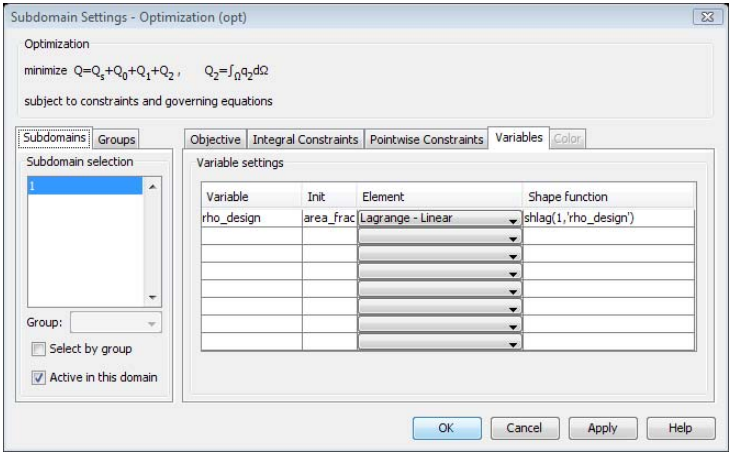
Subdomain Settings—Optimization

1. Select **Optimization (opt)** from the **Model Tree**.
2. Open the **Subdomain Settings** dialog box.
3. Select Subdomain 1 and switch to the **Parameters** page.

4 Edit the fields according to the following table:

VARIABLE	INIT	ELEMENT
rho_design	area_frac	Lagrange - Linear

This defines shape functions for `rho_design`, which is the design variable used in the optimization. The initial value corresponds to a uniform distribution of the available material throughout the structure.



Next you can constrain the design variable to the range $[10^{-4}, 1]$. According to Equation 13-3 (2) the lower bound of this interval should be zero. However, this would cause the stiffness matrix of the plane stress application mode to become singular.

5 Click the **Pointwise Constraints** tab.

6 Type `1e-4` in the **lb** edit field, `rho_design` in the **Expression** edit field, and `1` in the **ub** edit field.

Next define the variable name and the expression for the integral constraint Equation 13-3 (1).

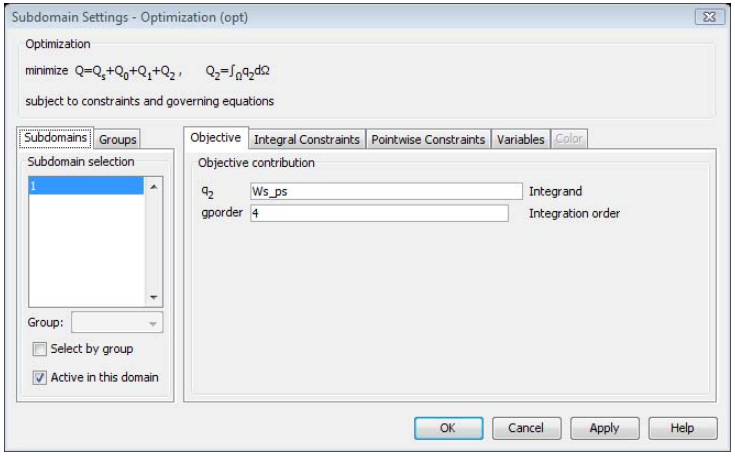
7 Click the **Integral Constraints** tab.

8 Enter `area_constr` in the **Name** field and `rho_design` in the $\mathbf{p_2}$ field.

Proceed to define the strain energy density as the objective function. Use the predefined variable `Ws_ps` from the Plane Stress application mode.

9 Click the **Objective** tab.

10 In the q_2 edit field, type `Ws_ps`.



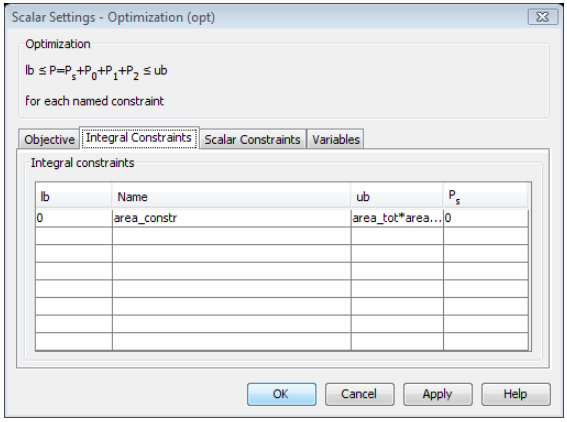
11 Click **OK**.

Scalar Settings—Optimization

Here you can define the bounds for the integral constraint, Equation 13-3 (1), which defines the amount of material available for design.

1 Choose **Physics>Scalar Settings**.

2 On the **Integral Constraints** page, in the first table row type `0` in the **lb** column, `area_tot*area_frac` in the **ub** column, and `0` in the P_s column.



3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 On the **Global** page, select the **Custom mesh size** check box.

3 In the **Maximum mesh size** edit field, type `7e-3`.

4 Click **OK**.

5 Click the **Mesh All (Free, Quad)** button on the Mesh toolbar.

COMPUTING THE SOLUTION—UNIFORM DISTRIBUTION

First solve the model for a uniform distribution of material, according to the initial value of the design parameter. Then, use this solution as a starting point for the optimization. By this procedure you can check that the initial solution looks reasonable. Alternatively, you can solve the full optimization problem in one go.

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

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

3 Make sure that **Optimization/Sensitivity** is not selected.

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

5 Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

The default plot shows the von Mises stress distribution in the structure. To view the initial distribution of the design variable, follow these steps:

1 Choose **Postprocessing>Plot Parameters**.

2 On the **General** page clear the **Geometry edges** check box.

3 Click the **Surface** tab.

4 From the **Predefined quantities** list, select **Optimization (opt)>rho_design**.

5 In the **Surface color** area, set the **Color table** to **GrayScale**. To make black correspond to material ($\rho = 1$) and white to void ($\rho = 0$), turn the color table on its head by selecting the **Reverse** check box.

6 Click **OK**.

COMPUTING THE SOLUTION—OPTIMIZATION

Now that you have obtained the initial solution, you continue by solving the optimization problem.

1 Open the **Solver Parameters** dialog box.

2 Select the **Optimization/Sensitivity** check box.

3 On the **Optimization/Sensitivity** page, set the **Analysis** to **Optimization**.

4 Click **OK**.

5 Click the **Solver Manager** button on the Main toolbar.

6 Select the **Current solution** check box in the **Initial value** area.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar to solve the model.

The optimization routine requires approximately 80 iterations and takes roughly 20–25 minutes depending on the computer. When the solver has finished, you should get the plot in Figure 13-11.

Stiffness Analysis of a Communication Mast's Diagonal Mounting

Introduction

Communication masts usually have a framework with a bolted triangular lattice design as illustrated in Figure 13-12. The diagonals of the framework are assembled from several parts and welded together.

When operating under a given wind load at a specific location, the antenna's total rotation angle should stay below a certain limit to ensure uninterrupted communications. For the type of mast in this model, the engineers have determined that its torsional stiffness is too low, and this effect is due to the geometry of the diagonal mountings. The goal is to increase the stiffness of such a diagonal mounting by first analyzing an existing 3D CAD geometry followed by an update of the geometry and a new analysis.

The model demonstrates the import of 3D CAD assemblies into COMSOL Multiphysics from a file and through the bidirectional interface to the SolidWorks

CAD software. This case also demonstrates the individual meshing of parts with the interactive meshing tools.

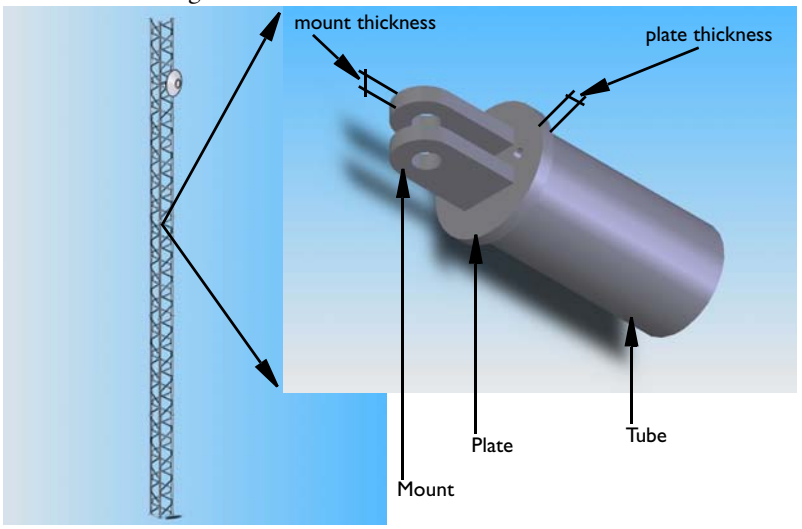


Figure 13-12: Mounting detail of a mast diagonal.

Model Definition

Start by importing and analyzing the diagonal mounting CAD assembly. The assembly includes only a short section of the diagonal tubing together with the other parts of the mounting as illustrated in Figure 13-12. Although a symmetry exists in both the geometry and load for this problem, this example models the entire assembly for illustrative purposes.

The geometry file is included in the model folder (`models/COMSOL_Multiphysics/Structural_Mechanics` in the COMSOL installation directory) both as a COMSOL Multiphysics binary file (`mast_diagonal_mounting_pt10_mt10.mphbin`) and as a Parasolid binary file (`mast_diagonal_mounting_pt10_mt10.x_b`). Importing the latter file requires the CAD Import Module.

After obtaining the stiffness of the assembly, assume that the geometry has been updated to improve the stiffness. Originally 10 mm, the plate thickness and mount thickness (see Figure 13-12) have been changed to 12 mm and 15 mm, respectively. You import the updated geometry file for the new analysis. These files are also included in the model folder with the name `mast_diagonal_mounting_pt12_mt15` with the

extensions `.mphbin` and `.x_b` for the COMSOL Multiphysics and the Parasolid binary format, respectively.

A third approach requires that both the CAD Import Module and SolidWorks software be installed on your computer. Here you use the bidirectional interface to SolidWorks to import and update the geometry. This method has the advantage that the boundary settings are saved between geometry updates. For complex problems this can result in considerable time savings. The necessary SolidWorks assembly and part files are included in the model folder; these are `mast_diagonal_mounting.sldasm`, `mount.sldprt`, `plate.sldprt`, and `tube.sldprt`.

MATERIAL PROPERTIES

Assume that the material is a structural steel. This is the default material with a Young's modulus of $2.0 \cdot 10^{11}$ N/m^2 and a Poisson's ratio of 0.33.

BOUNDARY CONDITIONS

Figure 13-13 shows the boundaries with an applied load and constrained displacements. Assume that the diagonal is loaded in tension by a force, F = 30 kN, which is transferred through the bolt to the mounting.

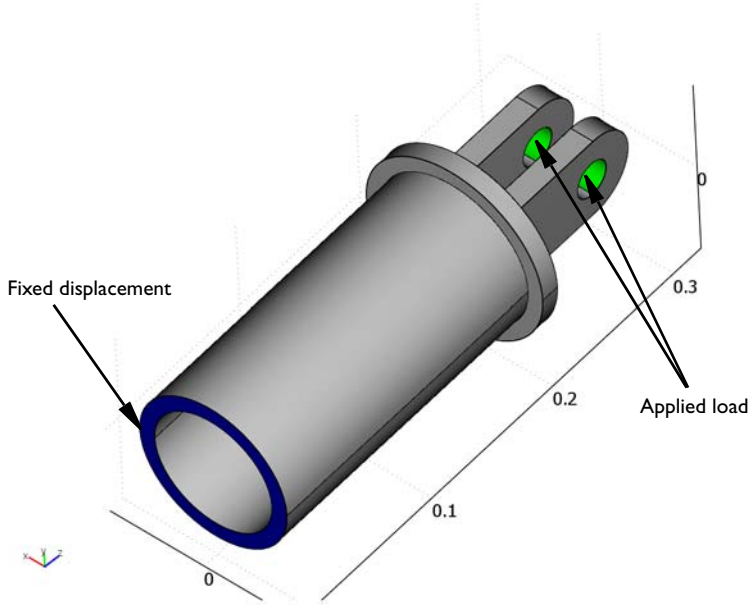


Figure 13-13: Boundaries with constrained displacements and applied loads.

Neglect contact conditions between the bolt and the mounting hole, and also neglect the constraint imposed on the mount by the bolt. Assume that the bolt fills out the entire hole volume. The load is distributed on the appropriate halves of the hole surfaces according to

$$p = \frac{F}{2(2r_{\mathrm{mh}}b_{\mathrm{mh}})} \cdot \frac{3}{2}\left(1 - \left(\frac{y}{r_{\mathrm{mh}}}\right)^2\right)$$

where r_{mh} and b_{mh} are the hole's radius and the thickness, respectively.

THE FINITE ELEMENT MESH

Next use the interactive meshing tool to individually mesh different parts of the diagonal mounting assembly. This way you can use both structured and unstructured meshes with various sizes on the different parts.

During the meshing procedure keep this in mind: for the identity boundary pairs, the destination boundary should have a finer mesh than the source boundary. The finite-element mesh consists of roughly 9000 tetrahedral elements and about 250 prism elements, giving a total number of approximately 50,000 degrees of freedom. Figure 13-14 shows a 3D view of the mesh.

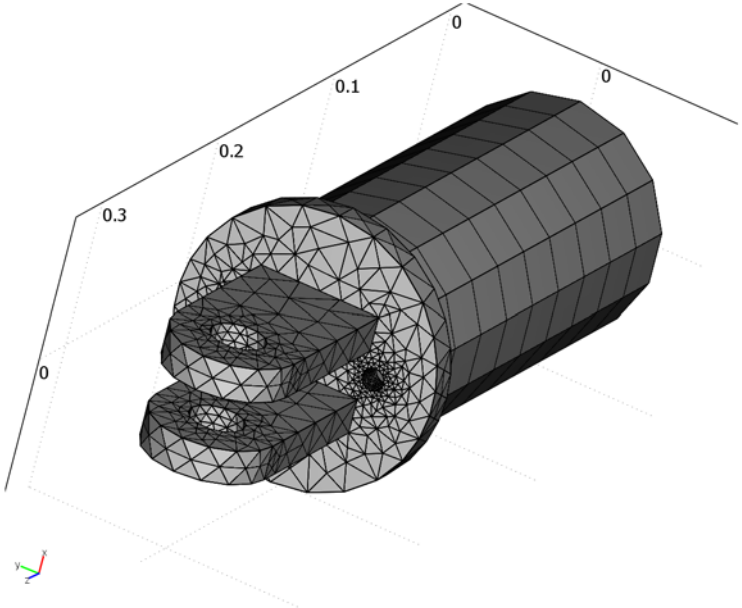


Figure 13-14: Finite-element mesh of the diagonal mounting assembly.

Results

Figure 13-15 shows the deformed shape of the diagonal mounting assembly with a boundary plot of the displacement in the axial direction of the diagonal. Calculate the stiffness of the mounting with the equation

$$S = \frac{F}{d_z}$$

where d_z is the average axial displacement at the midplane of the holes, and F is the applied load.

Compare this formula for the stiffness to an ideal stiffness, which would result if the diagonal tube were welded to the framework and placed under the same load. Calculate the ideal stiffness with the equation

$$S_{\text{id}} = \frac{E\pi(R_{\text{tb}}^2 - r_{\text{tb}}^2)}{L}$$

where r_{tb} and R_{tb} are the tube's inner and outer radii, and L is the total length measured in the axial direction up to the mid-plane of the mount holes. For the material under study, $E = 200$ GPa is the Young's modulus.

The stiffness ratio, $S_R = S/S_{id}$ is 0.38 for the case when the plate thickness and the mount thickness are 10 mm. With the updated geometry (plate thickness set to 12 mm and the mount thickness set to 15 mm), the stiffness ratio increases to 0.52.

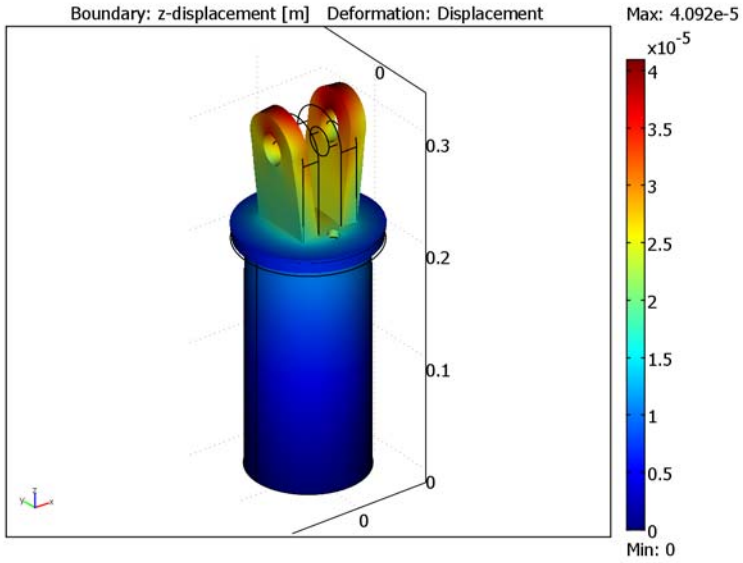


Figure 13-15: Deformed shape and boundary plot of the axial displacement for the mounting assembly with an end-plate thickness of 12 mm and mount thickness of 15 mm.

Model Library path: `COMSOL_Multiphysics/Structural_Mechanics/mast_diagonal_mounting_mphbin, mast_diagonal_mounting_parasolid, mast_diagonal_mounting_swlive`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator** go to the **New** page and select **3D** from the **Space dimension** list.

2 Select **COMSOL Multiphysics>Structural Mechanics>Solid, Stress-Strain>Static analysis**.

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

IMPORTING THE CAD GEOMETRY

Multiphysics Geometry File

1 On the **File** menu select **Import>CAD Data From File**.

2 In the **Files of type** list select **COMSOL Multiphysics file**.

3 Select the file `models/COMSOL_Multiphysics/Structural_Mechanics/mast_diagonal_mounting_pt10_mt10.mphbin` in the COMSOL installation directory.

4 Click **Import**.

Parasolid File

With the CAD Import Module you might also select the Parasolid file for import.

1 On the **File** menu select **Import>CAD Data From File**.

2 On the **Files of type** list select **Parasolid file**.

3 Select the file `models/COMSOL_Multiphysics/Structural_Mechanics/mast_diagonal_mounting_pt10_mt10.x_b` in the COMSOL installation directory.

4 Click **Import**.

SolidWorks Connection

With the CAD Import Module and SolidWorks software you might want to base the analysis on the SolidWorks assembly.

Have the file `mast_diagonal_mounting.sldasm` open in SolidWorks and carry out the following step in COMSOL Multiphysics:

On the **File** menu select **SolidWorks Connection>Initialize** to import the assembly into COMSOL Multiphysics.

Creating Boundary Pairs

1 Make sure all assembly parts are selected; if not, press Ctrl+A to select all parts.

The next step identifies the identity boundary pairs and creates the necessary identity constraints for the quantities that are equal on these boundaries.

2 Click the **Create Pairs** button on the Draw toolbar.

It is important that the source and destination domains be correctly defined for the identity pairs in the assembly. The destination should have a finer mesh than the source. For some of the identified identity boundaries you must interchange the source and destination so that they agree with the mesh you generate later on.

3 From the **Physics** menu select **Identity Pairs>Identity Boundary Pairs**.

4 In the **Identity pairs** list select **Pair 1**.

5 Click the **Interchange source and destination** button.

6 Repeat the previous two steps for **Pair 2** and **Pair 3**.

7 Click **OK** to close the **Identity Boundary Pairs** dialog box.

OPTIONS AND SETTINGS

Constants

1 On the **Options** menu select **Constants**.

2 Enter a variable with the **Name** `Force` and an **Expression** `30[kN]`.

3 Click **OK**.

Expressions

1 On the **Options** menu select **Expressions>Global Expressions**.

2 Enter expressions as given in the following table. Note that the last two expressions are for the load components; they specify both the magnitude and direction of the load that is applied in the opposite direction to the surface normal.

NAME	EXPRESSION
`mount_th_ac`	`mount_pos1-mount_pos2`
`mounthole_xarea`	`mount_th_ac*2*mounthole_r`
`tube_xarea`	`pi*(tube_R^2-tube_r^2)`
`Stiffness_ideal`	`2e11*tube_xarea/L_tot`
`Stiffness_current`	`Force/z_displ`
`Stiffness_ratio`	`Stiffness_current/Stiffness_ideal`
`mounthole_Fy`	`-Force/2/mounthole_xarea*3/2*(1-(y/mounthole_r)^2)*ny`
`mounthole_Fz`	`-Force/2/mounthole_xarea*3/2*(1-(y/mounthole_r)^2)*nz`

3 Click **OK**.

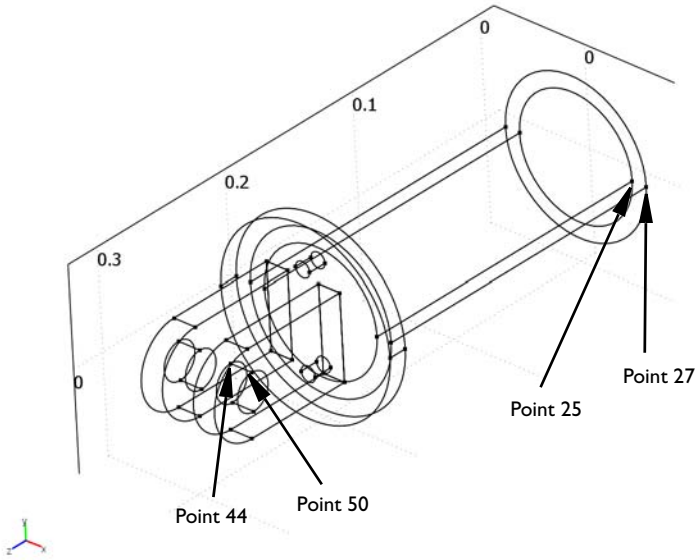
Integration Variables

Use integration coupling variables to make globally available the geometry dimensions as well as the average z displacement of the points on the hole midplanes.

1 On the **Options** menu select **Integration Coupling Variables>Point Variables**.

2 From the **Point selection** list choose 25.

3 Enter an expression with the **Name** `tube_r` and an **Expression** `x`.



4 Repeat the previous two steps for the following points and the corresponding expressions.

POINT SELECTION	NAME	EXPRESSION
27	`tube_R`	`x`
44	`mount_pos2`	`x`
50	`L_tot`	`z`
50	`mounthole_r`	`y`
50	`mount_pos1`	`x`
31, 32, 37, 38, 43, 44, 49, 50	`z_displ`	`w/8`

5 Click **OK**.

PHYSICS SETTINGS

Boundary Conditions

1 On the **Physics** menu select **Boundary Settings**.

2 On the **Boundaries** page locate the **Boundary selection** list and choose 22 and 30.

3 On the **Load** page enter `mounthole_Fy` in the $\mathbf{F_y}$ edit field and enter `mounthole_Fz` in the $\mathbf{F_z}$ edit field.

4 From the **Boundary selection** list choose 13.

5 On the **Constraint** page select the $\mathbf{R_x}$, $\mathbf{R_y}$, and $\mathbf{R_z}$ check boxes. Make sure their values are set to zero.

6 Click **OK**.

MESH GENERATION

Generate the mesh individually for the parts using the interactive meshing tool. Start by meshing the parts that should have an unstructured mesh by using the free mesher.

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

2 On the **Global** page locate the **Predefined mesh sizes** list and select **Fine**.

3 On the **Subdomain** page select Subdomains 3 and 4.

4 Click the **Mesh Selected** button.

5 On the **Global** page find the **Predefined mesh sizes** list and select **Finer**.

6 On the **Subdomain** page select Subdomain 1.

7 Click the **Mesh Selected** button. Click **OK**.

Now use the swept mesher on the tube.

1 On the **Mesh** menu select **Swept Mesh Parameters**.

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

3 From the **Subdomain selection** list select 2.

4 Click the **Mesh Selected** button.

5 Click **OK**.

Figure 13-14 shows the meshed assembly.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to start the analysis.

POSTPROCESSING AND VISUALIZATION

1 On the **Postprocessing** menu select **Plot Parameters**.

2 On the **General** page go to the **Plot type** area. Clear the **Slice** check box and select the **Boundary** and **Deformed shape** check boxes.

3 On the **Boundary** page go to the **Predefined quantities** list and select **z-displacement**.

4 Click **OK** to close the dialog box and to display the plot in Figure 13-15 on page 564.

5 On the **Postprocessing** menu select **Data Display>Global**.

6 From the **Predefined quantities** list select **Global Expressions>Stiffness_ratio**.

7 Click **OK**. The value of the stiffness ratio, 0.41, appears in the message log at the bottom of the user interface.

UPDATE OF CAD GEOMETRY

Click the **Draw Mode** button on the Main toolbar.

The following steps describe how to import the CAD geometry from a COMSOL Multiphysics geometry file and from a Parasolid file.

Multiphysics Geometry File

1 Press Delete to delete the current geometry (first make sure that the geometry is selected).

2 On the **File** menu select **Import>CAD Data From File**.

3 In the **Files of type** list select **COMSOL Multiphysics file**.

4 Select the file `mast_diagonal_mounting_pt12_mt15.mphbin`.

5 Click **Import**.

Parasolid File

1 Press Delete to delete the current geometry.

2 On the **File** menu select **Import>CAD Data From File**.

3 On the **Files of type** list select **Parasolid file**.

4 Select the file `mast_diagonal_mounting_pt12_mt15.x_b`.

5 Click **Import**.

SolidWorks Connection

Now you can control the plate and mount thicknesses of the SolidWorks assembly from COMSOL Multiphysics. This is possible if you define constants that have the same name as the variables defining these dimensions in the SolidWorks file.

1 On the **Options** menu select **Constants**.

2 Enter a variable with the **Name** `plate_thickness` and an **Expression** `12e-3`.

3 Enter a variable with the **Name** `mount_thickness` and an **Expression** `15e-3`.

4 Click **OK**.

5 On the **File** menu select **SolidWorks Connection>Update** to update and import the assembly into COMSOL Multiphysics.

Creating Boundary Pairs

Repeat the steps under "Creating Boundary Pairs" on page 565 only if you imported the COMSOL Multiphysics geometry or Parasolid file. Boundary pairs are retained with the SolidWorks connection and do not need to be specified again.

OPTIONS SETTINGS

Integration Variables

The names of the variables are retained. Select the points and enter the corresponding expressions as described in "Integration Variables" on page 566.

PHYSICS SETTINGS

Boundary Conditions

Repeat the steps under "Boundary Conditions" on page 567 only if you imported the COMSOL Multiphysics geometry or Parasolid file. Boundary conditions are retained with the SolidWorks connection and need not be specified again.

MESH GENERATION

Repeat the steps under "Mesh Generation" on page 568.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to start the analysis.

POSTPROCESSING AND VISUALIZATION

1 On the **Postprocessing** menu select **Data Display>Global**.

2 From the **Predefined quantities** list select **Global Expressions>Stiffness_ratio**.

3 Click **OK**. The value of the stiffness ratio, 0.58, appears in the message log at the bottom of the user interface.

Stresses in a Pulley

Introduction

This model contains a study of the stress distribution in a driving pulley. The analysis shows the stresses as functions of the pulley's angular velocity.

Model Definition

Figure 13-16 shows the pulley under study (to the right) and the external forces applied due to the driving belt.

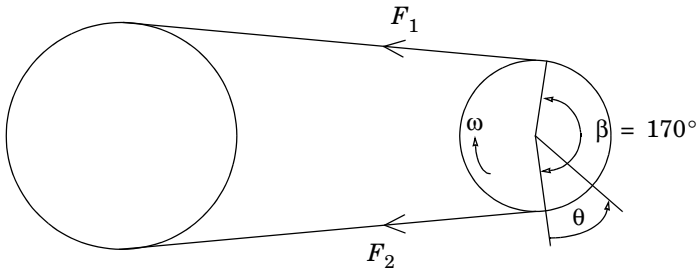


Figure 13-16: Pulley and driving belt with the external forces F_1 and F_2.

Here, F_1 and F_2 are the loads in the load side and in the slack side of the belt, respectively. The relationship between these forces is given by Reynold's equation (or Eytelwein's equation, as it is referred to in the German literature):

$$\frac{F_1}{F_2} = e^{\mu\beta}$$

where μ is the coefficient of friction and β is the contact angle between the belt and the pulley. This equation is valid if a condition of impending slippage between the belt and the pulley prevails.

It is also necessary to state that the peripheral force (the force that transmits the power) is

$$F_u = F_1 - F_2 = \frac{M}{r}$$

It is then possible to define F_2 as

$$F_2 = \frac{F_u}{(e^{\mu\beta} - 1)}$$

Now that you know the force in the slack side of the belt, you can derive the loads on the boundary of the pulley. In mechanics and the theory for flexible wires the following equilibrium equations appear:

$$F_n = \frac{S}{r}$$
$$F_t = \mu F_n$$

where F_n is the normal component and F_t the tangential component of the external forces, S is the tension force, and r is the radius.

If you apply these equations to this model, the loads on the boundary of the pulley become

$$F_n(\theta) = \frac{F_2}{r} e^{\mu\theta}$$

and

$$F_t(\theta) = \mu F_n(\theta)$$

where θ is the angle for which the forces are calculated (see Figure 13-16).

Due to the rotation of the pulley, inertia loads are generated. These loads can be calculated as

$$F_r = r\omega^2\rho$$

where r is the radius, ω is the rotation speed, and ρ is the density.

The pulley is fixed at its inner diameter and the inertia loads are active in the entire geometry.

A parametric analysis shows how the rotational speed affects the stress distribution in the pulley. Because the power at the pulley shaft remains constant, the torque (defined as the ratio of the power by the rotational speed) decreases with increased speed. This means that with increased rotational speed, the inertial load increases while the driving-belt force decreases.

Results and Discussion

The following plots show the von Mises stress distribution inside the pulley for different rotational speeds in rpm (revolutions per minute).

As is evident from the plots, the stress distribution changes as the rotational speed increases.

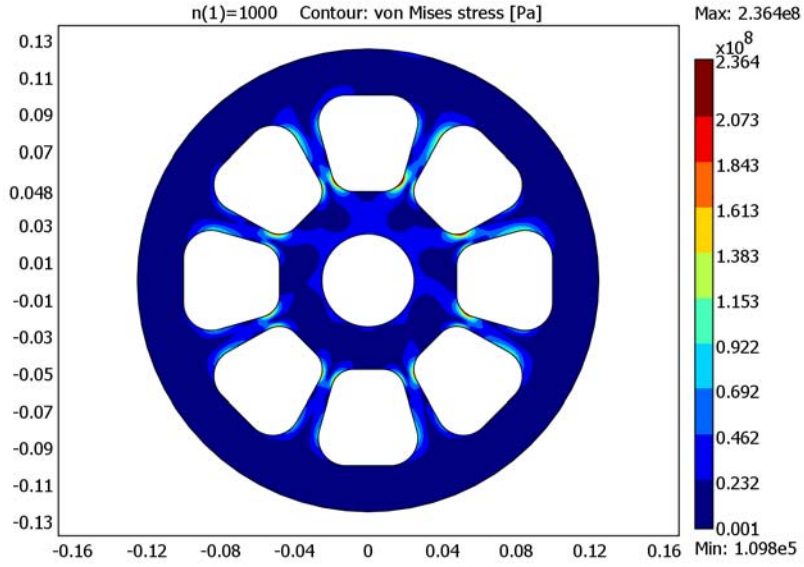


Figure 13-17: von Mises stress distribution at n = 1000 rpm.

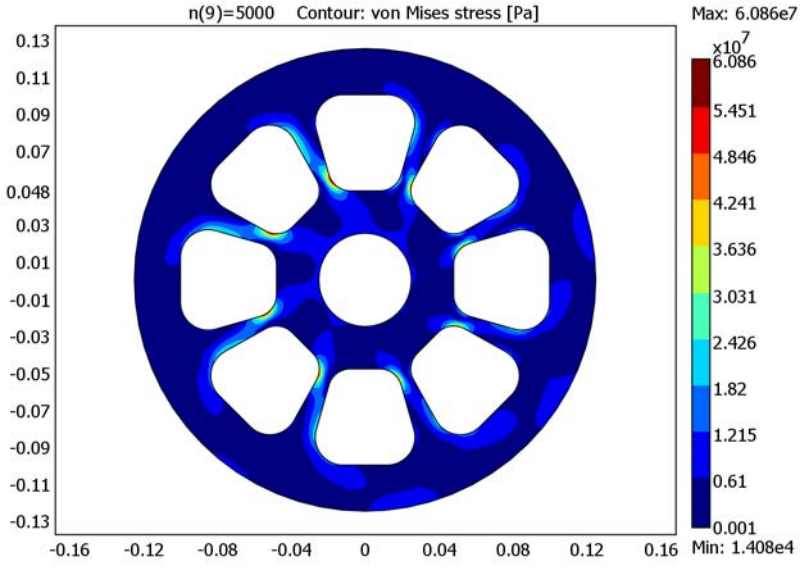


Figure 13-18: von Mises stress distribution at n = 5000 rpm.

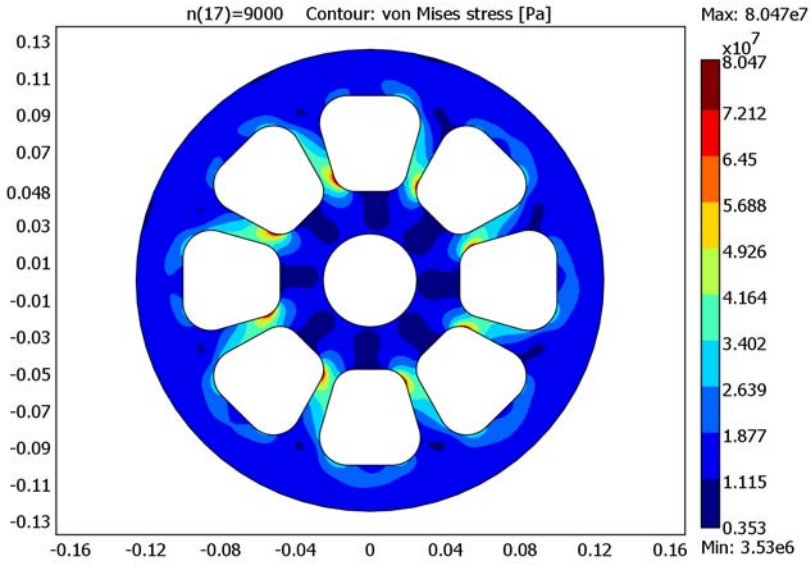


Figure 13-19: von Mises stress distribution at n = 9000 rpm.

At the point (0.019, 0.054), the von Mises stress is maximal for the first rotational speed (n = 1000 rpm). The plot in Figure 13-20 shows how the rotational speed affects the von Mises stress at this specific point. First the stress decreases, but then the effect of the inertial loads becomes dominating and the stress begins to increase.

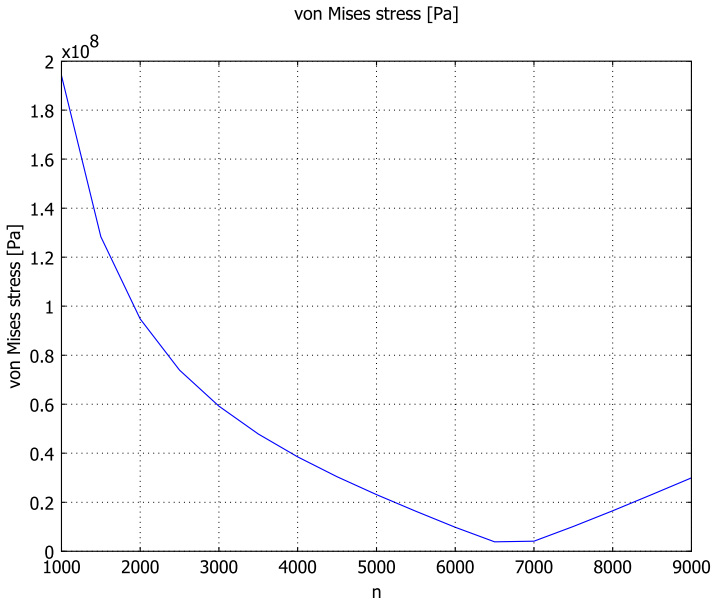


Figure 13-20: von Mises stress as function of rotational speed at point (0.019, 0.054).

Figure 13-21 shows the von Mises stresses in as part of the pulley evaluated using the accurate derivative recovery method. This makes the stress field smoother.

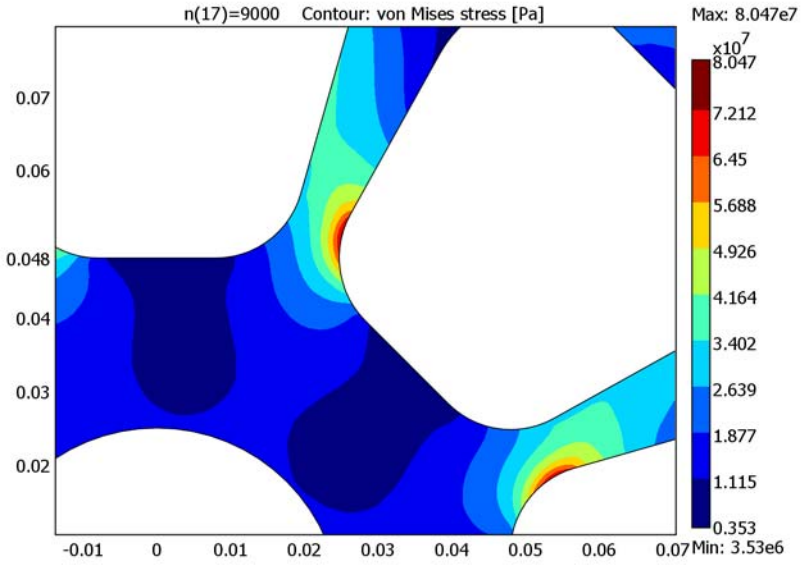


Figure 13-21: Von Mises stresses in a part of the pulley evaluated using accurate derivative recovery.

Modeling in COMSOL Multiphysics

To build the geometry, and especially the shape of the holes, use the tangent drawing tool.

When solving, adaptive mesh refinement helps to compute accurate stresses, as the stress concentration is not known in advance.

The accurate derivative recovery (see "Accurate Derivative Recovery" on page 471 of the *COMSOL Multiphysics User's Guide*) helps to produce a smooth stress field during postprocessing.

Model Library path: `COMSOL_Multiphysics/Structural_Mechanics/pulley`

MODEL NAVIGATOR

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

2 Select **COMSOL Multiphysics>Structural Mechanics>Plane Stress**, then click **OK**.

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
P	185[kW]	Power at pulley shaft
mu	0.5	Coefficient of friction between pulley and belt
beta	(170*pi/180)[rad]	Contact angle between pulley and belt
d	5[cm]	Thickness of the pulley
n	100	RPM

3 Open the **Scalar Expressions** dialog box available from the **Options>Expressions** menu.

4 Enter the following expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
r	sqrt(x^2+y^2)	Radius
theta	atan2(y,x)	Angle
omega	n/1[min]*2*pi[rad]	Rotational speed of the pulley
M	P/omega	Torque at pulley shaft
Fu	M/r	Peripheral force
F2	Fu/(exp(mu*beta)-1)	Belt force in slack side
C	F2/(r*d)	Variable used in load mode
Fn	-C*exp(mu*(theta+beta))	Normal component of the belt load
Ft	mu*C*exp(mu*(theta+beta))	Tangential component of the belt load

5 Choose **Options>Axes/Grid Settings**.

6 Specify axis and grid settings according to the following table. On the **Grid** page, clear the **Auto** check box to enter the grid spacing and extra grid point. When done, click **OK**.

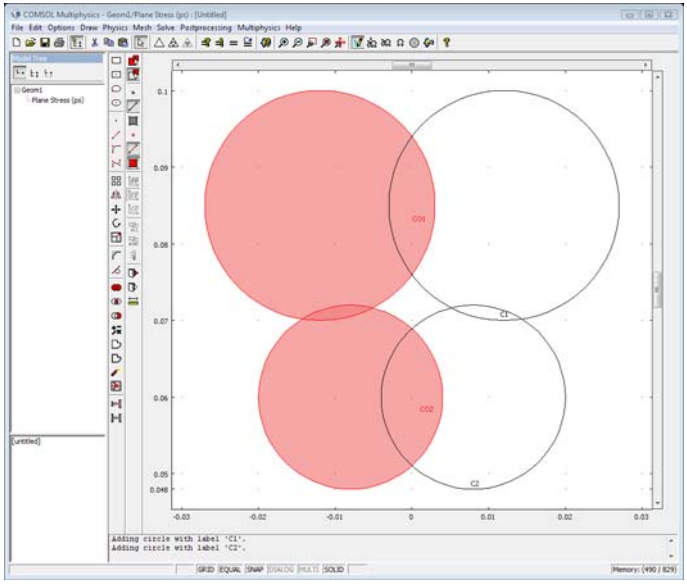
AXIS		GRID	
x min	-0.03	x spacing	1e-2
x max	0.03	Extra x	
y min	0.03	y spacing	1e-2
y max	0.11	Extra y	4.8e-2

GEOMETRY MODELING

1 Choose **Draw>Specify Objects>Circle** and define a circle centered at (1.2e-2, 8.5e-2) with a radius of 1.5e-2.

2 Draw another circle centered at (8e-3, 6e-2) with a radius of 1.2e-2.

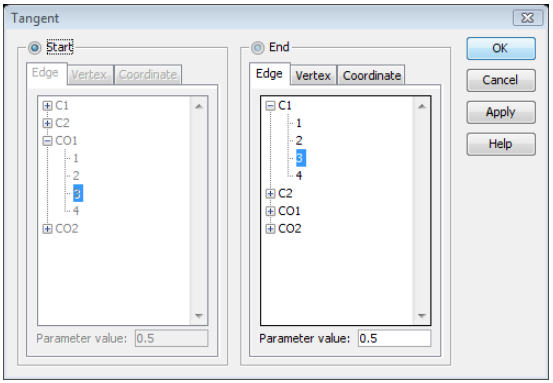
3 Select both circles and click the **Mirror** button on the Draw toolbar. Use the default setting for the reflection line and click **OK**.



4 Click the **Tangent** button on the Draw toolbar.

5 In the **Start** area, select Edge 3 of **CO1**.

6 Click the **End** button and select Edge 3 of **C1**.

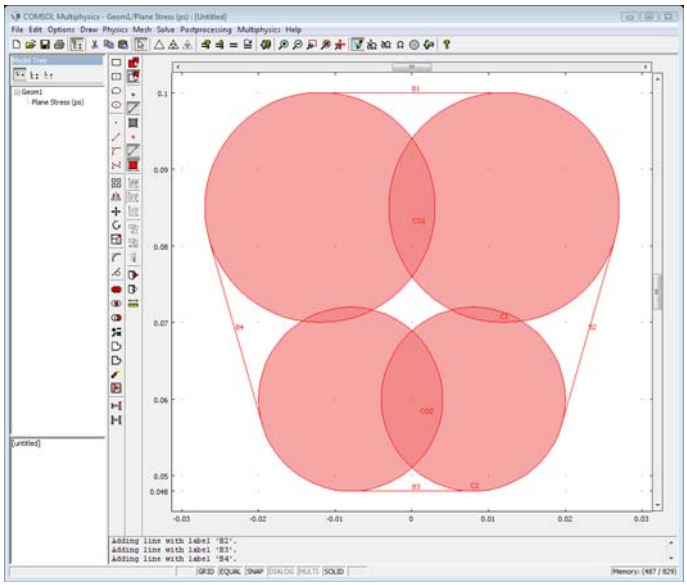


7 Click **OK**.

8 Draw three other tangents following the previous indication but this time with the start and end edges as in the table below.

START GEOMETRY OBJECT	START EDGE	END GEOMETRY OBJECT	END EDGE
C1	2	C2	2
C2	2	CO2	2
CO2	2	CO1	3

9 Press Ctrl+A to select all the geometry objects.



10 Click the **Coerce to Solid** button on the Draw toolbar.

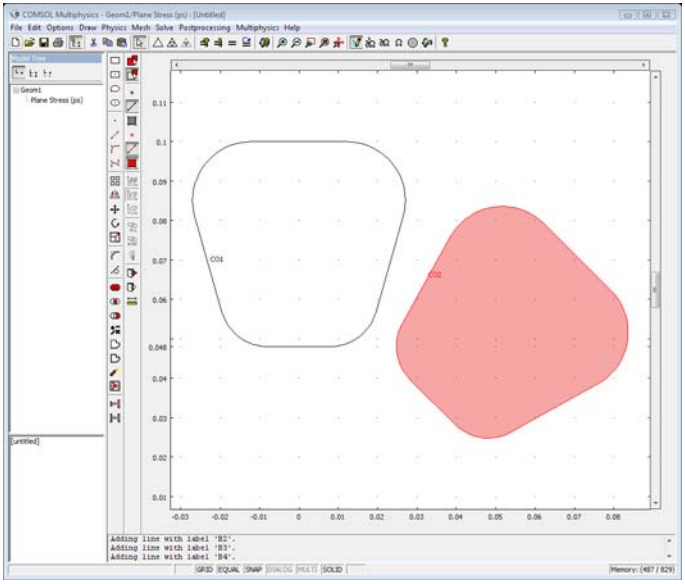
11 Click the **Delete Interior Boundaries** button on the Draw toolbar.

12 Press first Ctrl+C and then Ctrl+V to copy and paste the geometry.

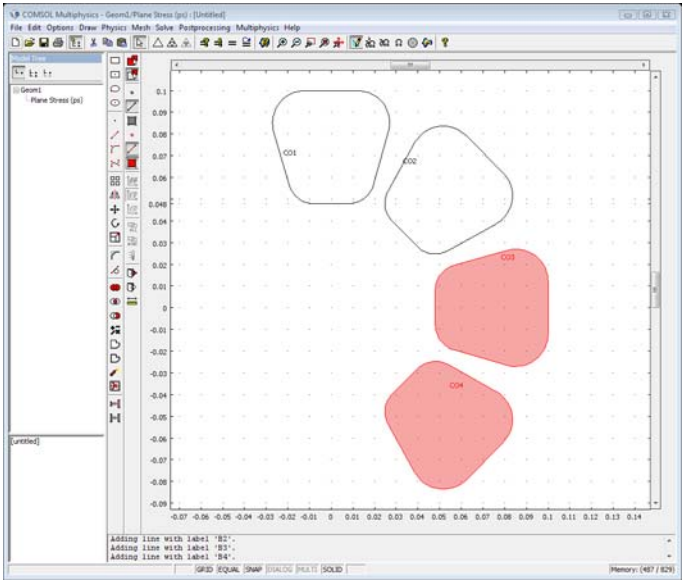
13 Click **OK** in the **Paste** dialog box.

14 Click **Rotate** and enter `-45` in the α edit field for the rotation angle.

15 Click **OK**.



16 Select both geometries, copy and paste them at the same location, and rotate the new geometries with an angle of –90°.



17 Copy and paste the new geometries and rotate them with an angle of –90°.

18 Repeat the last step once.

19 Click **Zoom Extents**.

20 Draw two circles centered at the origin with the radii 0.025 and 0.125, respectively.

21 Click **Zoom Extents**.

Next, split the right side of the exterior boundary to model the belt contact boundary (the belt and the pulley are in contact over an angle of 170°).

1 Draw a line from (0, 0.11) to (0, 0.13).

2 Click the **Rotate** button and type `-5` in the α edit field for the rotation angle.

3 Draw a line from (0, –0.11) to (0, –0.13).

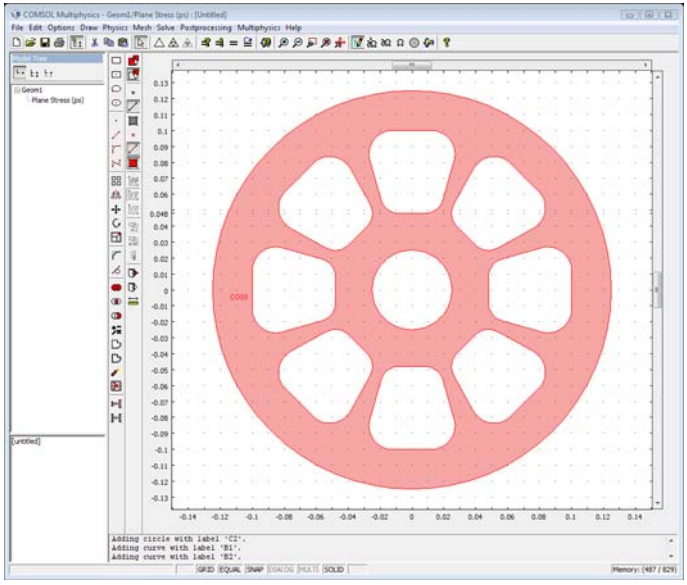
4 Click the **Rotate** button and type `5` in the α edit field for the rotation angle.

5 Select the outer circle C2 and the two lines, B1 and B2.

6 Click the **Coerce to Solid** button.

7 Select all objects (press Ctrl+A).

8 Click the **Difference** button.



PHYSICS SETTINGS

Subdomain Settings

1 From the **Physics** menu, open the **Subdomain Settings** dialog box.

2 On the **Material** page, click **Load**.

3 Select **Aluminum** from the library material.

4 In the **thickness** edit field type `d`.

5 Click the **Load** tab.

6 Type `r*omega^2*rho_ps*cos(theta)` in the **Body load x-dir.** edit field and `r*omega^2*rho_ps*sin(theta)` in the **Body load y-dir.** edit field.

This step is a transformation from cylindrical coordinates to the Cartesian coordinate system by entering the components of the radial load in the x and y directions.

7 Click the **Body load is defined as force/volume using the thickness** button.

8 Click **OK**.

Boundary Settings

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

2 Apply the following boundary conditions:

BOUNDARY	57, 58, 62, 63	
Page	Constraint	
	R_x	0
	R_y	0

BOUNDARY	67, 68	
Page	Load	
	F_x	`Fn*cos(theta)-Ft*sin(theta)`
	F_y	`Fn*sin(theta)+Ft*cos(theta)`

3 Click the **Edge load is defined as force/area using the thickness** button.

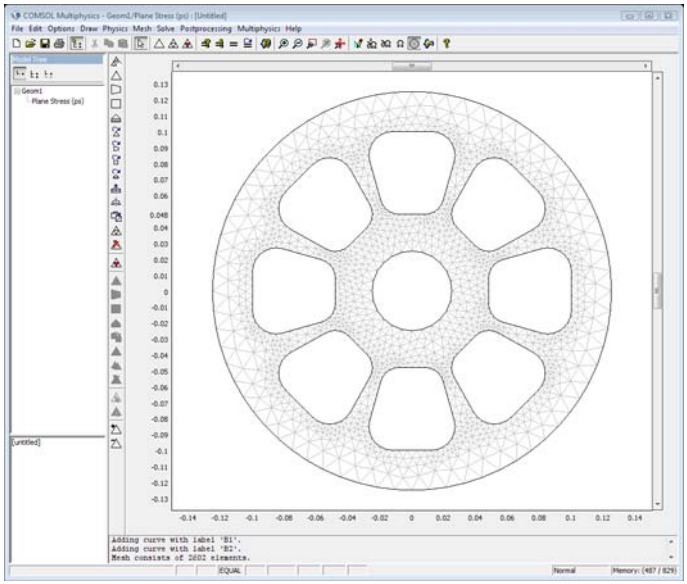
4 Click **OK**.

MESH GENERATION

You can expect the rate of change of stresses in the corner region to be high. Use an adaptive mesh algorithm to get a more suitable mesh size according to the stress concentration. It is therefore not necessary to start with a fine mesh. COMSOL

Multiphysics automatically detects areas with a high rate of change of stresses and refines them.

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



The total number of degrees of freedom should be around 11,460 (2656 elements).

COMPUTING THE SOLUTION

The rotational speed is the parameter of the parametric solver and varies from 1000 rpm to 9000 rpm in steps of 500 rpm.

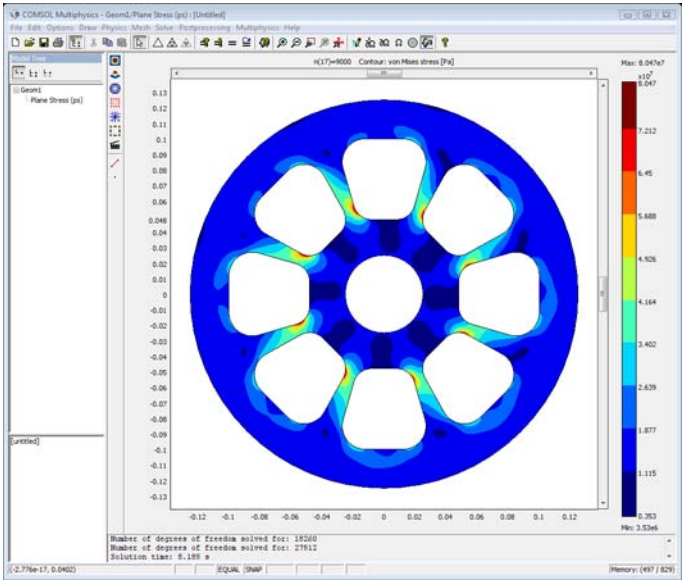
1. Open the **Solver Parameters** dialog box in the **Solve** menu.
2. Select **Parametric** from the **Solver** list.
3. Type `n` in the **Parameter names** edit field.
4. Type `range(1e3,5e2,9e3)` in the **Parameter values** edit field.
5. Select **Direct (SPOOLES)** in the **Linear system solver** list. The system matrix becomes symmetric, and this solver can make use of that symmetry to save memory.

   Use the adaptive mesh algorithm to refine the mesh during the calculation:
6. Select the **Adaptive mesh refinement** check box.
7. Click the **Adaptive** tab and type `1.3` in the **Increase number of elements by** edit field.
8. Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

The default plot gives the von Mises stress distribution for the highest rotational speed (9000 rpm). Use a filled contour plot to clearly see where different stress levels occur.



1 Open the **Plot Parameters** dialog box from the **Postprocessing** menu.

2 On the **General** page, clear the **Surface** check box in the **Plot type** area.

3 Click the **Contour** tab.

4 Select the **Contour plot** check box.

5 Select the **Recovery** check box to activate the accurate derivative recovery. You can compare the stress plot with and without accurate derivative recovery by selecting and clearing this check box. Notice how the stress field becomes smoother when the accurate derivative recovery is active.

6 Select the **Filled** check box at the bottom of the page to create filled contours.

7 Type 10 in the **Number of levels** edit field.

8 Click **Apply** to create the plot.

9 To visualize the results for different rotational speeds, use the solution for the desired rpm value by selecting it from the **Parameter value** list.

10 To get a line plot of the von Mises stress at a specific point as a function of the rotational speed, open the **Cross-Section Plot Parameters** dialog box.

11 On the **General** page, select all the solutions to plot from the **Solutions to use** list.

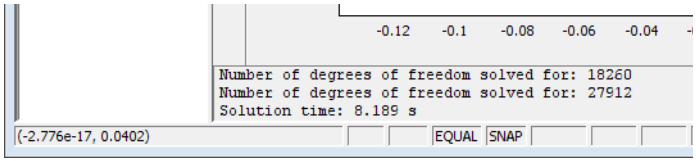
12 On the **Point** page, enter the coordinate of the point (0.019, 0.054).

13 Click **OK**.

14 Figure 13-20 shows the resulting plot.

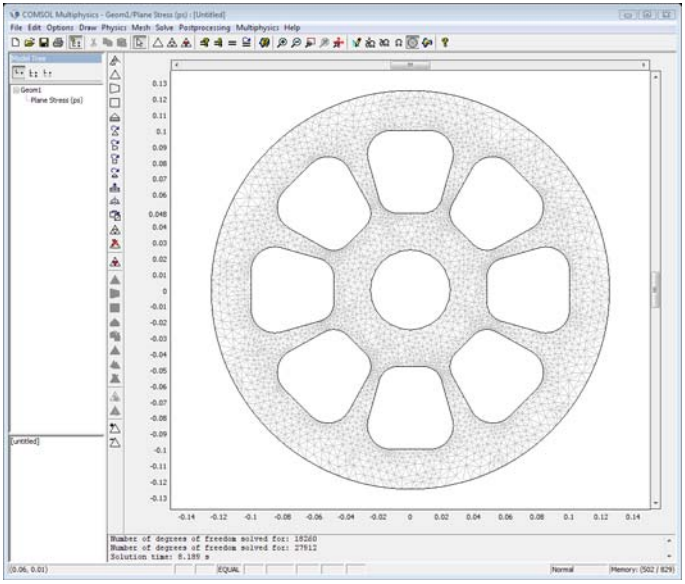
A Note About Adaptive Mesh Refinement

During the calculation the solver refines the mesh several time. You can verify this by looking at the message log at the bottom of the main user interface.



There are two mesh refinements: The first refinement gives about 19,500 DOFs, and the second refinement gives the final solution with about 31,200 DOFs.

Go to Mesh mode to see the refined mesh refined after the analysis.



The adaptive mesh algorithm, when coupled with a parametric analysis, only refines the mesh on the results based on the last parameter. In this specific case the variation of the gradient of the variable is not important enough to consider different meshes for the different parameters. In case of large variations of the gradients, we recommend to proceed using a manual mesh refinement in order to have a mesh that is suitable for all parameters.

14

Wave Propagation Models

Wave propagation models describe the propagation of electromagnetic waves, light, fluids, and more. For additional wave propagation models, see the chapters containing acoustics models, electromagnetics models, and fluid dynamics models.

Diffraction Patterns

Introduction

This example simulates a two-slit interference experiment with water waves or sound. The model mimics the plane-wave excitation with two thin waveguides leading to slits in a screen and computes the diffraction pattern on the other side of the screen.

Model Definition

Theory predicts amplitude minima along rays where the difference in travel distance is an odd multiple of half the wavelength, and maxima at even multiples. For $n = 0, \pm 1, \pm 2, \ldots$:

$$\begin{cases} \text{min}, & \sin\theta = \left(n + \frac{1}{2}\right)\frac{\lambda}{D} \\ \text{max}, & \sin\theta = n\frac{\lambda}{D} \end{cases}$$

In this model, the distance D between the slits is 2λ. Maxima should then be present at $\theta = 0°$ and $30°$, while minima should appear at $\theta = 14.48°$ and $48.59°$.

Equation

For time-harmonic propagation, the wave equation turns into the Helmholtz equation:

$$-\nabla \cdot (\nabla u) - k^2 u = 0, \qquad k = \frac{2\pi}{\lambda}$$

Boundary Conditions

The absorbing boundary conditions have the form

$$\begin{aligned} \mathbf{n} \cdot (\nabla u) + iku &= 2ik, && \text{inflow} \\ \mathbf{n} \cdot (\nabla u) + iku &= 0, && \text{outflow} \end{aligned}$$

where $\mathbf{n}$ is the outward boundary normal vector. This follows directly from the assumption that the total wave consists of an incident plane wave plus an outgoing plane wave, both at normal incidence:

$$u = u_1 e^{ikx} + u_2 e^{-ikx}$$

where the first term represents the outgoing wave and the second term the incident wave. For example, at the left boundary of a computational domain along the x axis, the normal derivative becomes

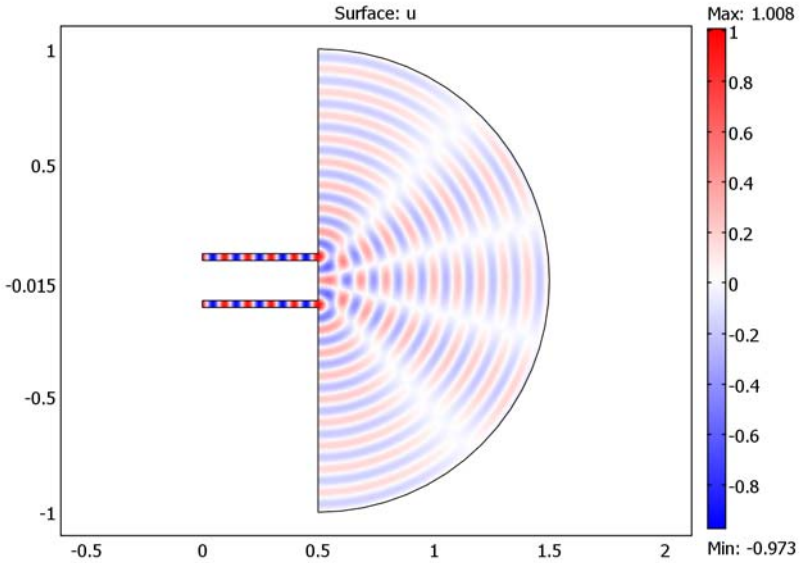
$$\frac{\partial u}{\partial n} = -\frac{\partial u}{\partial x} = -iku_1 e^{ikx} + iku_2 e^{-ikx} = -ik(u - 2u_2 e^{-ikx})$$

which means that

$$\frac{\partial u}{\partial n} + iku = 2iku_2$$

and for $u_2 = 1$, you get the absorbing boundary condition at the inflow for this model.

Results



The plot above shows the diffraction pattern clearly. The effect of quantization is that the numerical wavelength differs from λ, which results in a shift of the angles. You can correct for this effect by adjusting the value of k in the Helmholtz equation to the

element size. These practices are important for modeling the interference effects of monochromatic waves.

Model Library path: `COMSOL_Multiphysics/Wave_Propagation/diffraction_patterns`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **2D** from the **Space dimension** list.

2 In the list of application modes, open **COMSOL Multiphysics>PDE Modes** and then **PDE, Coefficient Form**.

3 Select **Stationary analysis**. Make sure that **Lagrange - Quadratic** elements are selected in the **Element** list.

4 Click **OK**.

OPTIONS AND SETTINGS

1 Open the **Axes/Grid Settings** dialog box.

2 Specify axis and grid settings according to the following table; when done, click **OK**.

AXIS		GRID	
x min	-0.75	x spacing	0.5
x max	2.25	Extra x	
y min	-1	y spacing	0.5
y max	1	Extra y	-0.015 0.015

3 Open the **Constants** dialog box.

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

NAME	EXPRESSION	DESCRIPTION
l	0.1	Wavelength (m)
k	2*pi/l	Wave number (rad/m)

GEOMETRY MODELING

1 Draw a circle with its center at (0.5, 0) and a radius of 1.

2 Draw a rectangle centered at (0, 0) with sides of 1 and 2 units for the x and y direction, respectively.

3 Select both objects and click the **Difference** button to create a half circle.

4 Draw a rectangle with its lower left corner at (0, -0.015) and upper right corner at (0.5, 0.015).

5 Click the **Move** button and set the y-displacement to `0.1`. Leave the x-displacement at 0.

6 Click **OK**.

7 Duplicate and place the rectangle by pressing Ctrl+C and then Ctrl+V.

8 Click the **Move** button again and set the x- and y-axis displacements to `0` and `-0.2`, respectively.

9 Select all objects.

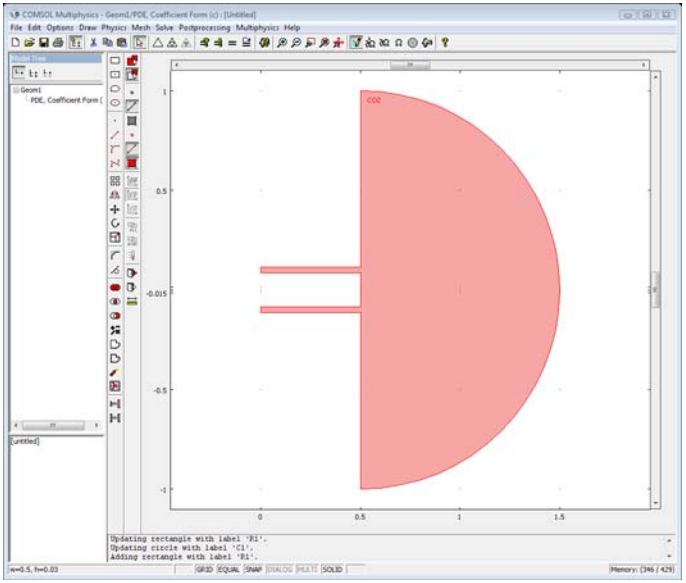
10 From the **Draw** menu, choose **Create Composite Object**.

11 In the **Set formula** edit field, type `CO1+R1+R2`.

12 Clear the **Keep interior boundaries** check box.

13 Click **OK**.

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



PHYSICS SETTINGS

Boundary Conditions

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

2 In the **Boundary Settings** dialog box, enter these boundary conditions (`i` denotes the imaginary unit):

SETTINGS	BOUNDARIES 1, 4 (INFLOW)	BOUNDARIES 2, 3, 5–9	BOUNDARIES 10, 11 (OUTFLOW)
Type	Neumann	Neumann	Neumann
q	`i*k`	0	`i*k`
g	`2*i*k`	0	0

Subdomain Settings

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

2 In the **Subdomain Settings** dialog box, enter the following PDE coefficients:

SETTINGS	SUBDOMAIN 1
c	1
a	`-k^2`
f	0

MESH GENERATION

1 In the **Free Mesh Parameters** dialog box, click the **Global** tab

2 Click the **Custom mesh size** button, then enter `0.03` in the **Maximum element size** edit field (approximately 3 second-order elements per wavelength).

3 Click the **Remesh** button, then click **OK**.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

By default, COMSOL Multiphysics plots the real part of the solution using the Rainbow color table. To make the diffraction pattern appear even more clearly, change to the WaveLight color table as follows:

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

2 On the **Surface** page, select **WaveLight** from the **Color table** list in the **Surface color** area.

3 Click **OK**.

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Benchmark Models

Benchmark models are those with known results from experiments and measurements, from analytical solutions and formulas, or from established benchmark problems published by organizations such as NAFEMS. Many of the other examples in the Model Library and the COMSOL Multiphysics modules are benchmark models as well. Most introductory models in the *COMSOL Multiphysics Modeling Guide* compare results to theoretical values or established benchmark data.

Isospectral Drums

Introduction

This example examines an interesting question posed by Mark Kac in 1966 (Ref. 1): "Can one hear the shape of a drum?"

Striking a drum excites a spectrum of vibration modes that together make up the instrument's characteristic sound or acoustic signal. These vibration modes correspond to the eigenmodes, or eigenfunctions, of the drum's membrane. Thus you can study this problem by solving eigenvalue problems for stretched membranes.

If you can find two differently shaped membranes that have identical eigenvalues—in other words, they are *isospectral*—then it is not possible to hear the shape of a specific drum.

In 1992, Gordon, Webb, and Wolpert (Ref. 2) showed that there are indeed sets of different planar shapes (nonisometric shapes) that are isospectral.

Work by Driscoll (Ref. 3) contains the following example of two planar shapes that sound the same.

Model Definition

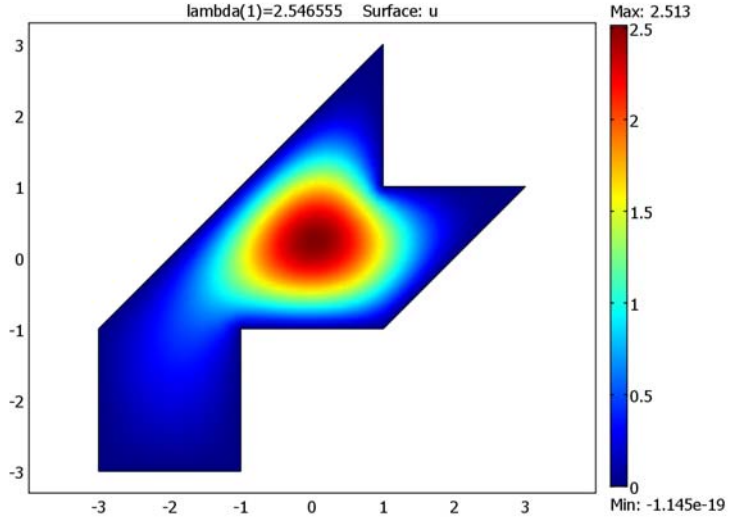
The model shows the eigensolutions (the eigenvalues and eigenmodes) in two isospectral domains. For both cases, use the solution to the same eigenvalue PDE:

$$\Delta u = \lambda u \tag{15-1}$$

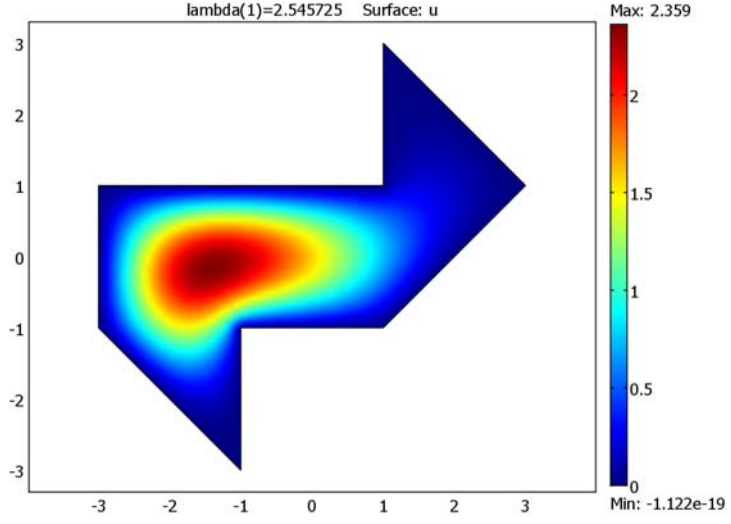
The membranes are fixed at the boundaries, that is, a homogeneous Dirichlet boundary condition applies for all boundaries.

Results

The eigenvalues show that the domains are isospectral. This is one of the eigenmodes for the first domain:



The eigenvalues are the same for the other domain. The sign of the eigenfunction is arbitrary and can vary from case to case:



Using Richardson extrapolation, the results for the first six eigenvalues of the two domains agree to at least five decimal places with the established values in Ref. 3.

Another postprocessing step shows that the eigensolutions are orthogonal by integrating the product of two different eigensolutions.

Modeling in COMSOL Multiphysics

Build two COMSOL Multiphysics models that solve the eigenvalue PDE on two different 2D domains and compare the sets of eigenvalues. To achieve higher accuracy in the results, use *Richardson extrapolation*, which increases the accuracy if you know the behavior of the numerical error.

The model also shows how to use the `with` operator to access different eigenmodes during postprocessing.

References

1. M. Kac, "Can one hear the shape of a drum?," *American Math. Mon.*,73 Part II (1966), pp. 1–23.

2. C. Gordon, D. Webb, and S. Wolpert, "Isospectral plane domains and surfaces via Riemannian orbifolds," *Invent. Math.*, 110 (1992), pp. 1–22.

3. T. Driscoll, "Eigenmodes of isospectral drums," *Technical Report-Center for Theory and Simulation in Science and Engineering*, Cornell University, Ithaca, N.Y., CTC95TR209, May 1995.

Model Library path: `COMSOL_Multiphysics/Benchmarks/isospectral_drum_1`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 In the **Application Modes** tree, choose **COMSOL Multiphysics>PDE Modes>PDE, Coefficient Form>Eigenvalue analysis**.

3 Make sure **Lagrange - Quadratic** elements are selected, then click **OK**.

GEOMETRY MODELING—THE FIRST ISOSPECTRAL DRUM

1 Press Shift and then click the **Line** button on the Draw toolbar.

2 In the **Line** dialog box, go to the **Coordinates** area and enter the following data:

PROPERTY	EXPRESSION
x	-3 -3 1 1 3 1 -1 -1
y	-3 -1 3 1 1 -1 -1 -3

3 From the **Style** list, select **Closed polyline (solid)**, then click **OK**.

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

PHYSICS SETTINGS

Subdomain Settings

The following equation describes a general eigenvalue PDE:

$$-\nabla \cdot (c\nabla u + \alpha u) + \beta \nabla u + au = d_a \lambda u$$

Thus, to implement the PDE in Equation 15-1 use the default values $c = 1$ and $d_a = 1$. All other coefficients are equal to 0 by default (the source term f is 1 but it is not part of the eigenvalue PDE).

Boundary Conditions

There is no need to change the boundary coefficients. The default Dirichlet condition $u = 0$ on the boundary is correct. This value corresponds to clamping the drum's membrane at the edges.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar to create a mesh.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to compute the solution. The default setting gives the six lowest eigenvalues.

POSTPROCESSING AND VISUALIZATION

Plot some of the eigenfunctions associated with the eigenvalues. Select the corresponding eigenvalue from the **Eigenvalue** list on the **General** page in the **Plot Parameters** dialog box. The plot shows the oddly shaped drum seen from above.

Model Library path: `COMSOL_Multiphysics/Benchmarks/isospectral_drum_2`

GEOMETRY MODELING—THE SECOND ISOSPECTRAL DRUM

1 Shift-click the **Line** button on the Draw toolbar.

2 Enter the following data in the **Coordinates** area of the **Line** dialog box:

PROPERTY	EXPRESSION
x	-3 1 1 3 1 -1 -1 -3
y	1 1 3 1 -1 -1 -3 -1

3 From the **Style** list, select **Closed polyline (solid)**, then click **OK**.

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

PHYSICS SETTINGS

In specifying PDE and boundary coefficients, follow the same procedure as for the first drum.

POSTPROCESSING

Showing that the Eigenmodes are Orthogonal

Use the `with` operator to access different eigenmodes in order to show that they are orthogonal:

1 From the **Postprocessing** menu, choose **Subdomain Integration**.

2 Select Subdomain 1.

3 Type `with(1,u)*with(2,u)` in the **Expression** edit field. This specifies an integrand that is the product of the first and the second eigenmode.

4 Click **OK**.

The value, which should be very small (on the order of 10^{-15}), appears in the message log at the bottom of the COMSOL Multiphysics user interface. Ideally, the result should be zero when the eigenmodes are orthogonal, but using a numerical method you can expect a small nonzero number.

Note: The following section requires that you run COMSOL Multiphysics with MATLAB.

To improve the accuracy of the eigenvalues, continue with MATLAB using Richardson extrapolation. First export the model:

From the **File** menu, choose **Export FEM Structure**. Then continue with the instructions on Richardson extrapolation in the section below.

Modeling Using the Programming Language

The following sequence of commands finds the eigenvalues and the corresponding eigenfunctions for the first drum:

1 Initialize the FEM structure and create the geometry and mesh:

```
clear fem
fem.shape = 2;
fem.sshape = 2;
fem.geom = poly2([-3,-3, 1, 1, 3, 1, -1, -1], ...
  [-3,-1,3,1,1,-1,-1,-3]);
fem.mesh = meshinit(fem);
fem.mesh = meshrefine(fem);
```

2 The eigenvalue PDE coefficients c and d for this problem are $c = 1$ and $d = 1$. Setting `h` to 1 ensures zero Dirichlet conditions on the boundaries:

```
fem.equ.c = 1;
fem.equ.da = 1;
fem.bnd.h = 1;
```

3 Create the extended mesh and call the eigenvalue solver. Find the resulting eigenvalues in the field `fem.sol.lambda`.

```
fem.xmesh = meshextend(fem);
fem.sol = femeig(fem);
```

4 To plot the fourth eigenfunction as a surface plot, type

```
postplot(fem,'tridata','u','solnum',4,'axisequal','on');
```

5 To model the second drum, replace the line defining the geometry with the following:

```
fem.geom = poly2([-3,-3, 1, 1, 3, 1, -1, -1], ...
  [-1,1,1,3,1,-1,-1,-3]);
```

RICHARDSON EXTRAPOLATION

The Richardson extrapolation part assumes that you have already created an FEM structure, either by exporting from COMSOL Multiphysics or by following the command-line instructions.

1. To begin, export or create the FEM structure for the first drum.
2. For the Richardson extrapolation, you need three meshes of different levels of refinement. To save the previous results, copy the FEM structure into three new FEM structures:

```
fem1 = fem;
fem2 = fem;
fem3 = fem;
```

3. First create a coarse mesh and solve the problem:

```
fem1.mesh = meshinit(fem1);
fem1.mesh = meshrefine(fem);
fem1.xmesh = meshextend(fem1);
fem1.sol = femeig(fem1);
```

   The field `fem1.sol.lambda` now contains the first six eigenvalues.

4. Second, create an intermediate mesh by refining the coarse mesh and then solve the problem:

```
fem2.mesh = meshrefine(fem1);
fem2.xmesh = meshextend(fem2);
fem2.sol = femeig(fem2);
```

5. Now create a fine mesh by refining again and solve the problem:

```
fem3.mesh = meshrefine(fem2);
fem3.xmesh = meshextend(fem3);
fem3.sol = femeig(fem3);
```

6. Now you can extrapolate these three results. To do so you must know the error behavior. The numerical eigenvalue λ_h differs from the exact eigenvalue λ according to

$$\lambda_h \approx \lambda + c_1 h^{4/3} + c_2 h^3 + \ldots$$

where h is the mesh parameter describing the length of the typical triangle edges. The exponent $4/3$ appears in the error due to the occurrence of concave corners in the geometry and does not depend on the element order. The second term corresponds to the standard error of the finite element method using second-order Lagrange elements.

Because you have three meshes with the parameters h, $h/2$, and $h/4$, and because you also have the three corresponding numerical eigenvalues λ_h, $\lambda_{h/2}$, and $\lambda_{h/4}$, you can solve for the unknowns λ, c_1, and c_2. This procedure yields a linear system

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & (1/2)^{4/3} & (1/2)^3 \\ 1 & (1/4)^{4/3} & (1/4)^3 \end{bmatrix} \begin{bmatrix} \lambda \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \lambda_h \\ \lambda_{h/2} \\ \lambda_{h/4} \end{bmatrix}$$

that you can solve by entering the following commands:

```
v = [1;1/2;1/4]*ones(1,3);
e = ones(3,1)*[0 4/3 4];
A = v.^e;
b = [fem1.sol.lambda;fem2.sol.lambda;fem3.sol.lambda];
x = A\b
lambda1 = x(1,:)
```

The vector `lambda1` now contains the extrapolated values for the first drum. Notice that the extrapolated values are all smaller than the corresponding non-extrapolated values. This is because solving an eigenvalue problem is related to solving a certain equivalent minimization problem, and a better numerical solution typically corresponds to a lower value. You can also observe the same effect when refining the mesh (see the vector `b` as created above).

Now export or create the FEM structure corresponding to the second drum and repeat the steps above. For comparison, remember to rename the `lambda1` vector, for example, `lambda2`.

Finally, compare the Richardson extrapolation results for the first six eigenvalues of the two domains and note that they agree to at least five decimal places.

```
2.537944    3.655510    5.175560    6.537563    7.248088    9.209311
2.537944    3.655512    5.175560    6.537560    7.248088    9.209319
```

Scientists have determined values for the first six eigenvalues, and they appear in the list below to approximately 12 decimal places (Ref. 3).

```
2.53794399980
3.65550971352
5.17555935622
6.53755744376
7.24807786256
9.20929499840
```

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