COMSOL MULTIPHYSICS

MEMS MODULE

MODEL LIBRARY

VERSION 3.4

COMSOL

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MEMS Module Model Library

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CONTENTS

Chapter 1: Introduction

Chapter 2: MEMS Actuator Models

Chapter 3: MEMS Sensor Models

Chapter 4: Microfluidics Models

Chapter 5: Models of Piezoelectric Devices

1

Introduction

The *MEMS Module Model Library* consists of a set of models that demonstrate the use of this module for modeling of various types of MEMS devices. The purpose of these models is to assist you in learning, by example, how to create sophisticated multiphysics models for design and analysis of microelectromechanical systems. In addition to serving as a reference, the model library can also give you a big head start if you are developing a model of a similar nature.

We have divided these models into four different groups:

- Actuator models
- Sensor models
- Microfluidics models
- Piezoelectric models

The models also illustrate the use of the various application modes in the MEMS Module that we used to build these models. Some models also make use of the PDE modes in COMSOL Multiphysics for equation-based modeling.

The book in your hands, the *MEMS Module Model Library*, provides details about a large number of ready-to-run models that illustrate real-world uses of the module.

Each model start with a model definition and results presentation. This part also includes information about how to implement the analysis using the MEMS Module. The last part of the model contains step-by-step instructions on how to build the model, perform the analysis, and finally visualize and postprocess the solution. For an overview of the functionality in the MEMS Module and a detailed introductory example, see the *MEMS Module User's Guide* and the *MEMS Module Reference Guide*. For more information on how to work with the COMSOL Multiphysics user interface, please refer to the *COMSOL Multiphysics User's Guide* or the *COMSOL Multiphysics Quick Start & Quick Reference* manual. An explanation on how to model using a programming language is available in yet another book, the *COMSOL Multiphysics Scripting Guide*.

Finally note that we supply these models as COMSOL Multiphysics Model MPH-files, available in the MEMS Module section on the Model Library page in the Model Navigator. You can open these models in COMSOL Multiphysics for immediate access making it possible to follow these examples every step along the way.

Model Library Guide

The table below summarizes key information about the entries in this model library. One column indicates which application modes (such as Plane Stress) the model includes. The solution time is the elapsed time measured on a machine running Windows Vista with a 2.6 GHz AMD Athlon X2 Dual Core 500 CPU and 2 GB of RAM. For models with a sequential solution strategy, the Solution Time column shows the elapsed time for the longest solution step. The following columns indicate the analysis type (such as eigenfrequency), and if multiphysics modeling or parametric studies are part of the model.

TABLE 1-1: MEMS MODULE MODEL LIBRARY MODELS

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	STATIONARY	EIGENFREQUENCY	TIME DEPENDENT	PARAMETRIC	MULTIPHYSICS
ACTUATOR MODELS	7							
Cantilever beam models	8							
Cantilever beam 2D	15	Plane Stress; Moving Mesh; Electrostatics	35 s				√	√

TABLE 1-1: MEMS MODULE MODEL LIBRARY MODELS

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	STATIONARY	EIGENFREQUENCY	TIME DEPENDENT	PARAMETRIC	MULTIPHYSICS
Cantilever beam 3D	21	Solid, Stress-Strain; Moving Mesh; Electrostatic	3 min	√				√
Comb drive	28	Plane Stress; Moving Mesh; Electrostatics	3 min	√			√	√
Capacitive 3D comb drive	44	Electrostatics	1 s	√				
Gecko foot	54	Solid, Stress Strain	20 s	√				
Microresistor beam	30*	Solid, Stress-Strain; Heat Transfer; Conductive Media DC	5 s	√				√
Micromirror	61	Solid, Stress-Strain	10 min	√			√	
Resonator models	73							
Resonator straight 2D	78	Plane Stress	2 s	√	√			
Resonator folded 2D	84	Plane Stress	4 s	√	√			
Resonator straight 3D	91	Solid, Stress-Strain	24 s	√	√			
Resonator folded 3D	99	Solid, Stress-Strain	29 s	√	√			
Thermoelastic damping models	106							
Thermoelastic damping 3D	115	Solid, Stress-Strain; Heat Transfer by Conduction	2 min					
Thermoelastic damping 2D	118	Plane Stress; Heat Transfer by Conduction	1 s					
Thermomechanical valve models	122							
Thermomechanical valve 2D	128	Plane Stress; Heat Transfer by Conduction; Conductive Media DC	27 s	√			√	√
Thermomechanical valve 3D	134	Solid, Stress-Strain; Heat Transfer by Conduction; Conductive Media DC	2 min	√			√	√
SENSOR MODELS	145							
Accelerometer models	146							

TABLE 1-1: MEMS MODULE MODEL LIBRARY MODELS

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	STATIONARY	EIGENFREQUENCY	TIME DEPENDENT	PARAMETRIC	MULTIPHYSICS
Accelerometer 2D	151	Plane Stress; Weak Form PDE	18 s			√		√
Accelerometer 3D	155	Solid, Stress-Strain; Weak Form PDE	2 min			√		√
MEMS gyroscope	161	Solid, Stress-Strain; Film Damping	11 min					
Piezoresistive elevator button	177	Solid, Stress-Strain; Electric Currents**	11 min			√		√
Pressure sensor 2D	194	Plane Stress; Weak Form PDE; Electrostatics	36 s	√				√
SAW gas sensor	212	Piezo Plane Strain	11 s		√			√
Thermal expansion in a MEMS device using the Material Library	227	Solid, Stress-Strain; Heat Transfer by Conduction	19 s	√				√
MICROFLUIDICS MODELS	241							
AC electrokinetic 2D	242	Electrostatics; Convection and Conduction; Incompressible Navier-Stokes; Diffusion and Convection; Diffusion	33 s			√		√
Electrokinetic valve 3D	294	Electrokinetic Flow; Incompressible Navier-Stokes; Conductive Media DC; Poisson's Equation	9 s			√		√
Fluid-structure interaction	294	Plane Strain with Fluid Interaction	2 min			√		√
Lamella mixer	307	Incompressible Navier-Stokes; Diffusion and Convection	53 s	√			√	√
Electroosmotic flow in a biochip	322	Electroosmotic Flow	1 s					

TABLE 1-1: MEMS MODULE MODEL LIBRARY MODELS

MODEL	PAGE	APPLICATION MODES	SOLUTION TIME	STATIONARY	EIGENFREQUENCY	TIME DEPENDENT	PARAMETRIC	MULTIPHYSICS
Low-voltage electroosmotic micropump	335	Electroosmotic Flow	17 s					
Electroosmotic mixer	349	Incompressible Navier-Stokes; Conductive Media DC	4 min			√		√
Star-shaped microchannel chip	364	Incompressible Navier-Stokes	33 s			√		
Microchannel H-cell	376	Flow with Species Transport	2 min				√	√
Inkjet model	390	Level Set and Laminar Flow	4 h			√		√
Filling of a capillary channel	404	Level Set and Laminar Flow	149 min			√		√
Hydrocarbon dehalogenation in a tortuous microreactor***	418	Incompressible Navier-Stokes	14 s	√				√
PIEZOELECTRICITY MODELS	435							
Piezoceramic tube	436	Piezo Axial Symmetry; Axial Symmetry Stress-Strain,	1 s	√				√
Piezoelectric shear actuated beam	449	Piezo Solid	7 s	√				√
Composite piezoelectric transducer	461	Piezo Solid; Solid, Stress-Strain	6 min		√		√	√

*In the *MEMS Module User's Guide*.

**This model requires the AC/DC Module.

***This model requires the COMSOL Reaction Engineering Lab.

We welcome any questions, comments, or suggestions you might have concerning these models. Contact us at `info@comsol.com` or call your local COMSOL representative.

Typographical Conventions

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

- A **boldface** font of the shown size and style indicates that the given word(s) appear exactly that way on the COMSOL graphical user interface (for toolbar buttons in the corresponding tooltip). For instance, we often refer to the **Model Navigator**, which is the window that appears when you start a new modeling session in COMSOL; the corresponding window on the screen has the title **Model Navigator**. As another example, the instructions might say to click the **Multiphysics** button, and the boldface font indicates that you can expect to see a button with that exact label on the COMSOL user interface.
- The names of other items on the graphical user interface that do not have direct labels contain a leading uppercase letter. For instance, we often refer to the Draw toolbar; this vertical bar containing many icons appears on the left side of the user interface during geometry modeling. However, nowhere on the screen will you see the term "Draw" referring to this toolbar (if it were on the screen, we would print it in this manual as the **Draw** menu).
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** means: Open the **COMSOL Multiphysics** folder, open the **Heat Transfer** folder, and select **Conduction**.
- A `Code` (monospace) font indicates keyboard entries in the user interface. You might see an instruction such as "Type `1.25` in the **Current density** edit field." The monospace font also indicates COMSOL Script codes.
- An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or in the Glossary. The names of books in the COMSOL documentation set also appear using an italic font.

2

MEMS Actuator Models

This chapter contains example models of MEMS actuators such as cantilever beams, comb drives, gecko feet, micromirrors, resonators, and thermomechanical microvalves. These models often include movements and geometry changes. Using the Moving Mesh (ALE) application mode you can include these effects in your own models, and the cantilever beam and comb drive models show how to do so. The Capacitive 3D Comb Drive model is an example of how to make a quick 3D analysis of the electrostatic field and calculate a base capacitance value based on that. Prestressed Micromirror and Thin-Film Resonator are pure continuum mechanics models. They demonstrate how you can model residual stresses using initial stress option. Two models, Microresistor Beam and Thermomechanical Microvalve, are examples of electro-thermal-structural couplings. In both models, the application is to move the structure by conducting a current through conductive layers and generate a temperature increase that leads to a displacement through thermal expansion. The Gecko Foot model uses assembly features and interactive meshing to model both the nanohair and microhair of a synthetic gecko foot.

Cantilever Beam

Introduction

The elastic cantilever beam is an elementary structure in MEMS design. This example shows the bending of a beam due to electrostatic forces. The primary problem the model addresses is the 2-way coupling between the deformations and the electric field. It solves the electrostatic equation in the air domain surrounding the beam using the *arbitrary Lagrangian-Eulerian* (ALE) method to account for geometry changes associated with the deformation. There are two versions: a 2D model and a 3D model. The 2D model uses the Plane Strain and the Electrostatics application modes from the MEMS Module and then the Moving Mesh (ALE) application mode from COMSOL Multiphysics. The 3D model uses the Solid, Stress-Strain application mode for the structural part.

Model Definition

Figure 2-1 and Figure 2-2 show the model geometry both in 2D and 3D. The cantilever beam, made of polysilicon (Young's modulus, E, for the material is 153 GPa, and its Poisson's ratio, ν, is 0.23), is fixed at one end but is otherwise free to move. It is coated with a thin conductive layer from the lower side. The beam resides in an air-filled chamber that is electrically insulated. However, the lower side of the chamber has an electrode that is grounded.

An electrostatic force caused by an applied potential difference between the two electrodes make the beam bend towards the grounded layer below it. To compute the electrostatic force, this example calculates the electric field in the surrounding air. The model considers a layer of air 20 μm thick both above and to the sides of the beam, and the air gap between the bottom of the beam and the grounded layer is initially 2 μm. As the beam bends, the geometry of the air changes continuously. Using the ALE method, the model takes this displacement into account when computing the potential field. Thus, the geometry deforms, and the electric field between the electrodes continuously changes as a result of the bending.

Figure 2-1: The cantilever-beam model's initial geometry. In 2D the beam has a length of 300 µm and a height of 2 µm, and it is fixed at the left boundary. The lower boundary of the surrounding air domain represents the grounded substrate.

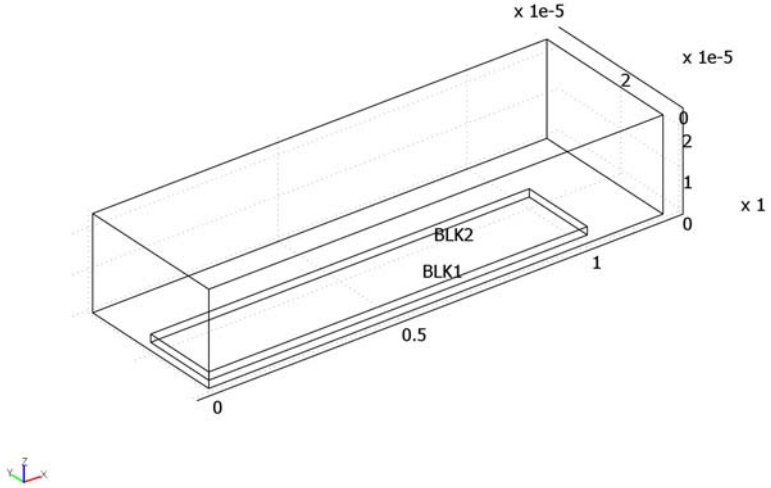


Figure 2-2: The cantilever beam's initial geometry in 3D. The beam is 100 µm long and 2 µm thick, and it is fixed at x = 0. The model uses symmetry on the zx-plane at y = 0, and thus it examines only a 20-µm wide section of the 40-µm wide beam. The lower boundary of the surrounding air domain represents the grounded substrate. The model has 20 µm of free air above and to the sides of the beam, while the gap below the beam is 2 µm.

This model solves the electric field within the air and the beam using the electrostatic equation

$$-\nabla \cdot (\varepsilon \nabla V) = 0 .$$

The model places the lower-boundary cantilever beam at a positive potential. The electric field is continuous from the polysilicon to air on the other boundaries. The lower boundary of the chamber is grounded, and all other boundaries are electrically insulated. The model solves the electrostatic equation on the deformed mesh that the Moving Mesh (ALE) application mode introduces.

The force density that acts on the electrode of the beam results from the Maxwell's stress tensor:

$$\mathbf{F}_{es} = -\frac{1}{2}(\mathbf{E} \cdot \mathbf{D})\mathbf{n} + (\mathbf{n} \cdot \mathbf{E})\mathbf{D}^T ,$$

where **E** and **D** are the electric field and electric displacement vectors, respectively, and **n** is the outward normal vector of the boundary. This force is always oriented along the normal of the boundary.

In 2D this model solves the structural deformation of the beam using the plane strain approximation.

Results

A positive feedback exists between the electrostatic forces and the deformation of the cantilever beam. The forces bend the beam and thereby reduce the gap to the grounded substrate. This action, in turn, increases the forces. At a certain voltage the electrostatic forces overcome the stress forces, the system becomes unstable, and the gap collapses. This critical voltage is called the *pull-in voltage*.

At applied voltages lower than the pull-in voltage, the beam stays in an equilibrium position where the stress forces balance the electrostatic forces. Figure 2-3 shows the potential field and the deformations for a 300 μm long 2D case. Similarly, Figure 2-4 shows the steady-state solution in a 100-μm long 3D case with 58 V applied. Because the cantilever's length in the 3D model is shorter (100 μm), the structure's stiffness is higher and a much higher applied voltage is required to achieve similar deformations as in the 2D model. Figure 2-5 shows the shape of the cantilever's deformation extracted from 3D results along the long edge.

When solving for a level higher than the pull-in voltage, the solution ceases to converge before the beam touches the substrate. This is an effect of the ALE method not being able to handle topology changes. By scanning over different applied voltages and using the parametric solver, you can study the beam's behavior and estimate the pull-in voltage. Figure 2-6 shows the deflection of the beam's end in a 2D model for different applied voltages.

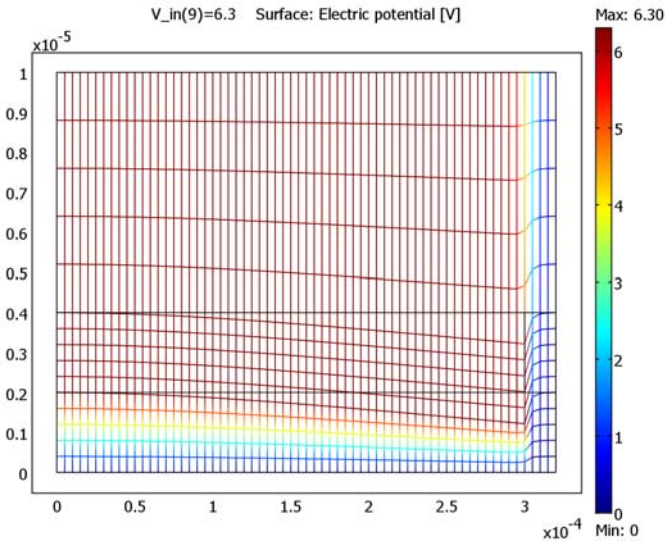


Figure 2-3: (2D model) The potential field and deformations at the cantilever beam's equilibrium position for an applied voltage of 6.3 V.

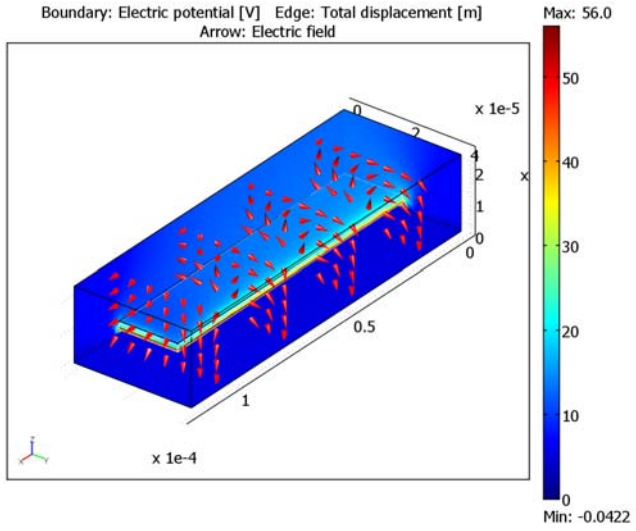


Figure 2-4: (3D model) Steady-state solution for the 3D cantilever-beam model with an applied voltage of 58 V. The boundaries display the electric potential; the arrows show the electric field; the black edges indicate the non-deformed beam geometry; and the white edges delineate the deformed geometry.

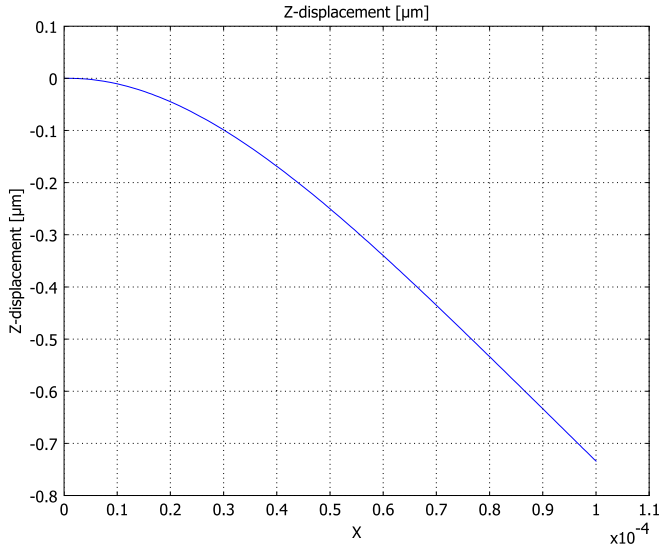


Figure 2-5: (3D model) The deformed shape of the cantilever along the long edge. This result is obtained from the 3D model.

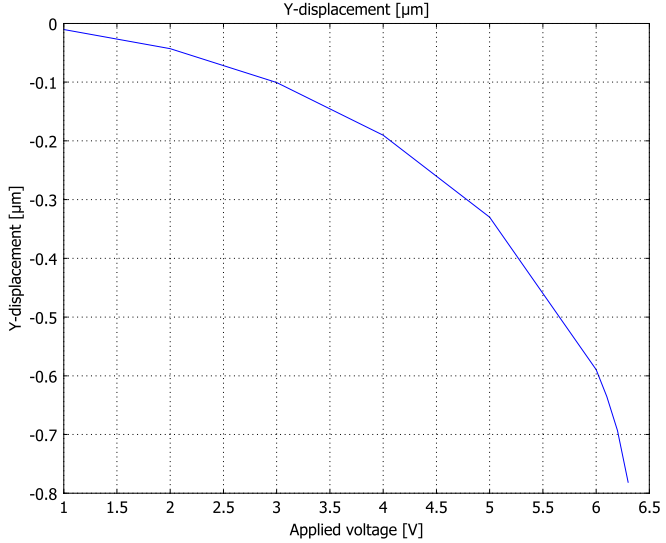


Figure 2-6: (2D model) Vertical displacement at the beam tip as a function of the applied voltage. The solution ceases to converge just before the beam touches the substrate.

The Figure 2-6 indicates that the pull-in voltage of the 300 µm long cantilever beam is somewhere between 6.3 V and 6.4 V. Using a finer mesh and computing the solution for a number of voltages in this range should reduce the size of this interval. For comparison, computations in Ref. 1 lead to the pull-in voltage of

$$V_{\mathrm{PI}} = \sqrt{\frac{4c_1 B}{\varepsilon_0 L^4 c_2^2 \left(1 + c_3 \frac{g_0}{W}\right)}}$$

where $c_1 = 0.07$, $c_2 = 1.00$, and $c_3 = 0.42$; g_0 is the initial gap between the beam and the ground plane; and

$$B = \hat{E} H^3 g_0^3.$$

If the beam has a narrow width (W) relative to its thickness (H) and length (L), $\hat{E}$ is Young's modulus, E. Otherwise, $\hat{E}$ is the plate modulus, $E/(1-\eta^2)$, where η is Poisson's ratio. Because the calculation in Ref. 1 uses a parallel-plate approximation for calculating the electrostatic force and because it corrects for fringing fields, these results are not directly comparable with those from the simulation. Inserting the data from the model in the formula and using an infinite width, W, to disable the fringing-field correction gives $V_{\mathrm{PI}} = 6.35$ V. Setting $W = 40$ µm results in $V_{\mathrm{PI}} = 6.28$ V. Here is some COMSOL Script code that calculates the analytical pull-in voltages:

```
% pull-in.m - calculates the analytical value for the pull-in
%   voltage
W = 40e-6; H = 2e-6; L = 300e-6;
gap = 2e-6;
c1 = 0.07; c2 = 1.00; c3 = 0.42;
E = 153e9;
nu = 0.23;
eps0 = 8.854e-12;
Ehat = E; % or = E/(1-nu^2);
B = Ehat*H^3*gap^3;
Vpi = sqrt((4*c1*B)/(eps0*L^4*c2^2*(1+c3*gap/W))); % or W -> inf
fprintf(1,'Pull in voltage is %f V \n', Vpi);
```

Modeling in COMSOL Multiphysics

COMSOL Multiphysics translates the application-mode equations between the fixed and moving frames. The program keeps track of the movements using the Moving Mesh (ALE) application mode and a transformation matrix, which you compute from the material displacements at the beam's boundaries. In this model the displacements are such that the forces' change of direction is almost negligible, but the

transformation might be needed if this serves as a template for a simulation that deals with larger deformations. Using the force transformation and support for large deformations in the Plane Strain application mode makes bending through large angles possible. Because the cantilever beam has a constant potential, the electrostatic forces are always perpendicular to its surface. To ensure that these forces have this orientation, the model uses the Electrostatics application mode's ability to calculate Maxwell's surface stress tensors on boundaries to define the electrostatic force.

In the 3D case, the large-deformation option doesn't dramatically affect the results. The difference in the z-displacement of the cantilever's tip between the large deformation being on and off is less than 1%. However, the solution time more than doubles when the large deformation is activated. Thus in the 3D case this exercise uses only the linear stress-strain relationship (where the large deformation is off).

Here the 2D case examines a parametric study in which the applied voltage varies. However, because the solution time for the parametric solution in the 3D case might expand to several hours, for 3D this example solves only the static solution. If more detailed studies are required, you should then also conduct a parametric or time-dependent analysis.

Reference

1. R.K. Gupta, *Electrostatic Pull-In Structure Design for In-Situ Mechanical Property Measurements of Microelectromechanical Systems (MEMS)*, Ph.D. thesis, MIT, 1997.

Model Library path: `MEMS_Module/Actuator_Models/ale_cantilever_beam_2d`

Model Library path: `MEMS_Module/Actuator_Models/ale_cantilever_beam_3d`

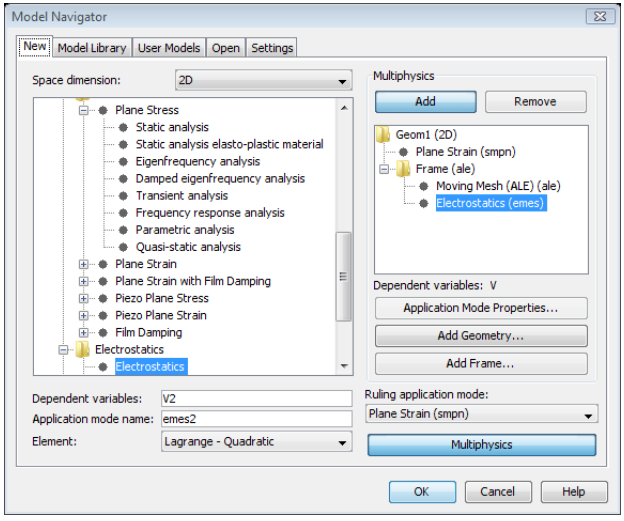
MODEL NAVIGATOR

1 In the **Model Navigator** select **2D** from the **Space dimension** list and then click **Multiphysics**.

2 From the list of application modes on the left side of the dialog box select **MEMS Module>Structural Mechanics>Plane Strain** and then click **Add**.

3 From the list of application modes select **COMSOL Multiphysics>Deformed Mesh>Moving Mesh (ALE)** and then click **Add**.

4 In the **Multiphysics** list on the right side of the dialog box select **Frame (ale)** then add **MEMS Module>Electrostatics>Electrostatics** to that list. As a result, the selected application modes in Model Navigator window look like this:



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

GEOMETRY MODELING

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

2 Clear the **Axis equal** check box, then click **OK**.

3 While holding down the Shift key, click the **Rectangle/Square** button on the Draw toolbar on the far left side of the graphical user interface; this action opens the **Rectangle** dialog box. Enter dimensions as in the following table, then click **OK**.

PROPERTY	VALUE
Width	300e-6
Height	2e-6
X	0
Y	2e-6

4 Repeat the procedure to make another rectangle but with these dimensions:

PROPERTY	VALUE
Width	320e-6
Height	10e-6
X	0
Y	0

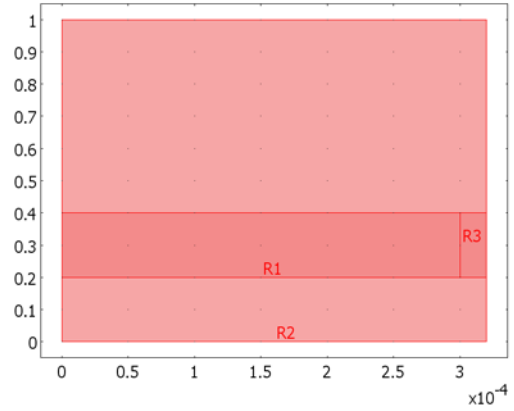
5 Click the **Zoom Extents** button on the Main toolbar at the top of the graphical user interface.

The inner rectangle represents the cantilever beam and the outer rectangle the surrounding air. These two objects would be enough to model the geometry with an unstructured mesh. However, in this model you use a mapped mesh, and for that purpose you add a rectangle that divides the air into three subdomains. This helps you create a rectangular mesh later on.

6 Repeat the procedure to create a third rectangle with these dimensions:

PROPERTY	VALUE
Width	20e-6
Height	2e-6
X	300e-6
Y	2e-6

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



Completed 2D model geometry.

PHYSICS SETTINGS

Subdomain Settings—Electrostatics

1 Go to the **Multiphysics** menu and make sure that **Electrostatics (emes)** is selected.

2 Open the **Physics>Subdomain Settings** dialog box and select Subdomains 1, 3, and 4. The default settings ($\varepsilon_r = 1$) corresponds to air, so keep them.

3 While still in that dialog box, select Subdomain 2. For the relative permittivity, ε_r, enter the value `4.5` (for polysilicon). Click the **Force** tab. In the first row enter `Fes`. The software automatically generates the variables `Fes_nTx_emes` and `Fes_nTy_emes` for the electrostatic force components. Later on you use these variables to define the boundary load in the Plane Strain application mode.

4 Click **OK**.

Boundary Conditions—Electrostatics

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

2 Select the **Interior boundaries** check box, then specify conditions as follows:

SETTINGS	BOUNDARIES 1, 3, 5, 7, 11–13	BOUNDARY 4	BOUNDARY 2	BOUNDARIES 6, 8, 9, 10
Boundary condition	Zero charge/ Symmetry	Electric potential	Ground	Continuity
V_0		`V_in`		

3 Click **OK**.

Subdomain Settings—Moving Mesh

1 From the **Multiphysics** menu, select **Moving Mesh (ale)**.

2 In the **Subdomain Settings** dialog box select the those for air (Subdomains 1, 3, and 4). Keep the default **Free displacement** setting.

3 While still in that dialog box select Subdomain 2. Inside the cantilever beam use **Physics induced displacement**. For the displacement variables, **dx** and **dy**, enter u and v, respectively. These are the displacements from the Plane Strain application mode.

4 Click **OK**.

Boundary Conditions—Moving Mesh

1 In the **Boundary Settings** dialog box, for the mesh displacements, **dx** and **dy**, enter the following values for outer settings (do not assign any settings for interior boundaries, which appear dimmed):

SETTINGS	BOUNDARIES 4, 6, 8	ALL OTHERS
dx	u	0
dy	v	0

2 Click **OK**.

Application Mode Properties—Plane Strain

1 From the **Multiphysics** menu, choose **Plane Strain (smpn)**.

2 From the **Physics** menu, open the **Properties** dialog box.

3 Click the **Application Mode Properties** button. From the **Large deformation** list, select **On**, then click **OK**.

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

The large-deformation option ensures that the solver uses a nonlinear stress-strain relationship to calculate the results in the Plane Strain application mode.

Subdomain Settings—Plane Strain

1 In the **Subdomain Settings** dialog box select Subdomain 2 and enter the following settings. Later on you use the parametric solver to find an estimate for the pull-in voltage, thus you only need to specify Young's modulus, E, Poisson's ratio, v, and the thickness.

SETTINGS	SUBDOMAIN 2
E	153e9
v	0.23

SETTINGS	SUBDOMAIN 2
α	4.15e-6
ρ	2330
thickness	20e-6

2 While still in the dialog box select Subdomains 1, 3, and 4. To make this application mode inactive outside the cantilever, clear the **Active in this domain** check box.

3 Click **OK**.

Boundary Conditions—Plane Strain

1 From the **Physics** menu, select **Boundary Settings**. In the resulting dialog box verify that the **Interior boundaries** check box is cleared.

2 Click the **Constraint** tab. Select Boundary 3. From the **Constraint condition** list select **Fixed**.

3 Click the **Load** tab. Enter boundary loads according to the following table; when finished, click **OK**.

SETTINGS	BOUNDARIES 3, 6, 8	BOUNDARY 4
F_x	0	Fes_nTx_emes
F_y	0	Fes_nTy_emes

Fes_nTx_emes and Fes_nTy_emes are automatically generated variables from the Electrostatics application mode (_emes) that define the x- and y-components of the electrostatic force, respectively.

4 Click **OK** to accept the boundary conditions.

MESH GENERATION

1 From the **Mesh** menu, open the **Mapped Mesh Parameters** dialog box.

2 Click the **Boundary** tab. Select Boundaries 1, 3, and 5.

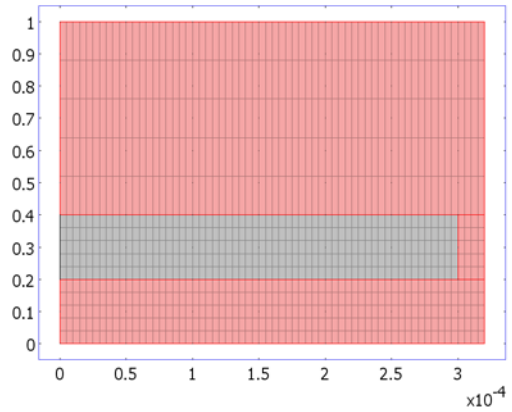
3 Check the **Constrained edge element distribution** check box and type 5 in the **Number of edge elements** edit field.

4 Repeat the previous step for Boundaries 6 and 10, in turn, using the values 60 and 4, respectively, for the **Number of edge elements**.

5 Click **Remesh**.

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

The completed mesh should look like that in the following figure.



Mesh for the 2D model.

COMPUTING THE SOLUTION

1. From the **Solver** menu, open the **Solver Parameters** dialog box.
2. Go to the **Solver** list and select **Parametric**.
3. In the **Parameter name** edit field, type `V_in`.
4. In the **Parameter values** edit field type `1:6, 6.1:0.1:6.3`. Because the cantilever deforms less at lower voltages, start with a long step (1.0 V) and then, when the solution gets closer to the pull-in value, use a shorter step (0.1 V).
5. Click **OK**.
6. Click the **Solve** button on the Main toolbar.

Note: If you try to solve the model for higher values of the applied voltage (for example, 6.4) the solver ceases to find a proper solution and you receive an error message ("Failed to find a solution for all parameters, even when using the minimum parameter step."). This indicates that you have exceeded the pull-in voltage. In that case, you can scroll up the log area of the solver's **Progress** window to find out the latest parameter values that the solver tried to use. That way you can get a more accurate estimate for the pull-in voltage.

POSTPROCESSING AND VISUALIZATION

The default plot shows the von Mises stress at the last successful parameter value $V_{in}(9) = 6.3$ V. To see deformations inside the cantilever beam, follow these instructions:

1. From the **Postprocessing** menu, open the **Plot Parameters** dialog box.
2. On the **General** page select the **Surface** check box. Make sure the check boxes for all other plot types are cleared.
3. Click the **Surface** tab. Go to the **Predefined quantities** list and select **Plane Strain (smps)>Total displacement**.
4. Click **Apply**.

To visualize the deformed mesh in the air domain, do as follows:

1. Click the **General** tab.
2. Clear the **Element refinement: Auto** check box and type 1 in the associated edit field. This makes a wireframe plot that represents the computational mesh.
3. Make sure that only the **Surface** and **Geometry edges** check boxes are selected.
4. Make sure that **Frame (ale)** is selected from the **Frame** list.
5. Click the **Surface** tab. From the **Predefined quantities** list on the **Subdomain Data** page, select **Electrostatics (emes)>Electric potential**. From the **Fill style** list in the **Coloring and fill** area, select **Wireframe**.
6. Click **OK**. This generates the plot in Figure 2-3 on page 11.

Next, plot the displacement of the cantilever beam's tip as a function of the voltage:

1. From the **Postprocessing** menu, select **Domain Plot Parameters**.
2. Click the **Title/Axis** button. Click the option button next to the **First axis label** edit field and enter the label `Applied voltage [V]`. Click **OK**.
3. Click the **Point** tab. From the **Point selection** list, select Point 5. From the **Predefined quantities** list, select **Plane Strain (smpn)>Y-displacement**. From the **Unit** list, select **um** to get the plot unit micrometer.
4. Click **OK** to close the dialog box and generate the plot in Figure 2-6.

Modeling Using the Graphical User Interface—3D Version

MODEL NAVIGATOR

1. In the **Model Navigator** select **3D** in the **Space dimension** list, then click **Multiphysics**.

2 From the list of application modes on the left side of the dialog box, select **MEMS Module>Structural Mechanics>Solid, Stress-Strain**. Click **Add**.

3 From the list of application modes, select **COMSOL Multiphysics>Deformed Mesh>Moving Mesh (ALE)** and then click **Add**.

4 In the **Multiphysics** list on the right side of the dialog box, select **Frame (ale)** then add **MEMS Module>Electrostatics>Electrostatics** to that list.

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

GEOMETRY MODELING

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

2 In the **Length** area, set **X** to `100e-6`, **Y** to `20e-6`, and **Z** to `2e-6`. In the **Axis base point** area, set **Z** to `2e-6`.

3 Click **OK**.

4 Repeat that procedure to make another block but this time set **X** to `120e-6`, **Y** to `40e-6`, and **Z** to `24e-6`.

5 Click **OK**.

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

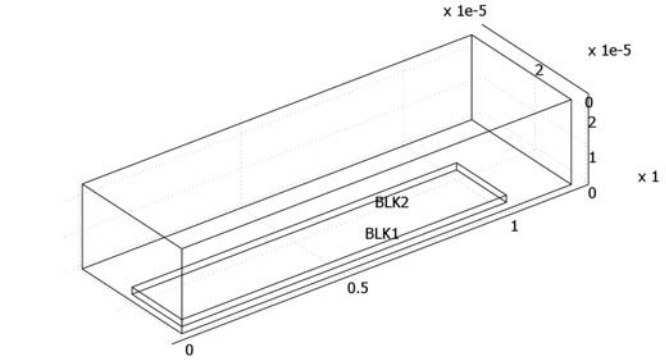


Figure 2-7: The geometry for 3D cantilever beam model. The inner block represents the cantilever beam and the outer rectangle the surrounding air. Symmetry is defined along the plane y = 0.

OPTIONS

Constants

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

2 Define a constant named `V0` by the expression `56[V]` and give it the description `Applied voltage`.

3 Click **OK**.

PHYSICS SETTINGS

Application Mode Properties—Solid, Stress-Strain

If you need more-precise results, try using the nonlinear stress-strain relationship. To do so select **Properties** from the **Physics** menu and set the **Large Deformation** property option to On. In this example, however, the final result differs less than 1% when the large deformation is not in use, so you can skip that step and continue directly from the subdomain settings.

Subdomain Settings—Solid, Stress-Strain

1 Go to the **Multiphysics** menu and make sure that the **Solid, Stress-Strain (smsld)** application mode is selected.

2 Open the **Physics>Subdomain Settings** dialog box and select Subdomain 1. To deactivate this application mode outside the cantilever, clear the **Active in this subdomain** check box.

3 While still in the dialog box, select Subdomain 2 and enter the following settings. Later on you use a static solver to find the cantilever's displacement. Thus, you only need to specify Young's modulus, E, and Poisson's ratio, ν.

PROPERTY	VALUE
E	153e9
ν	0.23
α	4.15e-6
ρ	2330

4 Click **OK**.

Boundary Conditions—Solid, Stress-Strain

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

2 Click the **Constraint** tab, then select Boundary 4. From the **Constraint condition** list select **Fixed**.

3 Select Boundary 5. From the **Constraint condition** list, select **Symmetry plane**.

4 Click the **Load** tab. Select Boundary 6, then enter the following settings:

PROPERTY	VALUE
F_x	dnTx_emes
F_y	dnTy_emes
F_z	dnTz_emes

Here, dn_Tx_emes, dnTy_emes, and dnTz_emes are automatically generated variables from the Electrostatics application mode that define the x-, y-, and z-components of the electrostatic force towards the air.

5 Click **OK** to accept the boundary conditions.

Subdomain Settings—Moving Mesh

1 From the **Multiphysics** menu, select **Moving Mesh (ALE)**.

2 In the **Subdomain Settings** dialog box select the air (Subdomain 1). Keep the default **Free displacement** settings.

3 While still in the dialog box, select Subdomain 2. Inside the cantilever beam use **Physics induced** displacement. For the displacement variables, **dx**, **dy**, and **dz**, enter u, v, and w, respectively. These are the displacements from the Solid, Stress-Strain application mode.

4 Click **OK**.

Boundary Conditions—Moving Mesh

1 In the **Boundary Settings** dialog box for the mesh displacements, enter these settings:

SETTINGS	BOUNDARIES 6, 7, 9, 11	BOUNDARIES 1, 3, 8, 10, 12	BOUNDARY 2
dx	u	0	not selected
dy	v	0	0
dz	w	0	not selected

2 Click **OK**.

Subdomain Settings—Electrostatics

1 From the **Multiphysics** menu, select **Electrostatics (emes)**.

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

3 For Subdomain 1, the default settings ($\varepsilon_r = 1$) corresponds to air, so keep them.

4 While still in the dialog box, select Subdomain 2. Clear the **Active in this domain** check box.

5 Click **OK**.

Boundary Conditions—Electrostatics

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

2 First select all the boundaries and change the **Boundary condition** to **Zero charge/ Symmetry**.

3 Next select only Boundary 3, and for the **Boundary condition** select **Ground**.

4 Finally select Boundary 6. Change the **Boundary condition** to **Electric potential**, and in the $\mathbf{V_0}$ edit field type `V0`.

5 Click **OK**.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar. The mesh consists of roughly 3700 elements.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button from the Main toolbar; the **Solver Parameters** dialog box then opens.

2 In the **General** page change **Linear system solver** to **FGMRES**. Keep the default **Preconditioner**: **Geometric multigrid**.

3 Click the **Settings** button; the **Linear System Solver Settings** dialog box then opens.

4 Select **Presmoother** from the tree on the left.

5 Change **Presmoother** to **Vanka**.

6 Type `1` into the **Number of iterations** field; The default 2 operates equally well, but additional time will be spend for extra iterations.

7 In the **Vanka update** area type `lm4 lm5 lm6` into the **Variables** field.

This defines the variables that produce zeros in the diagonal of the equation system matrix. lm4, lm5, and lm6 are the variables used on the boundaries of the Moving Mesh (ALE) application mode.

8 Select **Postsmoother** from the tree on the left.

9 Define same settings as for the presmoother (repeat steps 8–11).

10 Select **Coarse solver** from the tree on the left.

11 Change **Coarse solver** to **PARDISO**.

For some difficult problems the default UMFPACK solver can be a more stable choice. But in general the PARDISO solver is more memory efficient and with multiprocessor computers you benefit from the parallel operation of the solver.

12 Click **OK** to close the **Linear System Solver Settings** dialog box.

13 Click **OK** to close the **Solver Settings** dialog box.

14 Click the **Solve** button on the Main toolbar. It takes a few minutes to compute the solution.

POSTPROCESSING AND VISUALIZATION

The default plot show the von Mises stress slice plot. To see the deformed structure and the electrostatic fields inside the air, follow these instructions:

1 From the **Options** menu, select **Suppress>Suppress Boundaries**. Select Boundaries 8, 10, and 12. Click **OK**.

2 Click the **Camera Parameters** button on the Camera toolbar. Change the **Camera constraint** to **Z** and the **Mouse constraint** to **Horizontal**, then click **Close**. Using the mouse, rotate the graphics 180 degrees so that the tip of the cantilever points toward you.

3 From the **Postprocessing** menu, open the **Plot Parameters** dialog box. In the **Plot type** area on the **General** page, clear the **Slice** check box and select the **Boundary**, **Edge**, and **Arrow** check boxes.

4 Click the **Boundary** tab. From the **Predefined quantities** list on the **Boundary Data** page, select **Electrostatics (emes)>Electric potential**.

5 Click the **Edge** tab. In the **Edge color** area, click first the **Uniform color** option and then the **Color** button. From the palette on the **Edge Color** dialog box, select white. Click **OK**.

6 Click the **Arrow** tab and go to the **Subdomain Data** page. From the **Predefined quantities** list, select **Electrostatics (emes)>Electric field**. In the **Arrow positioning** area go to the **Number of points** edit fields and enter `4` for **x points**, `7` for **y points**, and `5` for **z points**. Go to the **Arrow parameters** area. Change the **Arrow type** to **Cone** and the **Arrow length** to **Normalized**. Clear the **Auto** check box for the **Scale factor** and enter a value of `0.5`.

7 Click **OK**.

8 On the Camera toolbar, click the **Scene Light** and **Headlight** buttons to turn them on.

To visualize the shape of the deformed cantilever, generate a domain plot:

1 From the **Postprocessing** menu, select **Domain Plot Parameters** and then click the **Line/ Extrusion** tab.

2 From the **Edge selection** list, select **13**.

3 From the **Predefined quantities** list in the **y-axis data** area, select **Solid, Stress-Strain (smsld)>Z-displacement**.

4 From the **Unit** list, select **um** to see the results in micrometers.

5 In the **x-axis data** area, select **X** from the drop-down list.

6 Click **OK**.

Comb Drive

Introduction

Rectangular comb drives find use in a variety of MEMS applications. The following model of an electrostatically actuated comb drive opens and closes a pair of microtweezers. To facilitate controlled partial engagement, this design gives the comb fingers jagged edges. This model comes from Isabelle P. F. Harouche and Dr. Cyrus Shafai of the Department of Electrical and Computer Engineering, University of Manitoba, Canada (Ref. 1).

Model Definition

Figure 2-8 shows the microtweezers (top) and a close-up of part of the comb drive (bottom). Applying a voltage across the gaps between the combs actuates the tweezers. The structure is made of polysilicon and has a thickness of a few micrometers.

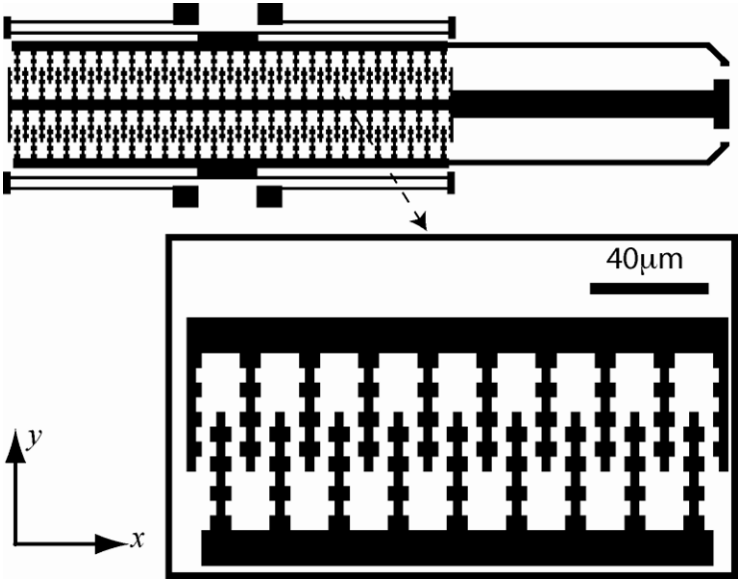


Figure 2-8: The microtweezers (top) and the comb-drive mechanism (bottom).

The model includes just a few of the teeth. It simulates only the comb drive and its attachment using double-folded beam springs. Taking advantage of symmetries means that you only have to set up a quarter of the geometry, see Figure 2-9.

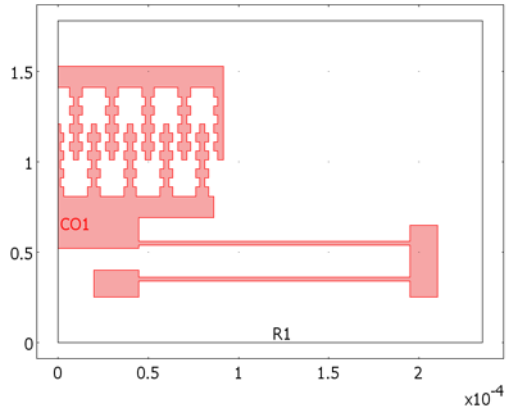


Figure 2-9: Initial (undeformed) model geometry.

The upper half of the comb is fixed, as is the end of the beam spring. The system applies an electric potential to the beam spring and the lower comb; the upper comb is grounded. In the air surrounding the comb drive, the model solves the electrostatic equation

$$-\nabla \cdot (\varepsilon \nabla V) = 0 .$$

The electrostatic force density is

$$F_{es} = \frac{\varepsilon E^2}{2},$$

and the simulation applies it to each comb as a perpendicular boundary load.

Modeling in COMSOL Multiphysics

Because electrostatic forces attract the combs to each other, any geometric change has an impact on the electric field between them. To account for this effect, the model uses an arbitrary Lagrangian-Eulerian (ALE) method implemented in COMSOL Multiphysics' Moving Mesh application mode. This application mode automatically keeps track of the movements and translate application mode equations between the fixed (reference) and moving frames.

In this model the displacements are relatively large. Therefore, you use the Plane Stress application mode's support for large deformations.

To define the electrostatic force, you use the Electrostatics application mode's Maxwell surface stress tensor boundary variables.

The geometry of this model is rather complex and thus the boundary conditions are laborious to enter. For an example that is faster and easier to set up, see the Cantilever beam model, which is a good introduction to using the Moving Mesh application mode.

Results and Discussion

The following two figures show the comb drive and the electric field at equilibrium for an actuation voltage of 600 V.

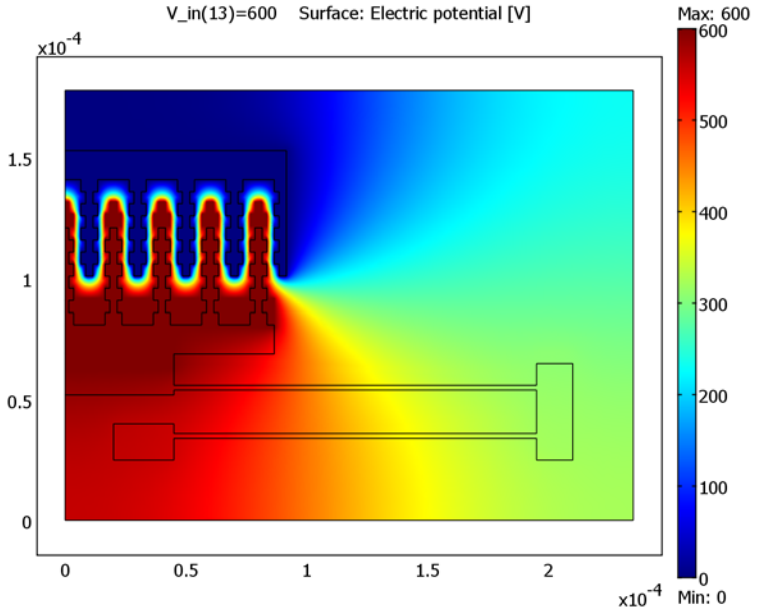


Figure 2-10: The electric-potential field for an actuation voltage of 600 V.

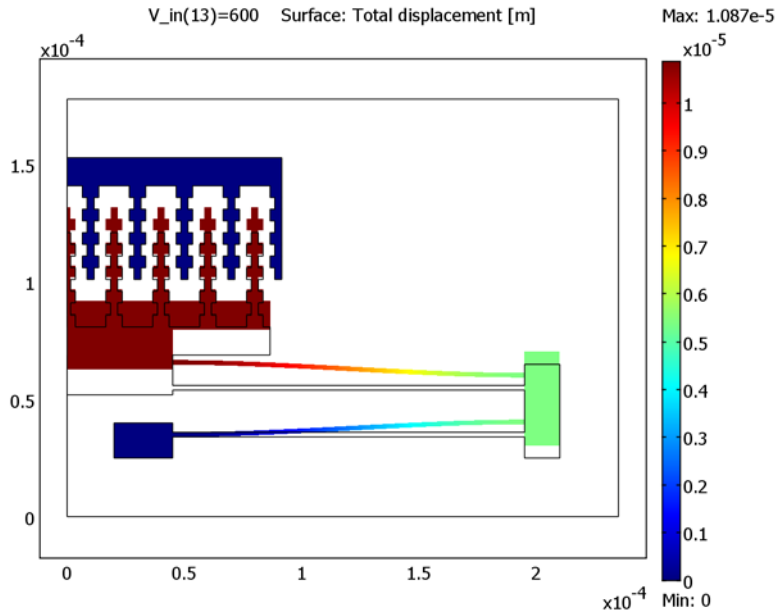


Figure 2-11: Displacements inside the comb drive at 600 V. The color scale that appears on the screen indicates displacements in the y direction.

The next figure plots the displacement at the tip of one of the fingers of the lower comb as a function of the actuation voltage. The teeth have some effect on the displacements, but in order to make step-by-step actuation possible (like a switch gear), they would need to be wider, almost touching each other.

To reduce actuation voltages it is common to construct comb drives with many more teeth than in this model. Preferably, you would model such comb drives using a periodic approximation, thereby allowing the simulation of only one pair of fingers. The model could handle plane stress analysis in a separate geometry using the parametric solver to find the displacement of the comb base as a function of the applied force. Then a boundary integration variable could integrate the force density and dictate the displacements.

Another extension of the model would include fringing-field effects. A full 3D model might not be realistic, but you could estimate the size of the fringing fields by modeling two fingers in both 2D and 3D. You could then include the result of this

simulation in the full 2D model as, for instance, an approximate correction factor applied directly to the actuation voltage.

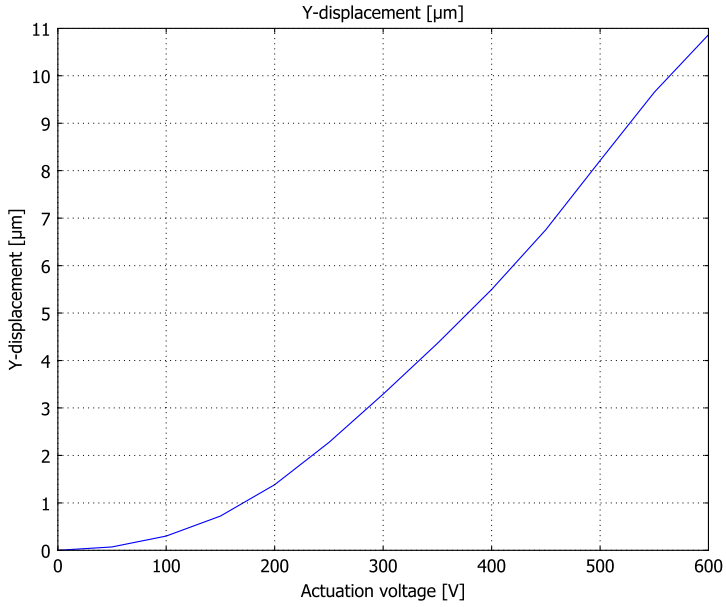


Figure 2-12: The displacement of the innermost comb finger as a function of the actuation voltage. For mid-range voltages the teeth suppress the displacement so that it is almost linear with voltage. Without teeth in the comb you could expect that the displacement would resemble a quadratic function of the voltage.

Reference

1. Isabelle P. F. Harouche and C. Shafai, "Simulation of shaped comb drive as a stepped actuator for microtweezers application," *Sensors and Actuators A: Physical*, 2005.

Model Library path: `MEMS_Module/Actuator_Models/comb_drive_2d`

MODEL NAVIGATOR

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

2 Click **Multiphysics**.

3 From the **Application Modes** list select **MEMS Module>Structural Mechanics>Plane Stress>Static analysis**.

4 Click **Add**.

5 Click the **Application Mode Properties** button. From the **Large deformation** list, select **On**, then click **OK**.

6 From the **Application Modes** list, select **COMSOL Multiphysics>Deformed mesh>Moving Mesh (ALE)**. Click **Add**.

7 Click the **Appliction Mode Properties** button and select **Winslow** in the **Smoothing method** list. Winslow smoothing works better for this model.

8 Click **OK** to close the **Appliction Mode Properties** dialog box.

9 In the **Multiphysics** list on the right side of the **Model Navigator**, select **Frame (ale)**.

10 From the **Application Modes** list, select **MEMS Module>Electrostatics>Electrostatics**.

11 Click **Add**.

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

GEOMETRY MODELING

Please follow these geometry-modeling steps carefully; the following discussion assumes that the boundary numbering is that resulting from these steps. After you complete the geometry it should have a total of 337 boundaries.

Notice also that you first enter the geometric objects as if they would be measured in micrometers (in other words, without the `e-6` after all numbers) and then, scale the entire geometry by 10^{-6} to have it in SI units. This approach reduces the amount of typing and avoids the likely error of forgetting to include `e-6` on one of the dimensions.

1 From the **Draw** menu, select **Specify Objects>Rectangle** to create rectangles (alternately, hold the Shift key and click on the **Rectangle/Square** button on the Draw

toolbar on the far left of the user interface). In the dialog box that opens, create four rectangles with these properties:

NAME	WIDTH	HEIGHT	X	Y
R1	7	5	-3.5	81
R2	3	5	-1.5	86
R3	7	5	6.5	106
R4	3	5	8.5	101

2 Select all the rectangles (use Ctrl+A) and click the **Array** button on the Draw toolbar.

3 Enter the data from this table:

DATA	EXPRESSION
X displacement	20
Y displacement	10
X size	5
Y size	4

4 Click **OK**.

5 Select all the rectangles and click the **Union** button on the Draw toolbar.

6 Create another rectangle with these properties:

NAME	WIDTH	HEIGHT	X	Y
R1	91.5	60	0	81

7 Select both objects and click the **Intersection** button on the Draw toolbar.

8 Create seven new rectangles with these properties:

NAME	WIDTH	HEIGHT	X	Y
R1	91.5	12	0	141
R2	86.5	12	0	69
R3	45	17	0	52
R4	150	2	45	54
R5	150	2	45	34
R6	25	15	20	25
R7	15	40	195	25

9 From the **Draw** menu select **Create Composite Object**.

10 In the dialog box that opens click **Select All**, then clear the **Keep interior boundaries** check box.

11 Click **OK**.

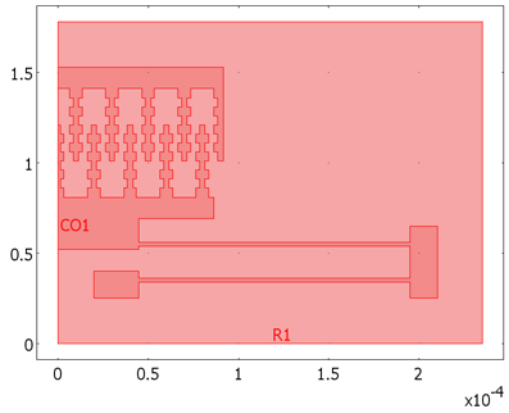
12 Create yet another rectangle:

NAME	WIDTH	HEIGHT	X	Y
R1	235	178	0	0

13 Select all the objects and click the **Scale** button. Enter `1e-6` for both the **X** and **Y** scale factors.

14 Click **OK**.

15 Click the **Zoom Extents** button.



The completed comb-drive geometry.

PHYSICS SETTINGS

Subdomain Settings—Electrostatics

1 From the **Multiphysics** menu, choose **Electrostatics (emes)**.

2 Open the **Subdomain Settings** dialog box, choose Subdomain 1, and verify that the relative permittivity, $\varepsilon_r = 1$.

3 Select Subdomains 2 and 3.

4 For the relative permittivity, ε_r, enter the value `4.5` (polysilicon).

5 Click the **Force** tab. On the first row enter `Fes`. COMSOL Multiphysics then automatically generates the variables `Fes_nTx_emes` and `Fes_nTy_emes` for the

electrostatic force components. Later on you will use these variables to define the boundary load in the Plane Stress application mode.

6 Click **OK**.

Boundary Conditions—Electrostatics

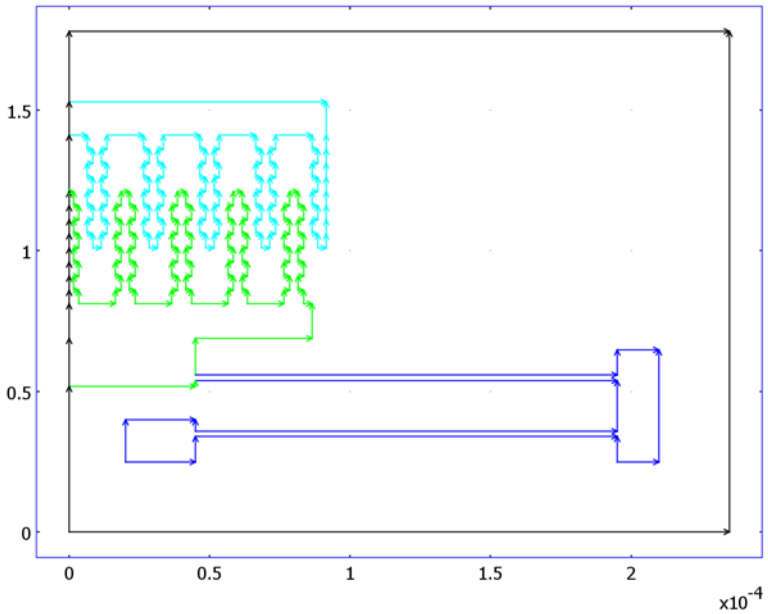
1 From the **Physics** menu, select **Boundary Settings**.

2 In the dialog box that opens, make sure that the **Interior boundaries** check box is selected.

3 Enter the settings in the following table. Note that the physical boundaries of the upper comb are all grounded, while those of the lower comb have an electric potential of V_{in}. The arms and the contact pads of the lower comb are electrically inactive. When you have entered all boundary conditions click the **Groups** tab and enter the group names. This helps you identify the boundaries if you want to make changes to the model.

SETTINGS	BOUNDARIES 1-3, 5-14, 16, 18, 20, 337	BOUNDARIES 85-87, 168-171, 173, 175, 331-336	BOUNDARIES 4, 15, 21-36, 69-84, 88-103, 136-167, 172, 174, 176, 209-240, 273-305	BOUNDARIES 17, 19, 37–68, 104–135, 177–208, 241–272, 306–330
Boundary condition	Zero charge/ symmetry	Continuity	Electric potential	Ground
V_0			`V_in`	
Group name	Zero charge/ symmetry	Continuity	`V_in`	Ground

4 Click **OK**.



Boundary conditions for the Electrostatics application mode. Grounded boundaries: cyan; electric potential (V_{in}): green; Zero charge/Symmetry boundaries: black; Continuity boundaries: blue.

Subdomain Settings—Moving Mesh

1. From the **Multiphysics** menu, select **Moving Mesh (ALE) (ale)**.
2. From the **Physics** menu, open the **Subdomain Settings** dialog box.
3. Select Subdomain 1 (air) and make sure that the **Free displacement** option is selected.
4. Select Subdomains 2 and 3 (comb drives).
5. Select the **Physics included displacement** check box. For the displacement variables **dx** and **dy**, enter the values u and v, respectively. These variables represent the displacements calculated in the Plane Stress application mode.
6. Click **OK**.

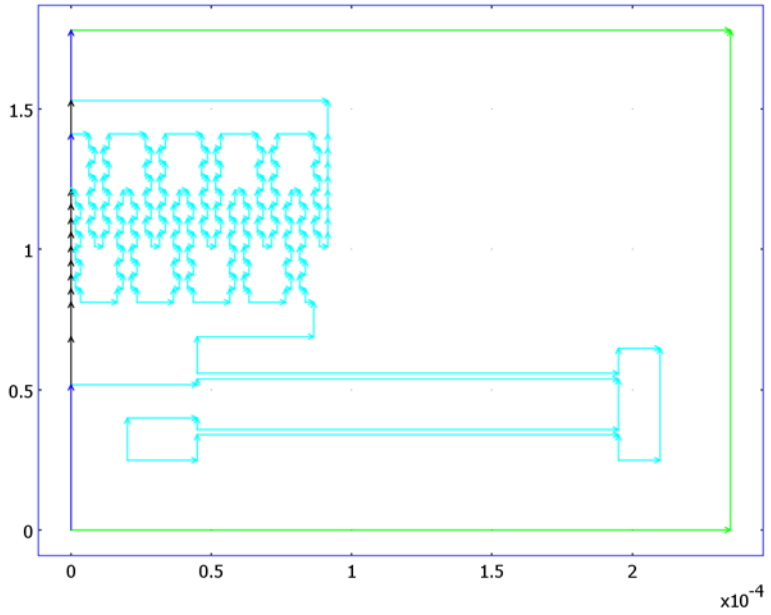
Boundary Conditions—Moving Mesh

1. From the **Physics** menu, select **Boundary Settings**. In the dialog box that opens, make sure that the **Interior boundaries** check box is not selected.

2 Enter the settings in the following table:

SETTINGS	BOUNDARIES 1,14, 18	BOUNDARIES 2, 20, 337	BOUNDARIES 4, 15, 17, 19, 21–336
dx	0	0	u
dy		0	v
Group name	Symmetry	Fixed	Comb drive

3 Click **OK**.



Boundary settings for Moving Mesh (ALE) application mode. Inactive boundaries: black; symmetry boundaries: blue; moving comb drive: cyan; the fixed outer boundaries: green.

Subdomain Settings—Plane Stress

1 From the **Multiphysics** menu, choose **Plane Stress (smps)**.

2 Open the **Subdomain Settings** dialog box.

3 Choose Subdomains 2 and 3, then enter these settings:

PROPERTY	VALUE
E	158e9
ν	0.22
thickness	2e-6

The thermal expansion coefficient (α) is needed only if you have included thermal expansion in the load settings. Similarly, the density (ρ) is used only in time-dependent, eigenfrequency, and frequency-response analyses. In this case you use a nonlinear parametric analysis, and it is therefore not necessary to enter these values.

4 While still in the dialog box, select Subdomain 1. To make sure that the application mode is inactive outside the comb drive, clear the **Active in this domain** check box.

5 Click **OK**.

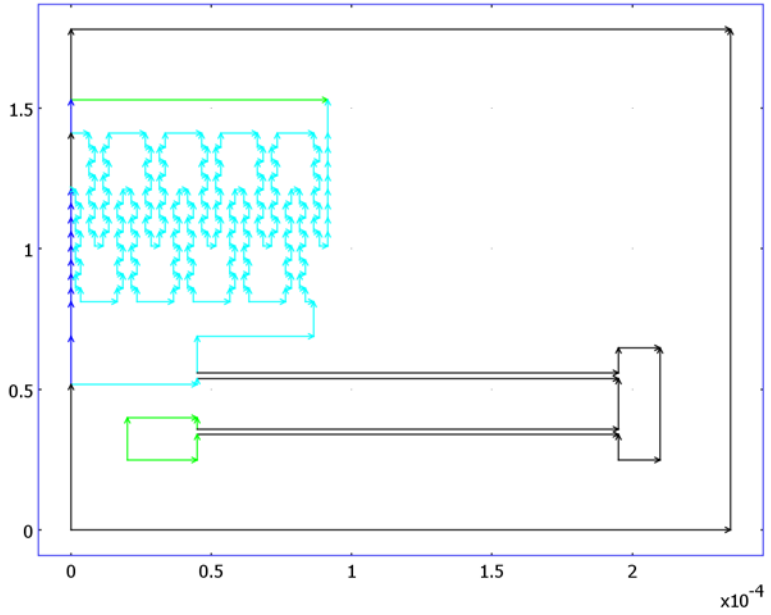
Boundary Conditions—Plane Stress

1 Open the **Boundary Settings** dialog box and make sure that the **Interior boundaries** check box is not selected.

2 On the **Constraint** and **Load** pages, define boundary conditions according to the following table. On the **Load** page, click the **Edge load is defined as load/area using the thickness** option button. This makes the loads from the Electrostatics application mode match the structural loads.

SETTINGS	BOUNDARIES 3, 5–13,16	BOUNDARIES 19, 85–87, 168, 170	BOUNDARIES 169, 171, 173, 175, 331–336	BOUNDARIES 4, 15, 17, 21–84, 88–167, 172, 174, 176–330
Constraint condition	Symmetry	Fixed	Free	
Edge load X dir.	0	0	0	Fes_nTx_emes
Edge load Y dir.	0	0	0	Fes_nTy_emes
Group name	Symmetry	Fixed	Free	Es force

3 Click **OK**.



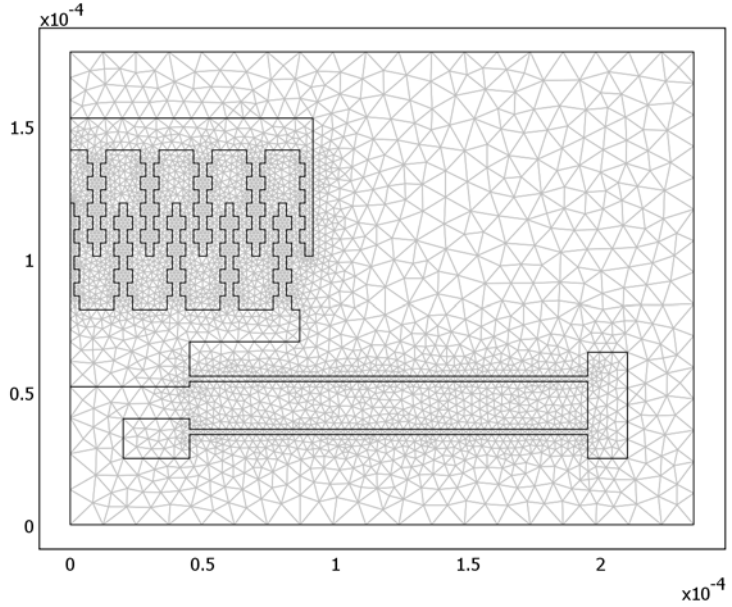
Boundary settings for the Plane Stress application mode. Electrostatically actuated boundaries: cyan; symmetry boundaries: blue; fixed boundaries: green; free boundaries (and inactive boundaries): black.

MESH GENERATION

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

2 On the **General** page, select **Fine** from the **Predefined mesh sizes** list.

3 Click the **Remesh** button and then click **OK**.



The mesh generated using the predefined settings for a fine mesh.

COMPUTING THE SOLUTION

1. From the **Solve** menu, choose **Solver Parameters**.
2. On the General page, select **Parametric** from the **Analysis** list.
3. In the **Parameter name** edit field type `V_in`, and in the **Parameter values** edit field type `0:50:600`.
4. Click the **Advanced** tab.
5. In the **Scaling of variables** area, select **Manual** from the **Type of scaling** list.
6. Type `V 100 u 1e-4 v 1e-4 x 1e-4 y 1e-4` in the **Manual scaling** edit field.

   This scales the variables using the magnitudes of the dependent variables (about 100 for the potential V and about 10^{-4} for the displacement (u, v, and w). The Lagrange multipliers have a magnitude of roughly 1 and do not need any scaling.
7. Click **OK**.
8. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The default results show von Mises stresses with colors on the deformed shape for the last parametric value, $V_{in}(12) = 600$ V. To study the electric potential in the moving frame do the following:

1. From the **Postprocessing** menu, select **Plot Parameters** to open the like-named dialog box.
2. On the **General** page, verify that only **Surface** plot type is selected and that the selection in the **Frame** list is **Frame (ale)**.
3. On the **Surface** page, select **Electrostatics (emes)>Electric potential** from the **Predefined quantities** list.
4. Click **Apply** to generate the plot displayed in Figure 2-10 on page 30.

   To see the deformation inside the comb drive do as follows:

5. On the **Surface** page, select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list.
6. Click **Apply** to generate the plot in Figure 2-11.

   It is also possible to visualize the deformed mesh in the air domain:

7. On the **General** page clear the **Auto Element refinement** check box, then type 1 in the associated edit field.
8. Click the **Surface** tab.
9. From the **Predefined quantities** list, select **Moving Mesh (ALE) (ale)>y-displacement (ale)**.
10. From the **Fill style** list, select **Wireframe**.
11. Click **OK**.

    The resulting plot is reproduced in Figure 2-13.

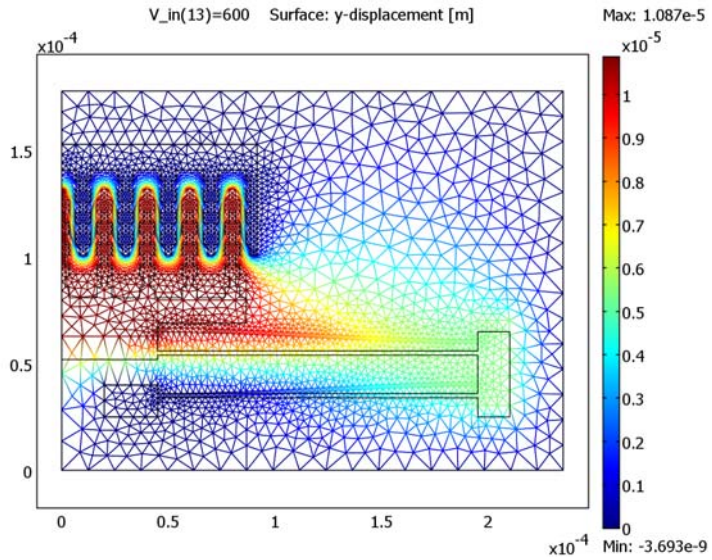


Figure 2-13: The deformed mesh at an actuation voltage of 600 V. The color scale that appears on the screen represents displacements in the y direction.

Next, plot the displacement of the central tooth as a function of the applied voltage:

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

13 On the **General** page, click the **Title/Axis** button. Select the option button next to the **First axis label** edit field, then enter the label `Actuation voltage [V]`. Click **OK**.

14 Click the **Point** tab. Select Point 12. From the **Predefined quantities** list, select **Plane Stress (smps)>Y-displacement**. From the **Unit** list, select **um** (for micrometers).

15 Click **OK**. The plot given in Figure 2-12 on page 32 appears in a new window.

Finally, to reproduce the plot that appears in the Model Navigator when you open the preconfigured model, do the following:

16 Go to the **Postprocessing** menu and select **Plot Parameters**.

17 On the **General** page select the **Element refinement Auto** check box.

18 Make sure that only the **Surface** check box is selected in the **Plot type** area.

19 On the **Surface** page, select **Electrostatics (emes)>Electric potential** from the **Predefined quantities** list.

20 From the **Fill style** list, select **Filled**, then click **OK**.

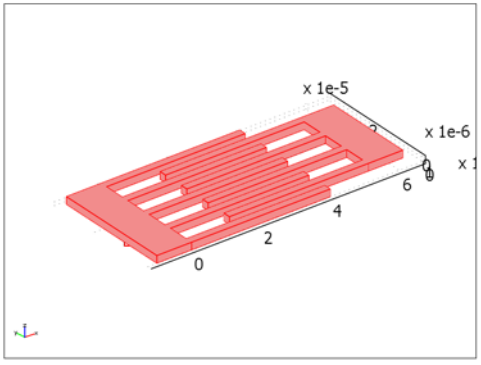
21 Click the **Zoom Extents** button on the Main toolbar.

Capacitive 3D Comb Drive

This model illustrates how to approach a 3D electrostatics problem, create a geometry using the array and extrusion tools, and compute capacitances using the Electrostatics application mode's port boundary condition.

Introduction

Capacitive comb drives are commonly used both as actuators and position sensors. For actuators, electrostatic forces typically pull on a MEMS flexure to provide highly accurate position control. The following model focuses on the other common usage of comb drives: position measurement. Many approaches exist for positional measurements with MEMS devices including changes in capacitance or inductance, optical schemes, and others. Of these, capacitance measurement is the most widely used, particularly in microaccelerometers.



A pair of interdigitated combs for capacitance-based position measurement. Note that the fingers of one comb do not touch those of the other.

Comb drives and capacitive sensors based on them consist of a series of interdigitated tines or fingers. In a pair of interdigitated combs (see the previous figure) the fingers of one comb do not touch those of the other comb, but they do slide in and out relative to each other with a variable overlap. The fingers in MEMS combs are typically a few microns wide and 40 to 100 microns long. The gap between the interdigitated tines is normally 0.5 to 2 microns.

You typically can get a rough idea of a drive's capacitance by approximating the 3D structure as multiple parallel-plate capacitors. This sizing approach is reasonable if the structures are tall compared to the gap and if fringing of the electrostatic field is negligible—which is not the case in most plated MEMS structures. In many cases the tine height is on the same order as its width as well as the gap between the tines; in fact, it can sometimes even be smaller. In these configurations electrostatic fringing dominates the field, and the parallel-plate approximation can be quite inaccurate, even for sizing. Here a quick 3D analysis of the electrostatic field gives a capacitance value that you can combine with the parallel-plate theory to provide considerable design information. Additionally, you can use the capacitance in reduced-order electrical circuit models to simulate the electrical system as a whole.

Theoretical Background

The energy required to charge a capacitor should equal that of the electrostatic field, which is

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

W_e is readily available in the Electrostatics application mode; the software calculates it by integrating across the domain

$$W_e = \int_{\Omega} (\mathbf{D} \cdot \mathbf{E}) d\Omega$$

where $\mathbf{D}$ is the electric displacement, and $\mathbf{E}$ is the electric field. The capacitance, C, is related to the charge on the two conductive plates, Q, and the voltage difference across those plates, ΔV, by

$$C = \frac{Q}{\Delta V}.$$

Now calculate C from the stored electric energy in the capacitor, W_e, and the voltage across the capacitor:

$$C = \frac{Q^2}{2W_e} = \frac{C^2 \Delta V^2}{2W_e} \Rightarrow C = \frac{2W_e}{\Delta V^2}. \qquad (2\text{-}1)$$

Results and Discussion

The next figure shows the electric potential on the comb drive's surfaces, the silicon substrate, and the bounding box. Calculating capacitance using the energy-storage distribution in the electric field and integrating over the volumetric domain leads to a value of 0.021 pF. Changing the geometry—for example, by shifting the fingers on the right side closer to those on the left—likewise changes the value of the stored energy and thus the capacitance.

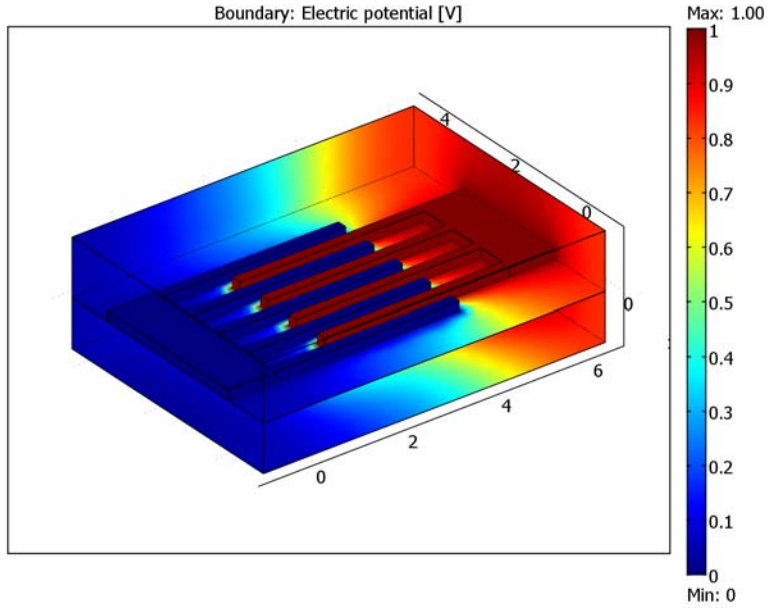


Figure 2-14: Electric potential on the surfaces of a comb drive.

Modeling in COMSOL Multiphysics

Static comb drives are relatively easy to set up in COMSOL Multiphysics. They typically consist of a series of interdigitated rectangles of the same size. Thus you can create one rectangle and reproduce it in a regular pattern it to create the fingers of a comb. Then simply copy, paste, and move the entire geometry to create a second comb. Finally recall that electrostatic fields have only one degree of freedom per node: the voltage. Therefore these types of models do not tend to lead to huge system matrices and memory requirements. True, you can make problems quite large, but you can generally expect quick solutions to reasonably complex 3D electrostatics problems.

To solve electrostatics problems in the MEMS Module, use the Electrostatics application mode, which solves for the electric potential.

Model Library path: `MEMS_Module/Actuator_Models/comb_drive_3d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator** to the **New** tab and select **3D** in the **Space dimension** list.

2 Select **Application modes>MEMS Module>Electrostatics>Electrostatics**.

3 Click **OK**.

GEOMETRY MODELING

Work-Plane Settings

1 From the **Draw** menu choose **Work-Plane Settings**.

2 Click the **Quick** tab, and on that page click the **x-y** button.

3 For the **z**-value use `0` (the default) and click **OK**.

Drawing the 2D Work Geometry

1 Shift-click the **Rectangle/Square** icon on the Draw toolbar and create a rectangle:

NAME	WIDTH	HEIGHT	BASE	X	Y
R1	40e-6	2e-6	Corner	0	0

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

3 From the **Draw** select first **Modify** and then **Array**.

4 In the **Array** dialog box enter these values:

DISPLACEMENT		ARRAY SIZE	
X	Y	X	Y
0	8e-6	1	5

5 Click **OK**.

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

7 Press Ctrl+A to select all the geometry objects.

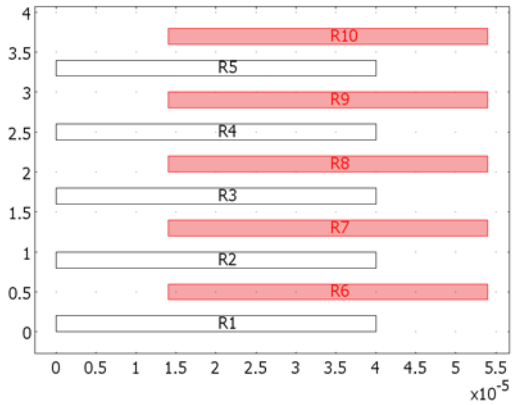
8 Press Ctrl+C and then Ctrl+V to copy and paste the selected objects.

9 In the **Paste** dialog box that appears, enter these values:

DISPLACEMENT	
X	Y
14e-6	4e-6

10 Click **OK**.

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



Creating the comb-drive geometry using a 2D work plane.

12 Select rectangle R10 and delete it.

13 Add two more rectangles:

	SIZE		POSITION		
NAME	WIDTH	HEIGHT	BASE	X	Y
R10	10e-6	26e-6	Corner	54e-6	4e-6
R11	10e-6	34e-6	Corner	-10e-6	0

14 Select the rectangles forming the left comb (R1, R2, R3, R4, R5, and R11).

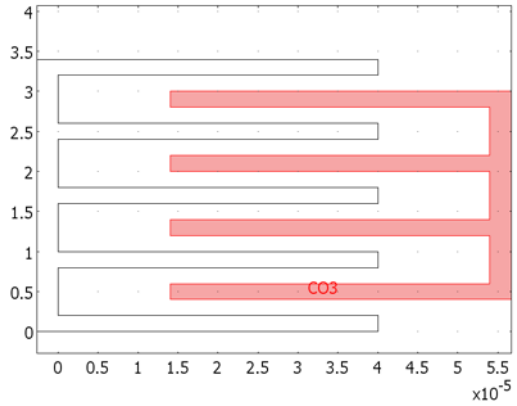
15 To create a composite object, click the **Union** button on the Draw toolbar.

16 Click the **Delete Interior Boundaries** button near the bottom of the Draw toolbar.

17 Select the rectangles that form the right comb (R6, R7, R8, R9, and R10).

18 Click the **Union** button.

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



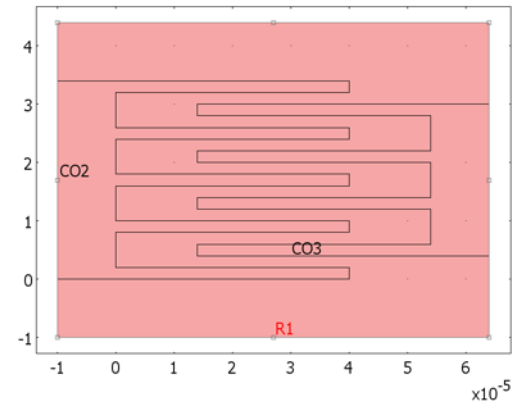
Two composite objects, one for each side of the comb.

Next draw the outline of the substrate and bounding air space for the analysis. In this case, extend the space 10 microns on either side of the comb teeth.

20 Create another rectangle:

	SIZE		POSITION		
NAME	WIDTH	HEIGHT	BASE	X	Y
R1	74e-6	54e-6	Corner	-10e-6	-10e-6

21 Click **Zoom Extents**.

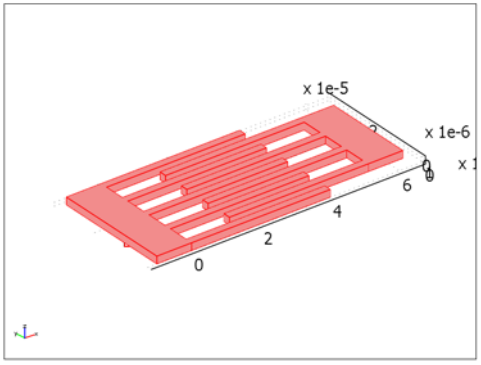


The comb with the substrate and bounding air space.

Extruding the Geometry

First extrude the two comb drives into a 3D geometry:

1. From the **Draw** menu, choose **Extrude**.
2. From the **Objects to extrude** list, select **CO2** and **CO3**.
3. In the **Distance** edit field, type `2e-6`.
4. Click **OK**.
5. Click then **Zoom Extents** button on the Main toolbar.



The extruded comb drive alone.

Now continue extruding, this time with the air surrounding the combs.

6. Switch back to the 2D window; to do so, go to the top of the work area and select the tab for **Geom2**.
7. From the **Draw** menu, choose **Extrude**.
8. In the **Objects to extrude** list, select **R1**.
9. In the **Distance** edit field, type `12e-6`.
10. Click **OK**.

    Because it is not necessary to model the electrostatic field inside the combs, subtract the comb geometries from the air; later you model the electrostatic field only in the air and substrate.
11. On the Draw toolbar, click the **Create Composite Object** button.
12. In the **Set formula** edit field, type `EXT3-EXT1-EXT2`.
13. Clear the **Keep interior boundaries** check box.

14 Click **OK**.

To complete the 3D geometry, extrude the silicon substrate under the two combs.

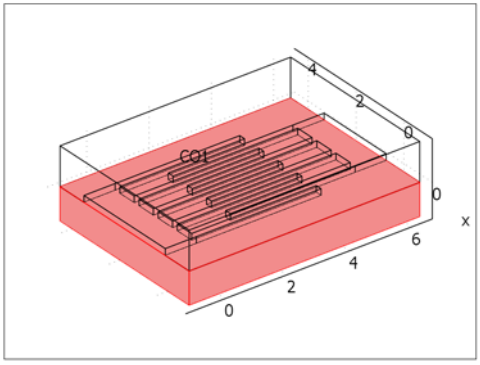
15 Click the **Geom2** tab to switch back to the 2D geometry.

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

17 From the **Objects to extrude** list, select **R1**.

18 In the **Distance** edit field, type `-10e-6`.

19 Click **OK**.



Extruding the geometry to create the silicon substrate below the combs.

PHYSICS SETTINGS

Subdomain Settings

The model consists of two subdomains: the first is the silicon substrate under the comb drives; the second is the surrounding air. Set a value of 11.9 for the substrate's relative permittivity and use the default value of 1.0 for the air.

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

2 Enter the following values for the subdomains; when finished, click **OK**.

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
ε_r (isotropic)	11.9	1.0
ρ	0	0

Boundary Conditions

Continue the physics settings by specifying the boundary conditions. The first comb is tied to the ground, and the second is defined as a port. You model the surrounding boundaries with the symmetry condition.

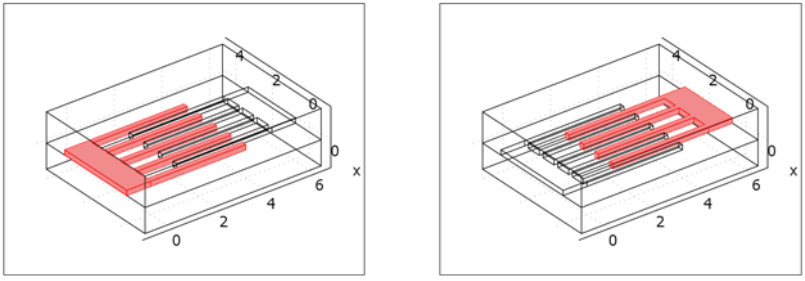
1 From the **Physics** menu, choose **Boundary Settings**.

2 On the **Conditions** page specify the following settings:

SETTINGS	BOUNDARIES 1–5, 7, 12, 13, 52, 53	BOUNDARIES 8–11, 14–27, 42–46	BOUNDARIES 28–41, 47–51
Boundary condition	Zero charge/ Symmetry	Ground	Port

3 While still in the **Boundary Settings** dialog box select one of the port boundaries and select the **Select by group** check box. Doing so selects all port boundaries. Then click the **Port** tab.

4 On the **Port** page, verify that the port number is 1. Then select the **Use port as input** check box, and from the **Input property** list select **Energy method**. Using these settings ensure that a unit voltage is forced on the boundaries of the second comb drive, and the capacitance value is integrated from electric energy density.



Boundary conditions for the two combs: The one on the left is grounded, and the one on the right is defined as a port. All other boundaries have symmetry conditions.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar. The resulting mesh consists of roughly 7800 elements.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar. The model contains about 12,400 degrees of freedom and COMSOL Multiphysics solves it in just a few seconds.

POSTPROCESSING AND VISUALIZATION

To see the voltage distribution on the surface of the comb drive (Figure 2-14), suppress some of the outer boundaries. The suppression visualization settings are available from the **Options** menu.

1. From the **Postprocessing** menu, select **Plot Parameters**.
2. In the dialog box that opens, click the **General** tab.
3. Clear the **Slice** check box and select the **Boundary** check box.
4. Click **OK**.
5. From the **Options** menu, choose **Suppress>Suppress Boundaries**.
6. Select Boundaries 1, 2, 4, 5, and 7.
7. Click **OK**.
8. On the Main toolbar, click the **Postprocessing Mode** button to return to the postprocessing plot.

Computing the Capacitance

As a final step, display the capacitance value computed by integrating the electric energy density over the geometry.

1. From the **Postprocessing** menu, choose **Data Display>Global**.
2. In the **Expression** edit field, type `C11_emes`.
3. Click **OK**.

The value of the integral, $2.1 \cdot 10^{-14}$—corresponding to 0.021 pF—appears in the message log at the bottom of the screen.

Gecko Foot

Introduction

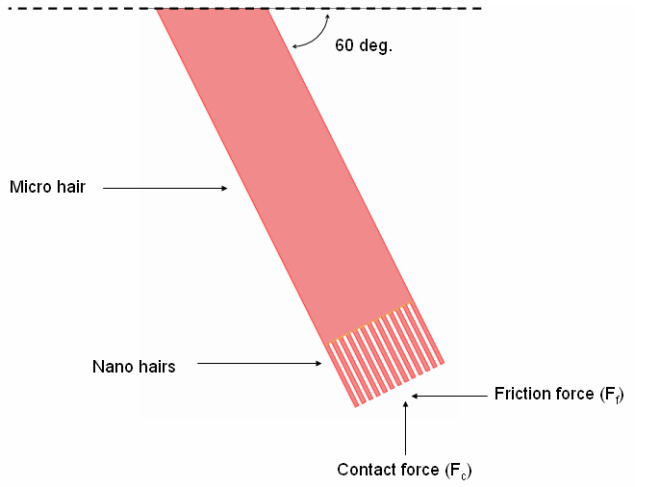
In nature, various species apply advanced techniques for specialized tasks. For instance, gecko lizards use dry adhesion forces such as Van der Waals forces to climb walls. Dry adhesion is an interesting phenomena for sticking because it requires no energy to hold on, and no residue is left on the surface. Gecko lizards have inspired researchers to develop synthetic gecko foot hairs to be used in, for example, robot application for purposes where humans cannot go.

Model Definition

Hair on a gecko foot is a very complex biological structure with hierarchical nano and micro sections. On its feet, a gecko has billions of nanoscale hairs that are in contact with surfaces while it climbs. These nanohairs are attached to microscale hairs, which are on the tip of a gecko's toes.

Critical design parameters for nanohairs to achieve the optimal sticking are hair length, detach angle, distance between nanohairs, and the cross section area of one hair. By varying these parameters, the hairs can stick onto very rough surfaces, but on the other hand they must be stiff enough to avoid sticking to each others. Proper material choices help achieving the design goals while providing the required adhesion force. Typically the Young's modulus for materials used in synthetic nanohair vary in between 1 GPa and 15 GPa.

This model contains the hierarchy of synthetic gecko foot hair where cantilever beams both in nano and micro scales describe the seta and spatula parts of one spatular stalk attached to a gecko foot. The basis of the analyzed structure is the micro stalk with these dimensions: width, 4.53 μm; height, 4.33 μm; and length, 75 μm. At the end of the micro hair, 169 nanohairs are attached and they have dimensions of 0.18 μm, 0.17 μm, and 3 μm, respectively. The micro hair is fixed at the far end, while the contact and friction forces appear as surface loads at the end of each nanohair. The free-body diagram of one micro/nanohair (see nearby figure) illustrates the applied forces, which are set to 0.4 μN for the contact force and 0.2 μN for the friction force with 60° contact angle to target surface. The structure is made of β-keratin with a Young's modulus of 2 GPa and a Poisson's ratio of 0.4. The model was inspired by Ref. 1.



Results and Discussion

The following plot shows the von Mises effective stress in the model, stress that reaches a maximum at 97.73 MPa. The total displacement is 13.01 µm. This information helps in selecting the material and certain criteria for polymers to be used in synthetic gecko foot design as well as in setting design parameters for the geometrical dimensions.

The maximum von Mises stress in the analyzed model is almost twice the value of the material's yield stress. Further analysis requires either a stronger material or some geometrical changes. An optimal solution likely depends on a combination of both these design parameters.

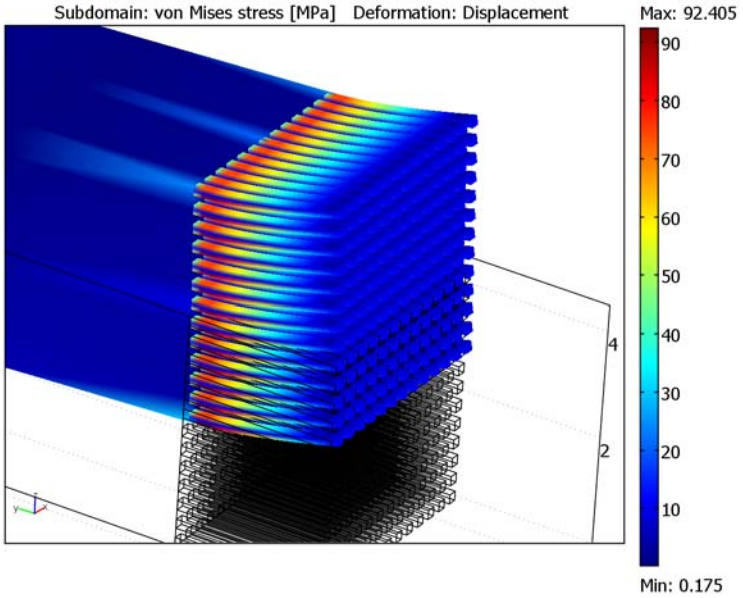


Figure 2-15: Von Mises stress in a synthetic Gecko foot with a length of the microbeam of 75 μm and nanohairs with a length of 3 μm. This plot shows only the end with the nanohairs.

References

1. G. Shah and I. Lee, "Finite Element Analysis of Gecko Foot Hairs for Dry Adhesive Design and Fabrication," Dept. of Mechanical Engineering—NanoRobotics Lab, Carnegie Mellon Univ., Pittsburgh.

2. M. Sitti and R.S. Fearing, "Synthetic Gecko Foot-Hair Micro/Nano-Structures for Future Wall-Climbing Robots," *Proc. IEEE Robotics and Automation Conf.*, Sept. 2003.

3. J. Vincent, *Structural Biomaterials*, rev. ed., Princeton University Press, 1990.

Model Library path: `MEMS_Module/Actuator_Models/gecko_foot`

MODEL NAVIGATOR

1. Open the Model Navigator to create a new model.
2. Select **3D** from the **Space dimension** list.
3. Select the **MEMS Module>Structural Mechanics>Solid, Stress-Strain** application mode.
4. Click **OK**.

OPTIONS AND SETTINGS

1. Choose **Options>Constants** to open the **Constants** dialog box.
2. Defined the following constants by typing the name, expression, and description into the table using a new row for each constant (the **Description** field is optional):

NAME	EXPRESSION	DESCRIPTION
Fc	0.4[uN]	Contact force
Ff	0.2[uN]	Friction force
Fcy	Fc*sin(pi/3)	Contact force, y component
Fcz	Fc*cos(pi/3)	Contact force, z component
Ffy	Ff*cos(pi/3)	Friction force, y component
Ffz	Ff*sin(pi/3)	Friction force, z component
Area	0.17[um]*0.18[um]	Cross-sectional area of the spatulae

3. Click **OK**.

GEOMETRY MODELING

To be able to mesh the microscale and nanoscale sections independently, use the assembly feature, which keeps each geometry object as a separate part. First create the microscale part as a block. Then create one of the nanohairs and use the array feature to create an array of identical nanohairs.

1. From the **Draw** menu, choose **Use Assembly**.
2. Click the **Block** button on the Draw toolbar. Enter the following dimensions in the **Length** area: **X**: `4.53e-6`, **Y**: `75e-6`; **Z**: `4.33e-6`.

   Use the default values for all other properties, then click **OK** to create the block.

3 Click the **Block** button on the Draw toolbar to create another block. Enter the following dimensions in the **Length** area: **X**: `0.18e-6`, **Y**: `3e-6`; **Z**: `0.17e-6`. Enter the following base point in the **Axis base point** area: **x**: `0`, **y**: `-3e-6`; **z**: `0`.

   Use the default values for all other properties, then click **OK** to create the block.

4 Make sure that the second block (BLK2) is selected.

5 Click the **Array** button on the Draw toolbar to make an array of blocks similar to BLK2. Together they form a group of 13×13 nanohairs. Enter the following values in the **Displacement** area: **x**: `(4.53e-6-0.18e-6)/12`, **y**: `0`; **z**: `(4.33e-6-0.17e-6)/12`. Enter the following values in the **Array size** area: **x**: `13`, **y**: `1`; **z**: `13`.

6 Click **OK**.

7 Press Ctrl+A to select all the objects.

8 Choose **Mate Objects** from the Draw menu. In the **Mate Objects** dialog box, clear the **Create imprints** check box, then click **OK**.

   This final step creates the identity pairs that connect the parts to form a continuous field problem in the entire assembly. There are a total of 169 pairs, one for each nanohair. There is no need to create imprints of the nanohairs because the displacement field is continuous across the entire assembly, and there are no loads or constraints where the nanohairs meet the microsection.

PHYSICS SETTINGS

Subdomain Settings

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

2 Select all the subdomains and then enter the following material properties on the **Material** page: **E**: `2e9` (Young's modulus), ν: `0.4` (Poisson's ratio).

3 Click **OK**.

Boundary Conditions

Specify the loads and constraints.

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

2 Select Boundary 83.

3 Select **Fixed** from the **Constraint condition** list.

4 Use the zoom tools and rotate the geometry so that you can reach the ends of all nanohairs. Then disable the zoom and rotate operations by clicking the **Orbit/Pan/Zoom** button on the Camera toolbar so that you can use the mouse to select boundaries.

5 Using the mouse, select the ends of all the nanohairs. The following table contains the numbers for all these boundaries:

2	8	14	20	26	32	38	44	50	56	62	68	74
86	92	98	104	110	116	122	128	134	140	146	152	158
164	170	176	182	188	194	200	206	212	218	224	230	236
242	248	254	260	266	272	278	284	290	296	302	308	314
320	326	332	338	344	350	356	362	368	374	380	386	392
398	404	410	416	422	428	434	440	446	452	458	464	470
476	482	488	494	500	506	512	518	524	530	536	542	548
554	560	566	572	578	584	590	596	602	608	614	620	626
632	638	644	650	656	662	668	674	680	686	692	698	704
710	716	722	728	734	740	746	752	758	764	770	776	782
788	794	800	806	812	818	824	830	836	842	848	854	860
866	872	878	884	890	896	902	908	914	920	926	932	938
944	950	956	962	968	974	980	986	992	998	1004	1010	1016

6 Click the **Load** tab.

7 Enter the following loads: $\mathbf{F_x}$: `0`, $\mathbf{F_y}$: `(-Fcy+Ffy)/Area`, $\mathbf{F_z}$: `(Fcz-Ffz)/Area`.

8 Click **OK**.

MESH GENERATION

Create swept meshes for each subdomain, which is possible due to the assembly geometry where each block is an individual part.

1 Choose **Mesh>Interactive Meshing>Mesh Selected (Mapped).** This creates a mapped 2D mesh on all nanohair ends.

2 Choose **Mesh>Swept Mesh Parameters**.

3 Select all subdomains except Subdomain 14 (the microsection).

4 On the **Element Layers** page select the **Manual specification of element layers** check box, then type `8` in the **Number of element layers** edit field.

5 Click the **Mesh Selected** button, then click **OK**.

This creates hexahedral mesh elements for all the nanohairs. Next create another swept hexahedral mesh for the microsection.

1 Choose **Mesh>Mapped Mesh Parameters**.

2 Select Boundary 83 (the back end of the microsection).

3 Click the **Edge** tab, then select Edges 162, 163, 164, and 168.

4 Select the **Constrained edge element distribution** check box and type 5 in the **Number of edge elements** edit field.

5 Click the **Boundary** tab, then click the **Mesh Selected** button. Click **OK**.

6 Choose **Mesh>Swept Mesh Parameters**.

7 Select Subdomain 14 (the microsection).

8 On the **Element Layers** page select the **Manual specification of element layers** check box, then type 10 in the **Number of element layers** edit field.

9 Click the **Mesh Selected** button, then click **OK**.

The total number of mesh elements should be approximately 1600.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to start the analysis.

POSTPROCESSING AND VISUALIZATION

1 Choose **Postprocessing>Plot Parameters**.

2 On the **General** page clear the **Slice** check box. Select the **Subdomain** and **Deformed shape** check boxes in the **Plot type** area.

3 Click the **Subdomain** tab.

4 Select **MPa** from the **Unit** list to display the von Mises stress in MPa instead of Pa.

5 Click **OK**.

Prestressed Micromirror

Introduction

One method of creating spring-like structures or inducing curvature in plated structures is to plate materials onto a substrate such that the layer has a residual stress after the plating process. The plating process can control this stress, which can be either compressive or tensile, even for similar materials. The automotive industry has studied this phenomenon at length because highly stressed chrome is appreciably shinier than nonstressed chrome. MEMS device manufacturers sometimes use this effect to create curved cantilevers or spring-loaded micromechanical structures that lift off the substrate when deliberately undercut by an etchant.

One such device is the electrostatically controlled micromirror. It is typically quite small, and arrays of such devices can implement a projection system. They serve as optical redirectors and similar reflection devices. This section shows the fundamentals of how to set up and solve lift-off of a prestressed plated device.

Model Definition

This single-physics model uses 3D structural analysis. The micromirror has a stiff, flat, reflective center portion, which is supported by four prestressed plated cantilever springs. To keep the mesh size small and the solution time reasonable, this exercise studies the plated structure with two layers. It also assumes that the plating process creates equal and opposite (compressive and tensile) initial stresses in the top and bottom layers. This convenience makes the model straightforward to set up. You can make the initial-stress distribution as complex as desired and set it up as shown in this example. Depending on the magnitude of the deformations, you are likely best advised to solve such simulations with a large-deformation analysis using a nonlinear or parametric nonlinear solver, noting that the latter is more likely to converge. Thus this illustrative model uses the large-deformation analysis type with both the linear and parametric linear solvers.

Note in particular that a 3D structure with thin layers such as the one in this model leads to a very large unstructured tetrahedral mesh. To avoid this case, this example first generates a 2D quadrilateral mesh by mesh mapping and then extrudes it into 3D to produce a mesh with hexahedral (brick) elements. This way you can have the mesh generator create structured elements with a high aspect ratio.

One of the key process parameters you wish to determine in this class of problem is generally what prestress level is necessary to result in a desired lift-off. Another common concern is how much effect variations in the prestress might have on displacement. A parametric study answers this question.

Results and Discussion

The following two images compare lift-off for aluminum and steel plates. The steel, being harder than aluminum, deforms less.

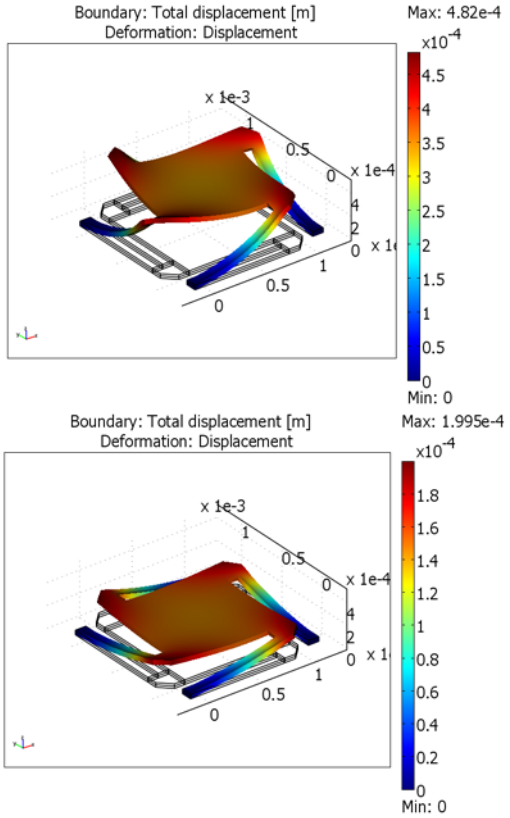


Figure 2-16: Lift-off for aluminum (top) and steel (bottom).

The following two figures show the mirror response to the different levels of applied prestress. According to Figure 2-17, the center point deflection is almost linearly dependent of the prestress. Figure 2-18 shows the mirror's curvature along its

centerline for different values of prestress. In line with expectations, increasing the stress bends the mirror more.

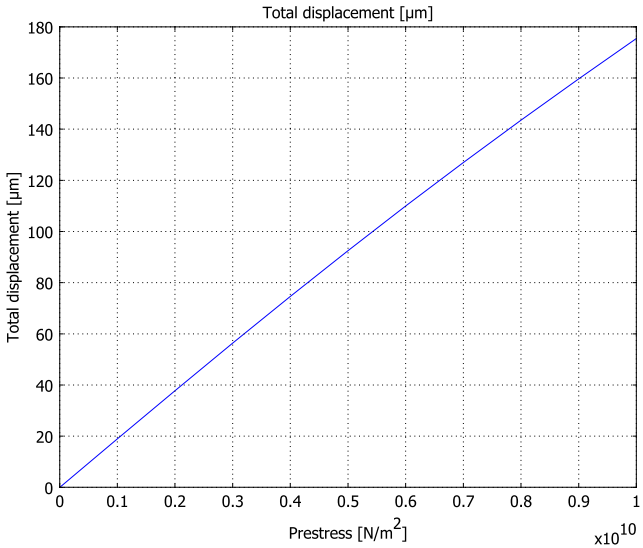


Figure 2-17: Vertical deflection of the center of the mirror for different prestress levels.

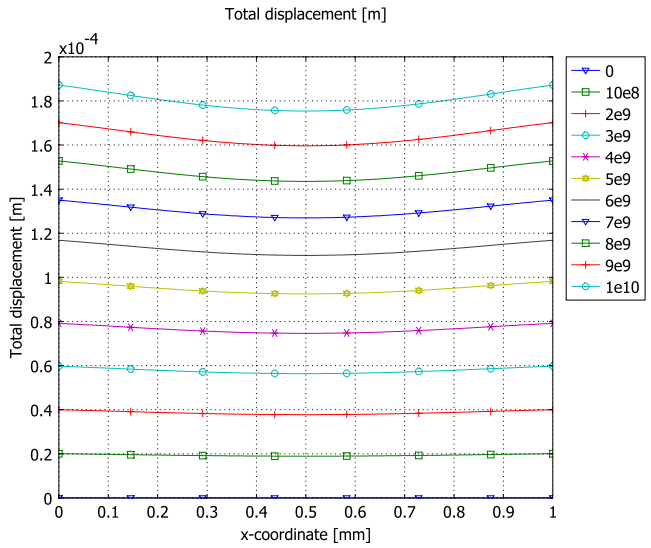


Figure 2-18: Mirror curvature along the centerline for different prestress levels.

Because of bonding the structure cannot move freely when it cools down, which causes residual stresses. The following plot shows this released stress state using the first principal stress after deformation.

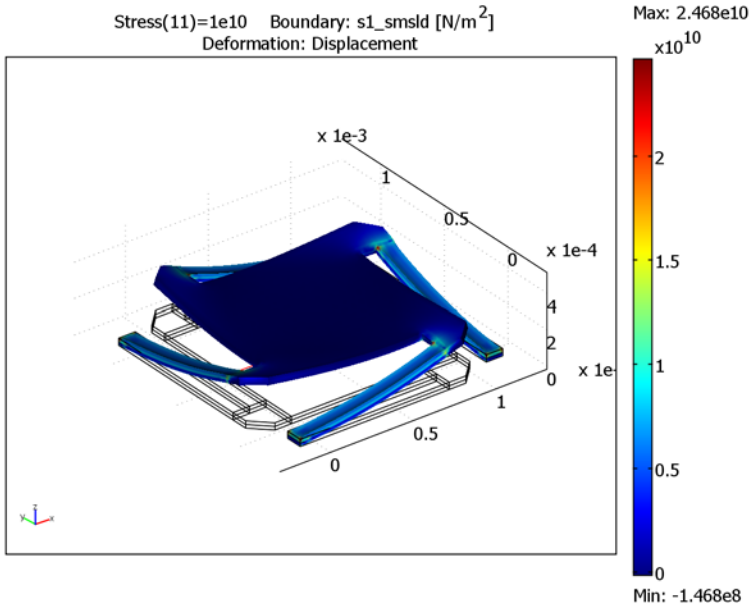


Figure 2-19: Plot of the first principal stress after deformation.

Reference

1. G. Kovacs, *Micromachined Transducers Sourcebook*, WCM McGraw-Hill, 1998.

Model Library path: `MEMS_Module/Actuator_Models/micromirror`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator** click the **New** tab. From the **Space dimension** list, select **3D**.

2 In the list of application modes select
MEMS Module>Structural Mechanics>Solid, Stress-Strain>Static analysis.

3 Click **OK**.

OPTIONS AND SETTINGS

Constants

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

2 Enter a variable with the **Name** `Stress`, the **Expression** `8[GPa]`, and the description `Initial normal stress`.

3 Click **OK**.

Work Plane

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

2 Click the **Quick** tab.

3 Choose the **x-y plane**, and for **z** use a value of `0`.

4 Click **OK**.

Axes and Grid Settings

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

2 Click the **Grid** tab.

3 Clear the **Auto** check box.

4 In both the **x spacing** and **y spacing** edit fields type `0.1`.

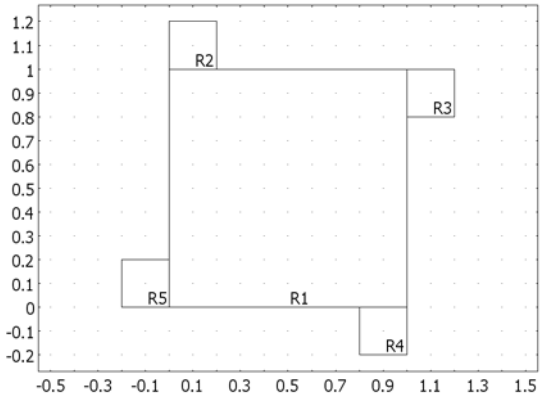
5 Click **OK**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar and create five rectangles:

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	1	1	Corner	0	0
R2	0.2	0.2	Corner	0	1
R3	0.2	0.2	Corner	1	0.8
R4	0.2	0.2	Corner	0.8	-0.2
R5	0.2	0.2	Corner	-0.2	0

2 Click the **Zoom Extents** button.



The initial geometry after drawing five rectangles.

These steps create the mirror along with support structure for the cantilevers. This assembly is made of a metal stiffer than the prestressed cantilever springs. Next chamfer the corners.

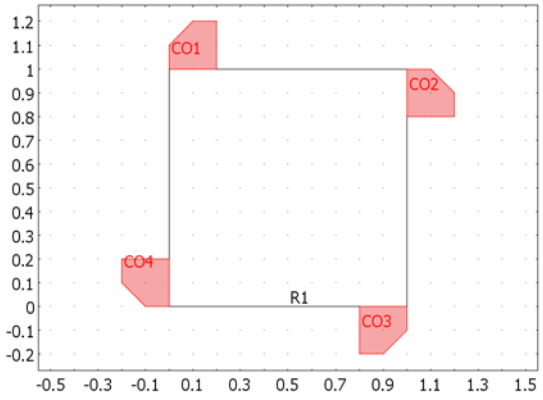
3 From the **Draw** menu, select **Fillet/Chamfer**.

4 Click the **Chamfer** option button.

5 In the **Distance** edit field, type `0.1`.

6 In the **Vertex selection** list, choose the four vertices **R2>4**, **R3>3**, **R4>2**, and **R5>1**.

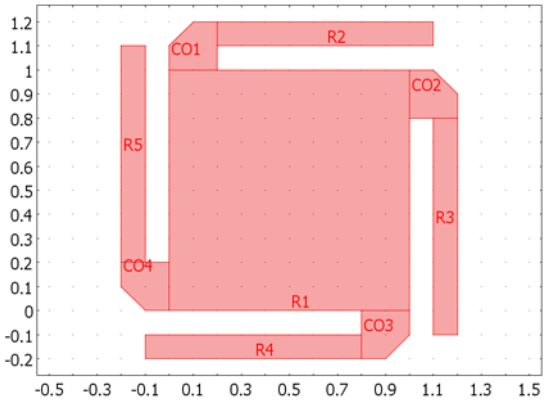
7 Click **OK**.



The mirror geometry after chamfering.

8 Use the **Rectangle/Square** tool and data from the following table to create the spring:

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	0.9	0.1	Corner	0.2	1.1
R2	0.1	0.9	Corner	1.1	-0.1
R3	0.9	0.1	Corner	-0.1	-0.2
R4	0.1	0.9	Corner	-0.2	0.2



The geometry with the springs added.

Rescaling the Geometry

1 From the **Edit** menu, choose **Select All**.

2 From the **Draw** menu, select **Modify** and then **Scale**.

3 In the **Scale factor** edit fields for **x** and **y**, type `1e-3`.

4 Click **OK**.

5 Click the **Zoom Extents** button.

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

7 Click the **Grid** tab.

8 Select the **Auto** check box.

9 Click **OK**.

CREATING A MAPPED MESH

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

2 Click the **Boundary** tab.

3 Select Boundaries 12, 16, 27, and 31.

4 Select the **Constrained edge element distribution** check box.

5 In the **Number of edge elements** edit field, type `6`.

6 Select Boundaries 3, 7, 13, 14, 20, 23, 30, and 39.

7 Select the **Constrained edge element distribution** check box.

8 In the **Number of edge elements** edit field, type `12`.

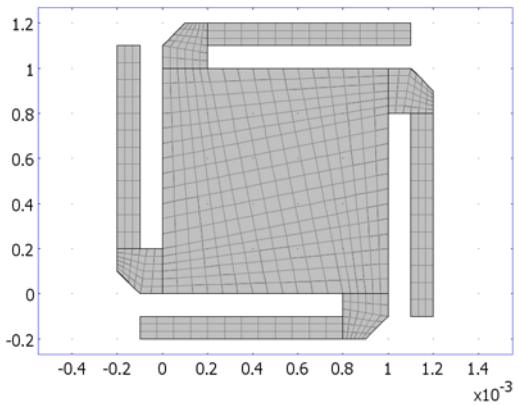
9 Next select Boundaries 4, 11, 19, 21, 24, 26, 32, and 36.

10 Select the **Constrained edge element distribution** check box.

11 In the **Number of edge elements** edit field, type `3`.

12 Click the **Remesh** button.

13 Click **OK**.



The geometry with the 2D mapped mesh.

EXTRUDING MESH INTO 3D

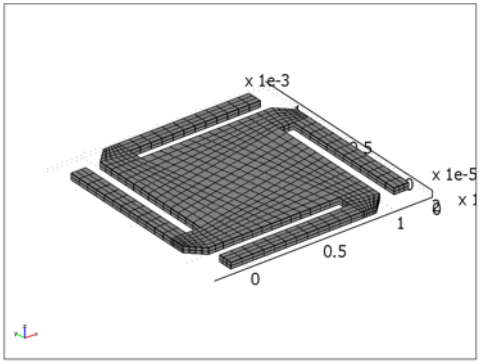
1 From the **Mesh** menu, select **Extrude Mesh**.

2 On the **Geometry** page, type `20e-6 40e-6` in the **Distance** edit field.

This specifies a 3D geometry meshed in two sections: a first section between the planes z = 0 and z = 20 µm, and a second section between z = 20 µm and z = 40 µm. On the **Mesh** page, you can specify the number of element layers for each

section. The default is in this case a single element layer per section. In general, the default number of element layers is a function of the 2D mesh-element size to give 3D prism elements of roughly the same size in all directions.

3 Click **OK**.



The geometry after extruding the mesh into 3D.

PHYSICS SETTINGS

Application Mode Properties

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

2 In the **Application Mode Properties** dialog box, change the value in the **Large deformation** list to **On**.

3 Click **OK**.

Subdomain Settings

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

2 In the **Subdomain Selection** list, select all subdomains (1–18).

3 Click the **Material** tab, then click the **Load** button.

4 From the **Basic Material Properties** list, choose **Aluminum 3003-H18**.

5 Click **OK**.

6 Click the **Initial Stress and Strain** tab.

7 From the **Subdomain selection** list, choose Subdomains 3, 5, 11, and 17.

8 Select the **Include initial stress** check box.

9 For both σ_{xi} and σ_{yi} enter the value `-Stress`.

10 From the **Subdomain selection** list, choose Subdomains 4, 6, 12, and 18.

11 Select the **Include initial stress** check box.

12 For both σ_{xi} and σ_{yi} enter the value `+Stress`.

13 Click **OK**.

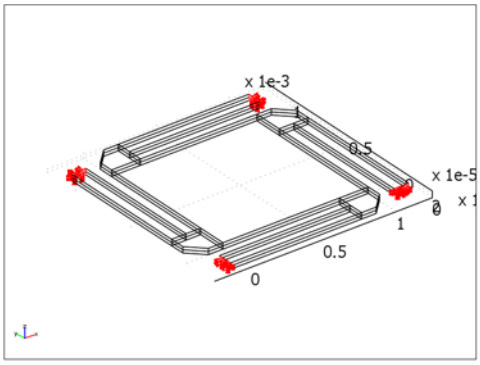
Boundary Conditions

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

2 In the **Boundary selection** list, select Boundaries 15, 16, 17, 20, 92, 95, 102, and 103 (see the image below).

3 On the **Constraint** page select, set the check boxes for **Constraint condition** list to **Fixed**.

4 Click **OK**.



Geometry with the fixed boundaries highlighted.

COMPUTING THE SOLUTION

For large stress values this model is very nonlinear and needs a lot of solver steps to converge. Thus you need to increase the default number of allowed steps before solving the model.

1 From the **Solve** menu, select **Solver Parameters**.

2 Verify that the **Analysis** list has selection **Static** and that the **Auto select solver** is selected.

3 Go to the **Stationary** page.

4 In the **Maximum number of iterations** field, type `50`.

5 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

Generate Figure 2-16 on page 62 with the following steps.

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

2 On the **General** page, clear the **Slice** check box in the **Plot type** area.

3 Select both the **Boundary** and **Deformed shape** check boxes.

4 Click the **Deform** tab.

5 Clear the **Auto** check box, and in the **Scale factor** edit field type `1.0`.

6 Click **OK**.

7 Click the **Zoom Extents** button.

8 Click the **Headlight** button on the Camera toolbar on the left side of the user interface.

STIFFENING THE CENTER SECTION

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

2 In the **Subdomain selection** list, choose 1, 2, 7–10, and 13–16.

3 On the **Material** page, click the **Load** button.

4 From the **Basic Material Properties** list, choose **Steel AISI 4340**.

5 Click **OK** twice.

6 Click the **Solve** button.

The resulting plot is shown in Figure 2-16 on page 62.

DISPLACEMENT VS. PRESTRESS

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, choose **Parametric**.

3 Click the **General** tab. In the **Parameter name** edit field, type `Stress`.

4 In the **Parameter values** edit field, type `0:1e9:10e9`. Click **OK**.

5 Click the **Solve** button. The analysis can require several minutes to complete.

POSTPROCESSING AND VISUALIZATION

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

2 In the **Solutions to use** list, verify that all solutions are selected. If not, click in the list and press Ctrl+A.

3 Click the **Title/Axis** button. Select the option button next to the **First axis label** edit field, then enter the label `Prestress [N/m<sup>2</sup>]`. Click **OK**.

4 Click the **Point** tab. In the **y-axis data** area, select **Solid, Stress-Strain (smsld)>Total displacement** from the **Predefined quantities** list and **um** from the **Unit** list.

5 In the **Coordinates** area, change the **x**, **y**, and **z** values to `0.5e-3`, `0.5e-3`, and `40e-6`, respectively.

6 Click **Apply**.

The resulting plot appears in Figure 2-17 on page 63.

7 On the **General** page, click the **Title/Axis** button. Click the **Auto** option button for the **First axis label**, then click **OK**.

8 On the **Line/Extrusion** page, click the **Line plot** option button.

9 In the **y-axis data** area, select **Solid, Stress-Strain (smsld)>Total displacement** from the **Predefined quantities** list and **um** from the **Unit** list.

10 In the **x-axis data** area, click the lower option button, then click **Expression**. From the **Predefined quantities** list, select **Geometry and Mesh>x-coordinate**. From the **Unit** list, select **mm**, then click **OK**.

11 Change the values in the **Cross-section line data** area as follows:

NAME	VALUE	NAME	VALUE	NAME	VALUE
x0	0	y0	0.5e-3	z0	40e-6
x1	1e-3	y1	0.5e-3	z1	40e-6

12 Click the **Line Settings** button. From the **Line marker** list, select **Cycle**. Select the **Legend** check box, then click **OK** to close the **Line Settings** dialog box.

13 Click **OK**.

The results appear in Figure 2-18 on page 63.

Visualizing the Released Stress State

Follow the steps below to create Figure 2-19 on page 64.

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

2 Click the **Boundary** tab.

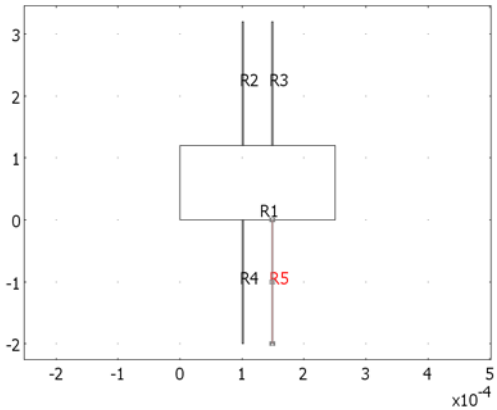
3 Find the **Boundary data** area, and in the **Expression** edit field type `s1_smsld`.

4 Click **OK**.

Residual Stress in a Thin-Film Resonator

Introduction

Almost all surface-micromachined thin films are subject to residual stress. The most common is likely thermal stress, which accompanies a change in temperature and is due to the difference in the coefficient of thermal expansion between the film and the substrate. The examples in this section show how to add thermal residual stress to a structural-mechanical model and observe how it changes the structure's resonant frequency.



A thin-film resonator with four cantilever beam springs.

For a lateral resonator with four cantilever-beam springs, the resonant frequency is

$$f_0 \approx \frac{1}{2\pi}\sqrt{\frac{4Etb^3}{mL^3} + \frac{24\sigma_r tb}{5mL}}$$

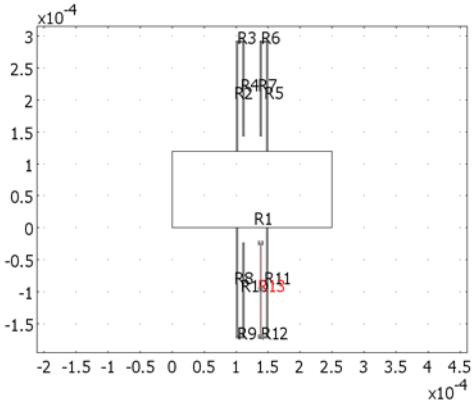
where m is the mass of the resonator plate, E is Young's modulus, t is the thickness, L is the length, b is the width, and σ_r is the residual stress in the cantilevers. The stress is typically a sum of external stresses, the thermal stress, and intrinsic components. Assuming the material is isotropic, the stress is constant through the film thickness, and the stress component in the direction normal to the substrate is zero. The stress-strain relationship is then

$$\sigma_r = \left(\frac{E}{1-\nu}\right)\varepsilon$$

where ν is Poisson's ratio.

A process deposits a thin film onto a thick substrate at a high temperature. When the assembly cools to room temperature, the film and the substrate shrink differently and cause strain in the film. The strain comes from $\varepsilon = \Delta\alpha\Delta T$ where $\Delta\alpha$ is the difference between the thermal-expansion coefficients, and ΔT is the difference between the deposition temperature and the normal operating temperature.

You can relieve thermal residual stress in thin-film spring structures by folding the flexures as shown in the next figure. The flexures relieve axial stress because each is free to expand or contract in the axial direction.



The film resonator with folded cantilever beam strings.

The basic folded structure is a U-shaped spring. For springs in series, the equivalent spring constant is

$$\frac{1}{k_{eq}} = \frac{1}{k_1} + \frac{1}{k_2} + \frac{1}{k_3}$$

The first and last springs are cantilever beams. You obtain the spring constant for them from $k = 3EI/L^3$, where I is the moment of inertia. For a rectangular beam with a rotation about the y-axis, the moment of inertia is $I = wt^3/12$, where w is the width and t is the structure's thickness. You can treat the second spring as a column with a spring constant of $k = AE/L$, where A is the cross-sectional area $A = wt$. Assuming the spring thickness and width are the same everywhere, the equation comes to

$$L_{eq}^3 = L_1^3 + \frac{wt^2 L_2}{4} + L_3^3,$$

which can help estimate the lengths of the folded springs.

Model Definition

This example took the dimensions and the material properties presented in the following tables from the example in Chapter 27.2.5 in Ref. 1. It calculates the lengths of the folded cantilever using the equivalent spring-constant relationship.

This simulation models thermal residual stress using the thermal expansion option in the Structural Mechanics application mode. It calculates the coefficient of thermal expansion using the stress-strain relationship. It sets the deposition temperature to 605 °C (see Chapter 16.13.2.3 in reference Ref. 1)..

TABLE 2-1: DIMENSIONS OF THE STRUCTURE.

PARAMETER	STRAIGHT CANTILEVERS	FOLDED CANTILEVERS			SHUTTLE MASS
		L1	L2	L3	
Length	200 μm	170 μm	10 μm	146 μm	250 μm
Width	2 μm				120 μm
Thickness	2.25 μm				2.25 μm

TABLE 2-2: MATERIAL PROPERTIES OF THE STRUCTURE.

PROPERTY	VALUE
Material	polysilicon
Young's modulus	155 GPa
Poisson's ratio	0.23
Density	2330 kg/m^3
T_0	605 °C
T_1	25 °C

In order to determine the eigenfrequencies for the case with residual stress, you must use the large-deformation analysis available in the structural mechanics application modes. First solve for the residual stress using a nonlinear solver. Then store the linear solution and solve for the eigenfrequencies using that stored solution. To obtain the eigenfrequency without the stress, solve the problem using the initial settings.

Results and Discussion

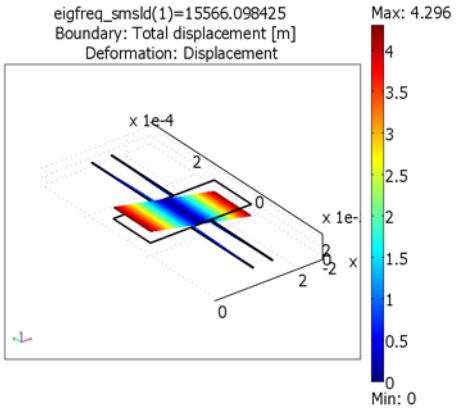
Table summarizes the resonant frequencies for the first horizontal eigenmode. For the 2D models this is the lowest found eigenmode, but for the 3D models this is the second mode. In 3D modes, the lowest resonance corresponds to eigenmode with rotational movement. You can see these modes for the resonator with straight cantilevers in the pictures below the table.

The von Mises stress is close to 50 MPa in the legs of the resonators with straight cantilevers. But for folded cantilevers, the stress is much less, about 140 kPa (See pictures in the step-by-step instructions). The analytical reference value for straight cantilevers was calculated using 50 MPa stress.

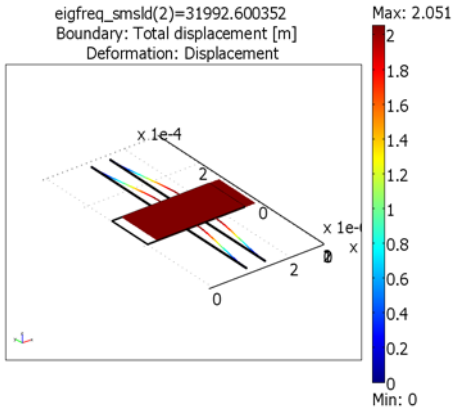
As the table shows, the resonant frequency for the straight cantilevers increases significantly when the model includes residual stress. Moreover, the model results agree closely with the analytical estimates. By folding the springs you can decrease the sensitivity to stress.

TABLE 2-3: RESONANT FREQUENCIES WITH AND WITHOUT RESIDUAL STRESS.

	STRAIGHT CANTILEVERS			FOLDED CANTILEVERS	
	ANALYTICAL	2D MODEL	3D MODEL	2D MODEL	3D MODEL
Without stress	15.0 kHz	14.8 kHz	14.8 kHz	14.0 kHz	14.1 kHz
With residual stress	33.1 kHz	31.9 kHz	32.0 kHz	14.0 kHz	14.1 kHz



The first and rotational eigenmode of the resonator with straight cantilevers.



The second and horizontal eigenmode of the resonator with straight cantilevers.

Reference

1. M. Gad-el-Hak, ed., *The MEMS Handbook*, CRC Press, London, 2002, ch. 16.12 and 27.2.5.

Model Library path: `MEMS_Module/Actuator_Models/resonator_straight_2d`

Model Library path: `MEMS_Module/Actuator_Models/resonator_folded_2d`

Model Library path: `MEMS_Module/Actuator_Models/resonator_straight_3d`

Model Library path: `MEMS_Module/Actuator_Models/resonator_folded_3d`

MODEL NAVIGATOR

1 Open the **Model Navigator**, click the **New** tab, and in the **Space dimension** list select **2D**.

2 In the list of application modes, select **MEMS Module>Structural Mechanics>Plane Stress>Static analysis**.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box enter the following names and expressions; the descriptions are optional. When finished, click **OK**.

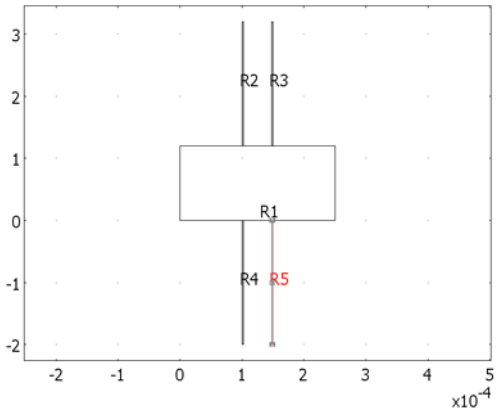
NAME	EXPRESSION	DESCRIPTION
E	155[GPa]	Young's modulus
nu	0.23	Poisson's ratio
rho	2330[kg/m^3]	Density
sigma	50[MPa]	Residual stress
epsilon	sigma*(1-nu)/E	Residual strain
T1	605[degC]	Deposition temperature
T0	25[degC]	Room temperature
daT	epsilon/(T1-T0)	Coefficient of thermal expansion (1/K)

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar to create these five rectangles:

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	250e-6	120e-6	Corner	0	0
R2	2e-6	200e-6	Corner	100e-6	120e-6
R3	2e-6	200e-6	Corner	148e-6	120e-6
R4	2e-6	200e-6	Corner	100e-6	-200e-6
R5	2e-6	200e-6	Corner	148e-6	-200e-6

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



Initial geometry for the thin-film resonator in 2D with straight cantilevers.

PHYSICS SETTINGS

Application Mode Properties

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

2 In the **Application Mode Properties** dialog box, go to the **Large deformations** list and select **On**. Click **OK**.

Subdomain Settings

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

2 Select all subdomains by first clicking in the **Subdomain selection** list or the drawing area and then pressing Ctrl+A.

3 Enter the following values on the **Material** page of the **Subdomain Settings** dialog box; when finished, click **OK**.

QUANTITY	VALUE	DESCRIPTION
E	E	Young's modulus
ν	nu	Poisson's ratio
α	daT	Thermal expansion coefficient
ρ	rho	Density
thickness	2.25e-6	Thickness

Boundary Conditions

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

2 In the **Boundary selection** list, select Boundaries 5, 9, 15, and 19.

3 On the **Constraint** page, set the **Constraint condition** list to **Fixed**.

4 Click **OK**.

MESH GENERATION

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

2 Verify that **Normal** is selected from the **Predefined mesh sizes** list.

3 Click **Custom mesh size**.

4 In the **Resolution of narrow regions** field type 2.

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

COMPUTING THE SOLUTION—EIGENMODES WITHOUT STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Eigenfrequency**.

3 Click **OK**.

4 Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

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

2 On the **General** page, choose from the **Eigenfrequency** list the mode you want to plot. The first eigenfrequency is approximately 14 kHz

3 Click the **Surface** tab.

The default plot in this page is the von Mises stress. Because the solution from the Eigenfrequency analysis is scaled, the stress levels is arbitrarily scaled also. Thus, it is more informative to plot, for example, the Total displacement.

4 Select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list.

5 Click the **Deform** tab.

6 Select the **Deformed shape plot** check box.

7 Click **OK**.

PHYSICS SETTINGS—THERMAL STRAINS

Subdomain Settings

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

2 Select all subdomains.

3 On the **Load** page, enter the values in the following table; when done, click **OK**.

PROPERTY	SETTING/VALUE	DESCRIPTION
Include thermal expansion	Selected	
Temp	T0	Strain temperature
Tempref	T1	Strain ref. temperature

COMPUTING THE SOLUTION—STATIC RESIDUAL STRESS

Using the steps below, solve the model and store the solution for later use.

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Static**, then click **OK**.

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

4 From the **Solve** menu, choose **Solver Manager**.

5 Click the **Initial Value** tab.

6 Click the **Store Solution** button at the bottom of the dialog box.

7 In the **Values of variables not solved for and linearization point** area, select **Stored solution**.

It is important to define the linearization point correctly. Using this information, the stress stiffening effect enters into the following eigenfrequency solution computed below.

8 Click **OK**.

POSTPROCESSING AND VISUALIZATION—STATIC RESIDUAL STRESS

To gain information about the thermally generated stresses change the surface plot back to von Mises stress:

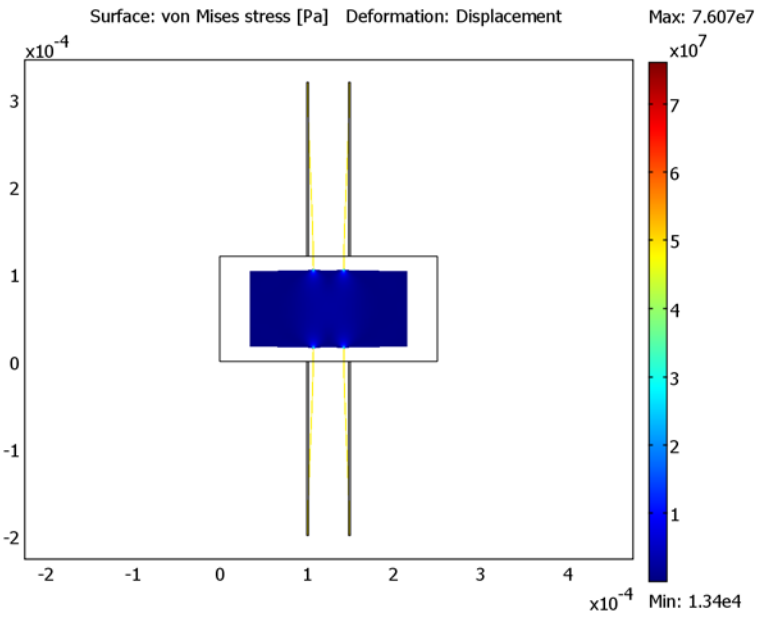
1 From the **Postprocessing** menu, choose **Plot Parameters**.

2 Click the **Surface** tab.

3 Select **Plane Stress (smps)>von Mises stress** from the **Predefined quantities** list.

4 Click **OK**.

.



Deformed shape of the geometry for the thin-film resonator in 2D with straight cantilevers.

Next create a cross-section plot to inspect the stress distribution in more detail.

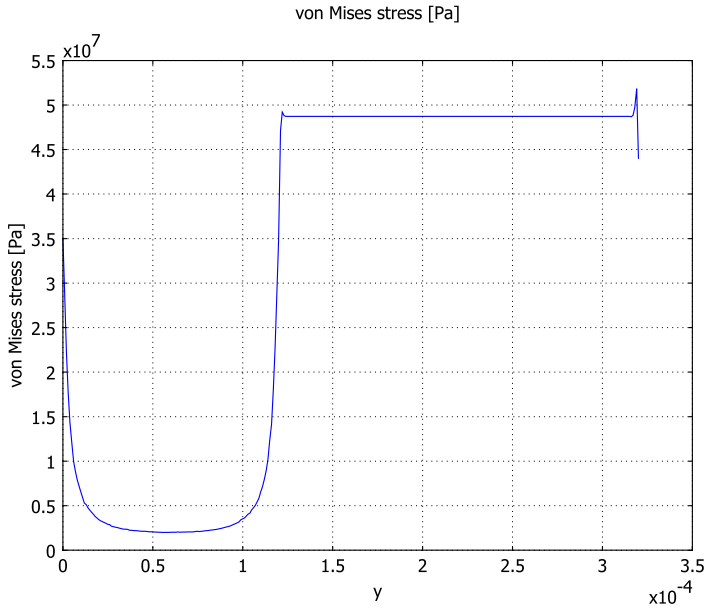
1 From the **Postprocessing** menu choose **Cross-Section Plot Parameters**.

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

3 Enter the following values:

PARAMETER	VALUE
Plot type	Line plot
Predefined quantities	von Mises stress
x-axis data	y
CROSS-SECTION LINE DATA	
x0	101e-6
x1	101e-6
y0	0
y1	320e-6
Line resolution	321

4 Click **OK**.



Line plot of von Mises stress going first through the resonator body and then through one of the legs.

COMPUTING THE SOLUTION—EIGENMODES WITH THERMAL STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

1 From the **Solve** menu choose **Solver Parameters**.

2 From the **Analysis** list select **Eigenfrequency**.

3 Click **OK**.

4 Click the **Solve** button on the Main toolbar. The value of the eigenfrequency appears in the message log. Notice that the first eigenfrequency has changed to approximately 31,950 Hz.

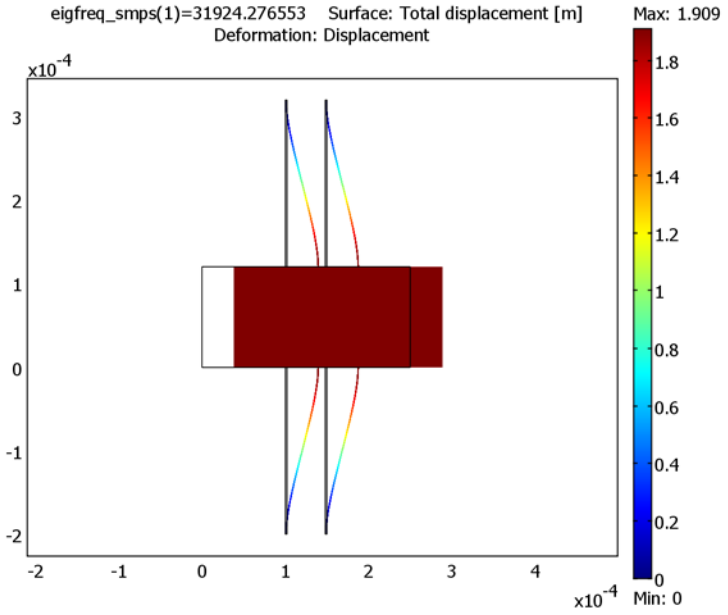
POSTPROCESSING AND VISUALIZATION

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

2 Click the **Surface** tab.

3 Select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list.

4 Click **OK**.



Deformation associated with the first eigenfrequency for the thin-film resonator in 2D with straight cantilevers.

Modeling Using the Graphical User Interface—2D, Folded Cantilevers

MODEL NAVIGATOR

1 Open the **Model Navigator**, click the **New** tab, and in the **Space dimension** list select **2D**.

2 Click the **New** tab, and in the list of application modes select **MEMS Module>Structural Mechanics>Plane Stress>Static analysis**.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box enter the following names and expressions; the descriptions are optional. When finished, click **OK**.

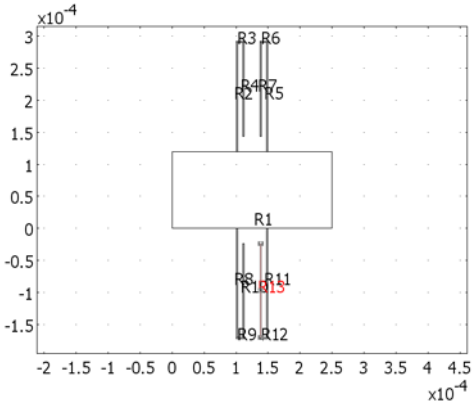
NAME	EXPRESSION	DESCRIPTION
E	155[GPa]	Young's modulus
nu	0.23	Poisson's ratio
rho	2330[kg/m^3]	Density
sigma	50[MPa]	Residual stress
epsilon	sigma*(1-nu)/E	Residual strain
T1	605[degC]	Deposition temperature
T0	25[degC]	Room temperature
daT	epsilon/(T1-T0)	Coefficient of thermal expansion

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar to create these 13 rectangles:

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	250e-6	120e-6	Corner	0	0
CANTILEVER 1					
R2	2e-6	170e-6		100e-6	120e-6
R3	12e-6	2e-6		100e-6	290e-6
R4	2e-6	146e-6		110e-6	144e-6
CANTILEVER 2					
R5	2e-6	170e-6		148e-6	120e-6
R6	12e-6	2e-6		138e-6	290e-6
R7	2e-6	146e-6		138e-6	144e-6
CANTILEVER 3					
R8	2e-6	170e-6		100e-6	-170e-6
R9	12e-6	2e-6		100e-6	-172e-6
R10	2e-6	146e-6		110e-6	-170e-6
CANTILEVER 4					
R11	2e-6	170e-6		148e-6	-170e-6
R12	12e-6	2e-6		138e-6	-172e-6
R13	2e-6	146e-6		138e-6	-170e-6

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



Initial geometry for the thin-film resonator in 2D with folded cantilevers.

PHYSICS SETTINGS

Application Mode Properties

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

2 In the **Application Mode Properties** dialog, go to the **Large deformations** list and select **On**.

Subdomain Settings

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

2 Select all subdomains.

3 On the indicated pages, specify the following settings; when finished, click **OK**.

SETTINGS	VALUE	DESCRIPTION
MATERIAL PAGE		
E	`E`	Young's modulus
ν	`nu`	Poisson's ratio
α	`daT`	Thermal expansion coefficient
ρ	`rho`	Density
thickness	`2.25e-6`	Thickness
LOAD PAGE		
Include thermal expansion	selected	

SETTINGS	VALUE	DESCRIPTION
Temp	T0	Strain temperature
Tempref	T1	Strain ref. temperature

Boundary Conditions

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

2 In the **Boundary selection** list, select Boundaries 22, 24, 34, and 36.

3 On the **Constraint** page, set the **Constraint condition** list to **Fixed**.

4 Click **OK**.

MESH GENERATION

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

2 Verify that **Normal** is selected from the **Predefined mesh sizes** list.

3 Click **Custom mesh size**.

4 In the **Resolution of narrow regions** edit field type 2.

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

COMPUTING THE SOLUTION—EIGENMODES WITHOUT STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Eigenfrequency**.

3 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

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

2 On the **General** page, choose the mode you want to plot from the **Eigenfrequency** list; the first eigenfrequency is approximately 14 kHz.

3 Click the **Surface** tab.

The default plot in this page is the von Mises stress. Because the solution from the Eigenfrequency analysis is scaled, the stress levels will be arbitrarily scaled also. Thus, it is more informative to plot for example the Total displacement.

4 Select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list.

5 Click the **Deform** tab.

6 Select the **Deformed shape plot** check box.

7 Click **OK**.

PHYSICS SETTINGS—THERMAL STRAINS

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

2 Select all subdomains.

3 On the **Load** page, enter the values in the following table; when finished, click **OK**.

SETTINGS	VALUE	DESCRIPTION
Include thermal expansion	selected	
Temp	T0	Strain temperature
Tempref	T1	Strain ref. temperature

COMPUTING THE SOLUTION—STATIC RESIDUAL STRESS

Using the steps below, solve the model and store the solution for later use.

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Static**, then click **OK**.

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

4 From the **Solve** menu, choose **Solver Manager**.

5 Click the **Initial Value** tab.

6 Click the **Store Solution** button at the bottom of the dialog box.

7 In the **Values of variables not solved for and linearization point** area select **Stored solution**.

It is important to define the linearization point correctly. Using this information, the stress stiffening effect enters into the following eigenfrequency solution computed below.

8 Click **OK**.

POSTPROCESSING AND VISUALIZATION—STATIC RESIDUAL STRESS

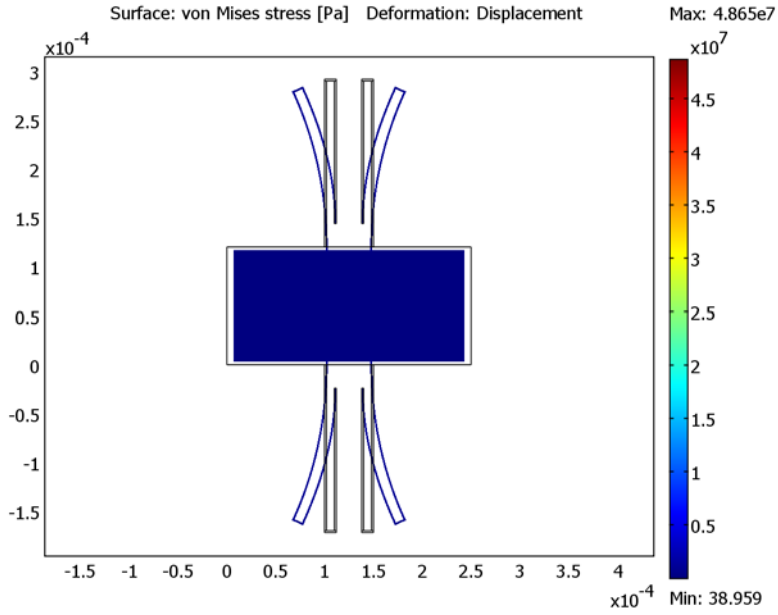
To gain information about the thermally generated stresses change the surface plot back to von Mises stress:

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

2 Click the **Surface** tab.

3 Select **Plane Stress (smps)>von Mises stress** from the **Predefined quantities** list.

4 Click **OK**.



Deformed shape of the geometry for the thin-film resonator in 2D with folded cantilevers.

Next create a cross-section plot to inspect the stress distribution in more detail:

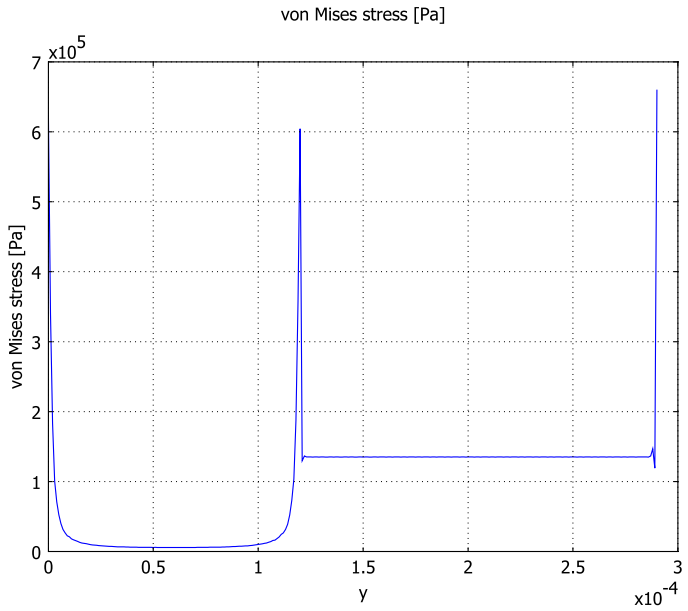
1 From the **Postprocessing** menu, choose **Cross-Section Plot Parameters**.

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

3 Enter these values; when done, click **OK**.

PARAMETER	VALUE
Plot type	Line plot
Predefined quantities	von Mises stress
Expression	`mises_smps`
x-axis data	y
CROSS-SECTION LINE DATA	
x0	`101e-6`
x1	`101e-6`
y0	0

PARAMETER	VALUE
yl	290e-6
Line resolution	291



Line plot of von Mises stress going first through the resonator body and then through one of the legs.

COMPUTING THE SOLUTION—EIGENMODES WITH STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

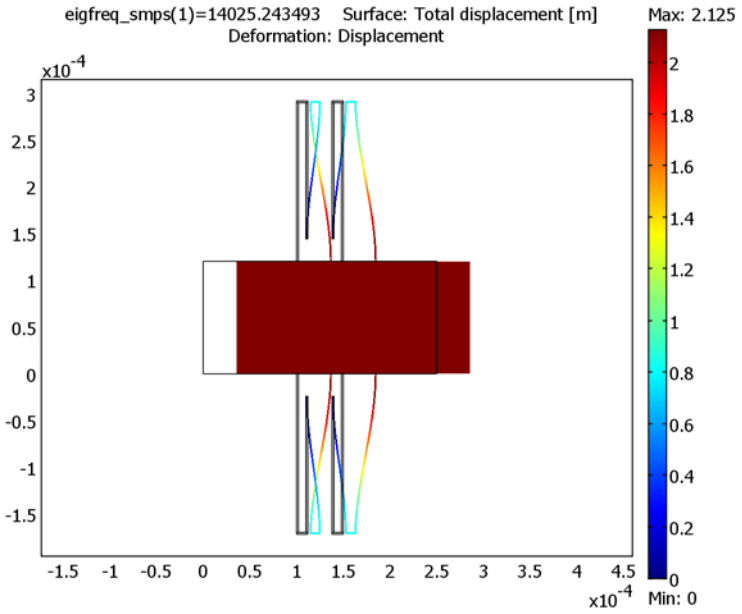
1. From the **Solve** menu, choose **Solver Parameters**.
2. From the **Analysis** list, select **Eigenfrequency**.
3. Click **OK**.
4. Click the **Solve** button on the Main toolbar. Notice that the first eigenfrequency is almost the same as without thermal stresses.

POSTPROCESSING AND VISUALIZATION

1. From the **Postprocessing** menu, choose **Plot Parameters**.
2. Click the **Surface** tab.

3 Select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list.

4 Click **OK**.



Deformation associated with the first eigenfrequency for the thin-film resonator in 2D with folded cantilevers.

Modeling Using the Graphical User Interface—3D, Straight Cantilevers

MODEL NAVIGATOR

1 In the **Model Navigator**, click the **New** tab. In the **Space dimension** list, select **3D**.

2 In the list of application modes, select
MEMS Module>Structural Mechanics>Solid, Stress-Strain.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, enter these variable names, expressions, and (optionally) descriptions; when done, click **OK**.

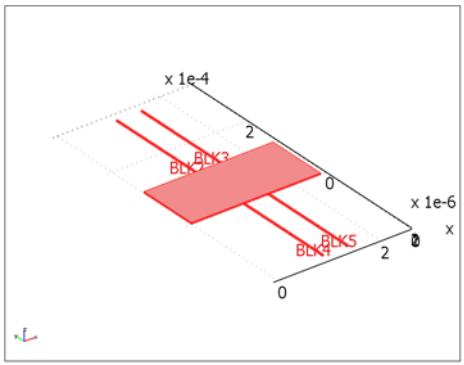
NAME	EXPRESSION	DESCRIPTION
E	155[GPa]	Young's modulus
nu	0.23	Poisson's ratio
rho	2330[kg/m^3]	Density
sigma	50[MPa]	Residual stress
epsilon	sigma*(1-nu)/E	Residual strain
T1	605[degC]	Deposition temperature
T0	25[degC]	Room temperature
daT	epsilon/(T1-T0)	Coefficient of thermal expansion

GEOMETRY MODELING

1 Shift-click the **Block** button on the Draw toolbar to create these five solid blocks; when complete, click **OK**.

NAME	LENGTH			AXIS BASE POINT		
	X	Y	Z	X	Y	Z
BLK1	250e-6	120e-6	2.25e-6	0	0	0
BLK2	2e-6	200e-6	2.25e-6	100e-6	120e-6	0
BLK3	2e-6	200e-6	2.25e-6	148e-6	120e-6	0
BLK4	2e-6	200e-6	2.25e-6	100e-6	-200e-6	0
BLK5	2e-6	200e-6	2.25e-6	148e-6	-200e-6	0

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



Initial geometry for the thin-film resonator in 3D with straight cantilevers.

PHYSICS SETTINGS

Application Mode Properties

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

2 In the **Application Mode Properties** dialog box, go to the **Large deformations** list and select **On**.

Subdomain Settings

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

2 Select all subdomains.

3 Enter the following values on the **Material** page of the **Subdomain Settings** dialog box; when finished, click **OK**.

PROPERTY	VALUE	DESCRIPTION
E	E	Young's modulus
ν	nu	Poisson's ratio
α	daT	Thermal expansion coeff.
ρ	rho	Density

Boundary Conditions

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

2 In the **Boundary selection** list, select Boundaries 7, 15, 21, and 29.

3 On the **Constraint** page, set the **Constraint condition** list to **Fixed**.

4 Click **OK**.

MESH GENERATION

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

2 Click the **Global** tab.

3 Verify that the selection from the **Predefined mesh sizes** list is **Normal**.

4 Click the **Advanced** tab.

5 For the **z-direction scale factor** enter `2.0`.

6 Click **Remesh**.

7 Click **OK**.

COMPUTING THE SOLUTION—EIGENMODES WITHOUT STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Eigenfrequency**.

3 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION—STATIC RESIDUAL STRESS

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

2 Click the **General** tab.

3 from the **Eigenfrequency** list, choose the mode you want to plot; the eigenmode for the horizontal movement has an eigenfrequency of approximately 14.8 kHz

4 Clear the **Slice** check box.

5 Select the **Boundary** and **Deformed shape** check boxes.

6 Click **OK**.

PHYSICS SETTINGS—THERMAL STRAINS

Subdomain Settings

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

2 Select all subdomains.

3 Go to the **Load** page and enter the values in the following table; when done, click **OK**.

SETTINGS	VALUE	DESCRIPTION
Include thermal expansion	yes	
Temp	T0	Strain temperature
Tempref	T1	Strain ref. temperature

COMPUTING THE SOLUTION—STATIC RESIDUAL STRESS

Using the steps below, solve the model and store the static solution for later use.

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Static**, then click **OK**.

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

4 From the **Solve** menu, choose **Solver Manager**.

5 Click the **Initial Value** tab.

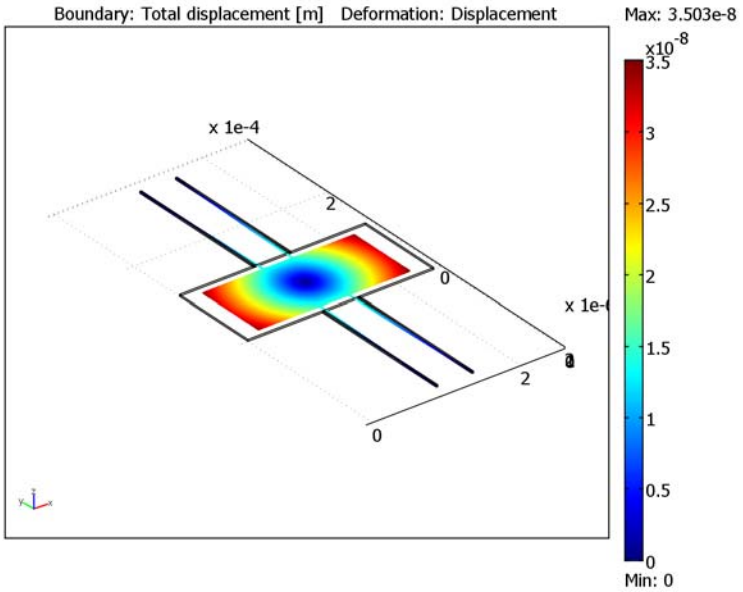
6 Click the **Store Solution** button at the bottom of the dialog box.

7 In the **Values of variables not solved for and linearization point** area select **Stored solution**.

8 Click **OK**.

POSTPROCESSING AND VISUALIZATION—STATIC RESIDUAL STRESS

According to the plot settings you defined before, the deformed plot with total displacement appears in the user interface:



Deformed shape of the geometry for the thin-film resonator in 3D with straight cantilevers.

Next create a cross-section plot to inspect the stress distribution in more detail.

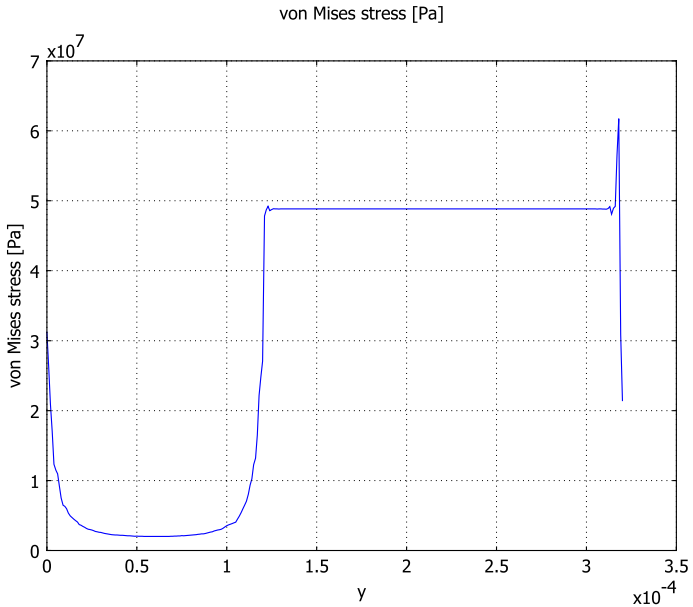
1 From the **Postprocessing** menu, choose **Cross-Section Plot Parameters**.

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

3 Enter the following values; when finished, click **OK**.

PARAMETER	VALUE
Plot type	Line plot
Predefined quantities	von Mises stress
Expression	`mises_smsld`
x-axis data	y
CROSS-SECTION LINE DATA	
x0	`101e-6`
x1	`101e-6`

PARAMETER	VALUE
y0	0
y l	320-6
z0	1.125e-6
z l	1.125e-6
Line resolution	321

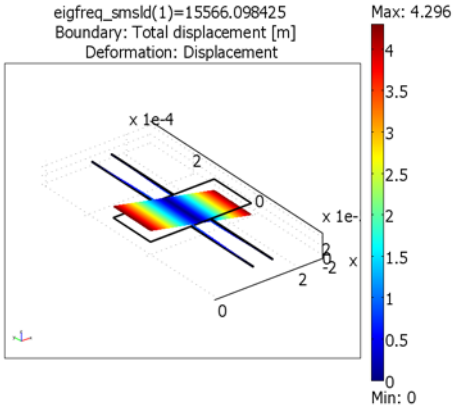


Line plot of von Mises stress going first through the resonator body and then through one of the legs.

COMPUTING THE SOLUTION—EIGENMODES WITH STRESSES

1. From the **Solve** menu, choose **Solver Parameters**.
2. From the **Analysis** list, select **Eigenfrequency**.
3. Click **OK**.
4. From the **Solve** menu, choose **Solver Manager**.

5 Click the **Solve** button. Observe the eigenfrequency from the plot title; the first found eigenmode corresponds to rotational movement.



Deformation associated with the first eigenfrequency for the thin-film resonator in 3D with straight cantilevers.

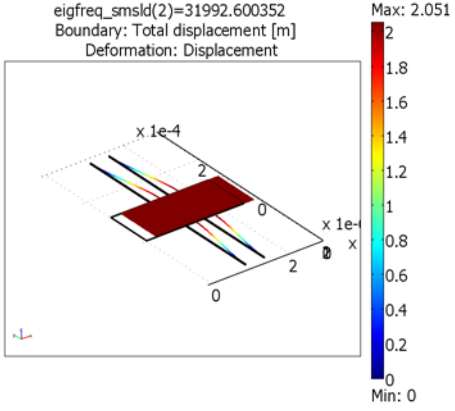
POSTPROCESSING AND VISUALIZATION—EIGENFREQUENCY

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

2 Click the **General** tab.

3 Go to the **Solution to use** area, and in the **Eigenfrequency** list select the second value, which should be near 32 kHz.

4 Click **OK**.



Deformation associated with the second eigenfrequency for the thin-film resonator in 3D with straight cantilevers.

MODEL NAVIGATOR

1 In the **Model Navigator** click the **New** tab, and in the **Space dimension** list select **3D**.

2 In the list of application modes select **MEMS Module>Structural Mechanics>Solid, Stress-Strain**.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box, enter these variable names, expressions, and (optionally) descriptions; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
E	155[GPa]	Young's modulus
nu	0.23	Poisson's ratio
rho	2330[kg/m^3]	Density
sigma	50[MPa]	Residual stress
epsilon	sigma*(1-nu)/E	Residual strain
T1	605[degC]	Deposition temperature
T0	25[degC]	Room temperature
daT	epsilon/(T1-T0)	Coefficient of thermal expansion

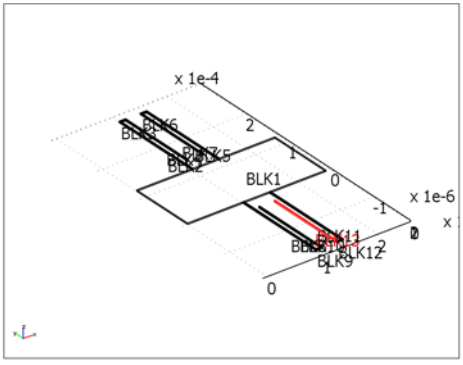
GEOMETRY MODELING

1 Shift-click the **Block** button on the Draw toolbar to create these 13 solid blocks; when finished, click **OK**.

NAME	LENGTH			AXIS BASE POINT		
	X	Y	Z	X	Y	Z
BLK1	250e-6	120e-6	2.25e-6	0	0	0
CANTILEVER 1						
BLK2	2e-6	170e-6	2.25e-6	100e-6	120e-6	0
BLK3	12e-6	2e-6	2.25e-6	100e-6	290e-6	0
BLK4	2e-6	146e-6	2.25e-6	110e-6	144e-6	0
CANTILEVER 2						
BLK5	2e-6	170e-6	2.25e-6	148e-6	120e-6	0

NAME	LENGTH			AXIS BASE POINT		
	X	Y	Z	X	Y	Z
BLK6	12e-6	2e-6	2.25e-6	138e-6	290e-6	0
BLK7	2e-6	146e-6	2.25e-6	138e-6	144e-6	0
CANTILEVER 3						
BLK8	2e-6	170e-6	2.25e-6	100e-6	-170e-6	0
BLK9	12e-6	2e-6	2.25e-6	100e-6	-172e-6	0
BLK10	2e-6	146e-6	2.25e-6	110e-6	-170e-6	0
CANTILEVER 4						
BLK11	2e-6	170e-6	2.25e-6	148e-6	-170e-6	0
BLK12	12e-6	2e-6	2.25e-6	138e-6	-172e-6	0
BLK13	2e-6	146e-6	2.25e-6	138e-6	-170e-6	0

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



Initial geometry for the thin-film resonator in 3D with folded cantilevers.

PHYSICS SETTINGS

Application Mode Properties

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

2 In the **Application Mode Properties** dialog box, go to the **Large deformations** list and select **On**.

3 Click **OK**.

Subdomain Settings

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

2 Select all subdomains.

3 On the **Material** page of the **Subdomain Settings** dialog box, enter the following values; when finished, click **OK**.

SETTINGS	VALUE	DESCRIPTION
MATERIAL PAGE		
E	E	Young's modulus
ν	nu	Poisson's ratio
α	daT	Thermal expansion coefficient
ρ	rho	Density

Boundary Conditions

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

2 In the **Boundary selection** list, select 34, 36, 52, and 54.

3 On the **Constraint** page, set the **Constraint condition** list to **Fixed**.

4 Click **OK**.

MESH GENERATION

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

2 Click the **Global** tab.

3 Verify that the selection from the **Predefined mesh sizes** list is **Normal**.

4 Click the **Advanced** tab.

5 For the **z-direction scale factor** enter `2.0`.

6 Click **Remesh**.

7 Click **OK**.

COMPUTING THE SOLUTION—EIGENMODES WITHOUT STRESSES

Follow the steps below to compute the eigenmodes with the applied stress stiffening:

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Eigenfrequency**.

3 Click **OK**.

4 Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

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

2 Go to the **General** page.

3 From the **Eigenfrequency** list, choose the mode you want to plot; The eigenmode for the horizontal movement has an eigenfrequency of approximately 14 kHz

4 Click the **Deform** tab.

5 Select the **Deformed shape plot** check box.

6 Click **OK**.

PHYSICS SETTINGS—THERMAL STRAINS

Subdomain Settings

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

2 Select all subdomains.

3 On the **Load** page, enter the values in the following table; when finished, click **OK**.

QUANTITY	VALUE	DESCRIPTION
Temp	T0	Strain temperature
Tempref	T1	Strain ref. temperature

COMPUTING THE SOLUTION—STATIC RESIDUAL STRESS

Using the steps below, solve the model and store the static solution for later use.

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Static**, then click **OK**.

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

4 From the **Solve** menu, choose **Solver Manager**.

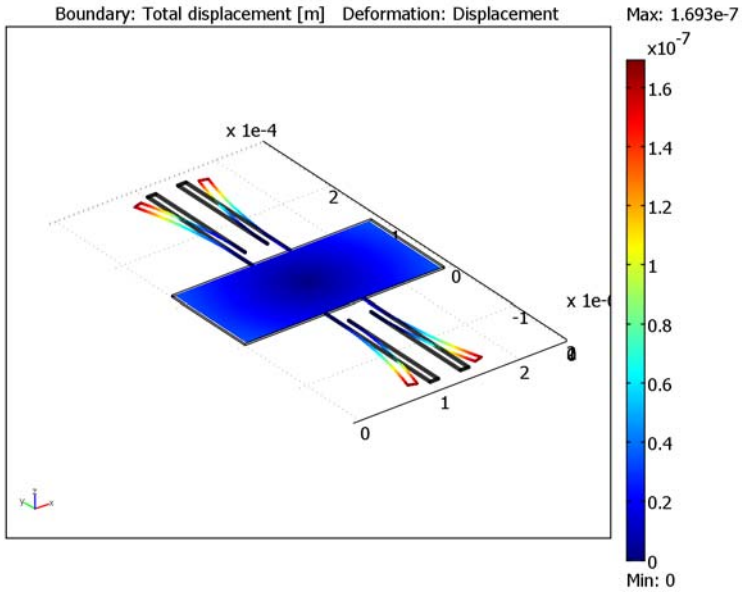
5 Click the **Initial Value** tab.

6 Click the **Store Solution** button at the bottom of the dialog box.

7 In the **Values of variables not solved for and linearization point** area select **Stored solution**.

8 Click **OK**.

According to the plot settings you defined before, the deformed plot with total displacement appears in the user interface:



Deformed shape of the geometry for the thin-film resonator in 3D with folded cantilevers.

Next create a cross-section plot to inspect the stress distribution in more detail.

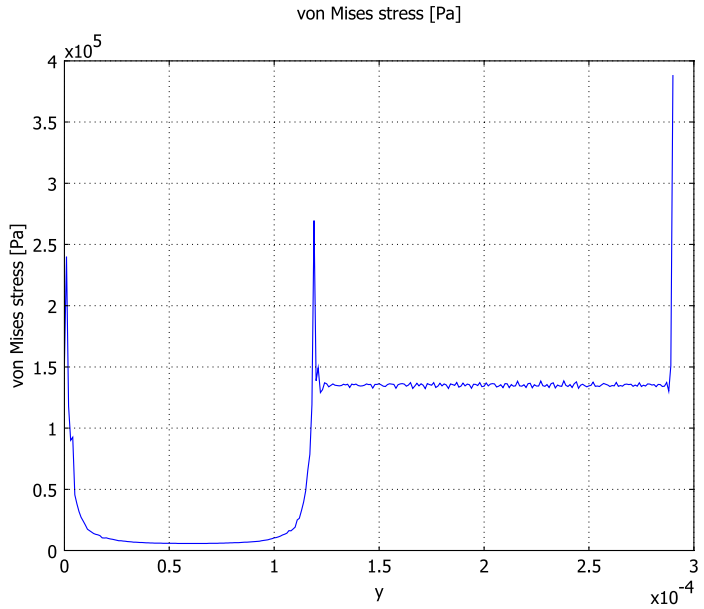
1 From the **Postprocessing** menu, choose **Cross-Section Plot Parameters**.

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

3 Enter the following values; when finished click **OK**.

PARAMETER	VALUE
Plot type	Line plot
Predefined quantities	von Mises stress
Expression	`mises_smsld`
x-axis data	y
CROSS-SECTION LINE DATA	
x0	`101e-6`
x1	`101e-6`

PARAMETER	VALUE
y0	0
yl	290e-6
z0	1.125e-6
zl	1.125e-6
Line resolution	291



Line plot of von Mises stress going first through the resonator body and then through one of the legs.

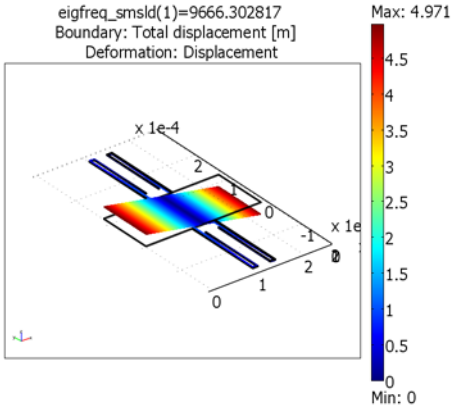
COMPUTING THE SOLUTION—EIGENMODES WITH STRESSES

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Eigenfrequency**.

3 Click **OK**.

4 Click the **Solve** button. Observe the eigenfrequency from the plot title; the first found eigenmode corresponds to rotational movement.



Deformation associated with the first eigenfrequency for the thin-film resonator in 3D with folded cantilevers.

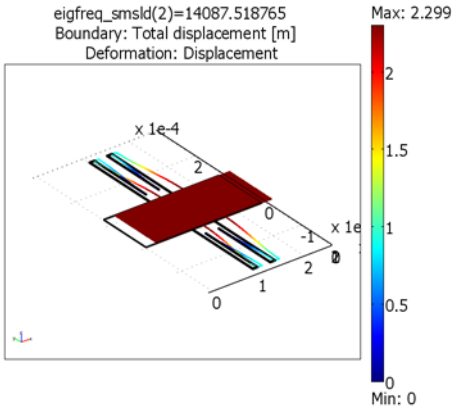
POSTPROCESSING AND VISUALIZATION—EIGENFREQUENCY

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

2 Click the **General** tab.

3 From the **Eigenfrequency** list, select the second value, which should be near 14 kHz.

4 Click **OK**.



Deformation associated with the second eigenfrequency for the thin-film resonator in 3D with folded cantilevers.

Thermoelastic Damping in a MEMS Resonator

Introduction

A high Q value is a key factor of a MEMS resonator. It it essential that the resonator vibrates consistently at the desired frequency and that it requires as little energy as possible to maintain its vibration. These features can be characterized by the resonator's Q value, which is a measure of the sharpness of its spectrum's peak. There are several ways to define the Q value, for example:

$$Q = \frac{2\pi W_0}{\Delta W} = \frac{\omega_0}{2\delta} = \frac{\omega_0}{\Delta\omega} \tag{2-2}$$

where W_0 is the total stored vibrational energy, ΔW is the energy lost per cycle, ω_0 is the natural angular frequency, δ is the damping factor (vibration decays exponentially with δt), and $\Delta\omega$ is the half power width of the spectrum.

In order to improve the resonator, the designer needs to consider all aspect that produce damping and noise to the system. For example, resonators are usually run in vacuum to minimize effects of air and squeeze-film damping.

Thermoelastic damping (Ref. 1, Ref. 2, and Ref. 3) is an important factor that the resonator designer needs to address. It is a result of a phenomenon called thermoelastic friction, which takes place when you subject any material to cyclic stress. The stress results in deformation, and the required energy is mostly stored as internal potential energy. However, materials heat under compressive stress and cool under tensile stress. Thus, due to the heat flow from warmer to cooler regions energy is also lost as nonrecoverable thermal energy. The amount of thermoelastic friction and damping depends on the rate of this energy loss. The magnitude of the energy loss depends on the vibrational frequency and on the structure's thermal relaxation time constant, which is the effective time the material requires to relax after an applied constant stress or strain. Therefore, the effect of thermoelastic dissipation, and consequently the damping, is most pronounced when the vibration frequency is close to the thermal relaxation frequency.

For simple structures, researchers have developed analytical expressions to estimate thermoelastic damping. According to Zener (Ref. 1 and Ref. 2), you can calculate the Q value for a resonator with a single thermal mode by:

$$\frac{1}{Q} = \left(\frac{E\alpha^2 T_0}{\rho C_p}\right)\left(\frac{\omega\tau}{1+(\omega\tau)^2}\right) \tag{2-3}$$

where E is the Young's modulus, α is the thermal expansion coefficient, T_0 is the resonator temperature at rest, ρ is the density, C_p is the heat capacity of the material, ω is the vibration angular frequency, and τ is the thermal relaxation time of the system. Thus it is easy to see that in order to have good Q value, the system needs to be designed so that ω is as far from $1/\tau$ as possible.

The natural frequency of a beam clamped at both ends can be calculated as (Ref. 4)

$$\omega_0 = a_0^2 \frac{h}{L^2}\sqrt{\frac{E}{12\rho}} \tag{2-4}$$

where a_0 equals 4.730; h and L are the thickness and length of the beam, respectively; and E and ρ are material parameters as above.

The thermal relaxation time of the beam is given by

$$\tau = \frac{\rho C_p h^2}{\pi^2 \kappa} \tag{2-5}$$

where κ is the thermal conductivity and other parameters are as above.

The problem is that Equations 2-3 through 2-5 are valid only for very simple structures. Therefore more advanced methods, such as FEA, are preferable.

This example shows how to model thermoelastic damping with COMSOL Multiphysics. To be able to compare with measurements and analytical expressions, this example illustrates a simple beam resonator in 2D and 3D. The Q value and natural frequency is solved with an eigenfrequency analysis that combines heat transfer and structural mechanics in one equation system. Thus the eigenmodes are thermoelastic.

This example was inspired by the work of Amy Duwel and others (Ref. 1).

Model Definition

Figure 2-20 shows the geometry. The resonator is a beam of silicon with length 400 µm, height 12 µm, and width 20 µm. The beam is fixed at both ends, and it vibrates in a flexural mode in the z direction (that is, along the smallest dimension). The model assume that the vibration takes place in vacuum. Thus there is no transfer of heat from the free boundaries. The model also assumes that the contact boundaries are thermally insulated.

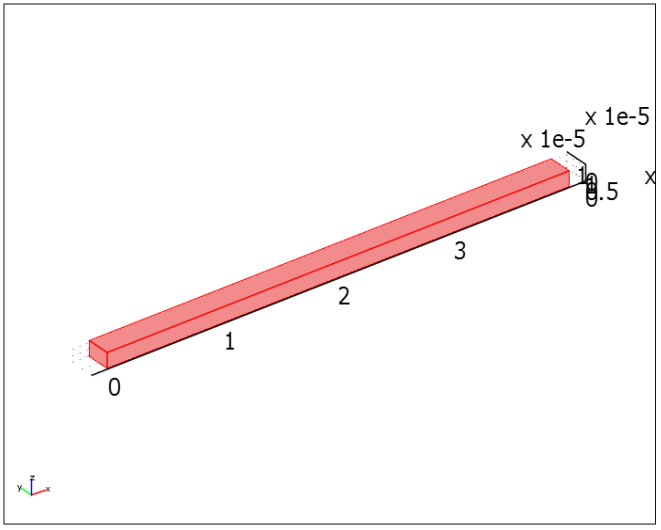


Figure 2-20: Geometry of the modeled beam. The beam is fixed at both ends.

Table 2-4 lists the physical properties of the beam material and the surroundings:

TABLE 2-4: MATERIAL PROPERTIES (POLYSILICON)

PROPERTY	VALUE
Young's modulus, E	157 GPa
Density, ρ	2330 kg/m^3
Poisson's ratio, ν	0.3
Thermal expansion coefficient, α	2.6·10^{-6} K^{-1}
Specific heat, C_p	700 J/(kg·K)
Thermal conductivity, k	90 W/(m·K)
Ambient and initial beam temperature, T_{init}	300 K

To gain information about the quality of the resonator, it is of interest to know its natural frequency and Q value. To do this, you run an eigenfrequency analysis to find the eigenvalues for this system. For a system with damping, the eigenvalue λ contains information about the natural frequency and Q value according to:

$$\begin{aligned} w_0 &= |\mathrm{Im}(\lambda)| \\ Q &= \left|\frac{\mathrm{Im}(\lambda)}{2\mathrm{Re}(\lambda)}\right| \end{aligned} \tag{2-6}$$

The eigenvalues appear as complex conjugates, and ω_0 and Q are therefore given as absolute values.

At this point, to avoid any confusion it is good to note that here Q refers to the resonator's quality, whereas later in this text Q_{heat} refers to the heat source term in the heat equation.

To model thermoelastic damping, you must consider both the thermal problem and the structural problem. Furthermore, there is a 2-way coupling between them: the strain rate heats or cools the material locally, which produces thermal strains.

The relation between the material stress σ and strain ε is given by

$$\sigma = D\varepsilon_{\mathrm{el}} = D(\varepsilon - \varepsilon_{\mathrm{th}}) \tag{2-7}$$

where $\varepsilon_{\mathrm{el}}$ and $\varepsilon_{\mathrm{th}}$ are the elastic and thermal strains, respectively, D is the 6×6 elasticity matrix, and all stresses and strains are denoted with 6-component vectors consisting of x, y, and z normal components followed by the xy, yx, and xz shear components.

It is possible to expand this for an isotropic material:

$$\begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{xz} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} \varepsilon_x - \alpha(T - T_{\mathrm{ref}}) \\ \varepsilon_y - \alpha(T - T_{\mathrm{ref}}) \\ \varepsilon_z - \alpha(T - T_{\mathrm{ref}}) \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \end{bmatrix} \tag{2-8}$$

where T is the strain temperature, T_{ref} is the stress-free reference temperature, and α is the thermal expansion coefficient.

The heat balance equation is

$$T\frac{\partial S}{\partial t} - \nabla \cdot (k\nabla T) = 0 \tag{2-9}$$

where k is the thermal conductivity. For a linear thermoelastic solid, the entropy per unit volume is:

$$S = \rho C_P \log(T/T_0) + S_{\text{elast}} \tag{2-10}$$

where T_0 is the reference temperature, the volumetric heat capacity ρC_P is assumed independent of the temperature, and

$$S_{\text{elast}} = \alpha_{\text{vec}} \cdot \sigma \tag{2-11}$$

where σ is the stress vector, and α_{vec} is the thermal expansion vector. For an isotropic material, Equation 2-11 simplifies into

$$S_{\text{elast}} = \alpha(\sigma_x + \sigma_y + \sigma_z) \tag{2-12}$$

For small deformations and small variation of the temperature, Equation 2-9 is linearized as:

$$\rho C_P \frac{\partial T}{\partial t} + T_0 \frac{\partial}{\partial t} S_{\text{elast}} - \nabla \cdot (k\nabla T) = 0 \tag{2-13}$$

Finally, the frequency decomposition for the temperature is performed

$$T = \tilde{T}(x_i)\exp(j\omega t) \tag{2-14}$$

where $j\omega = -\lambda$ is the complex angular frequency. Equation 2-13 gives

$$-\nabla \cdot (k\nabla \tilde{T}) = Q_{\text{heat}} \tag{2-15}$$

where the heat source term is

$$Q_{\text{heat}} = -j\omega(\rho C_P \tilde{T} + T_0 S_{\text{elast}}) \tag{2-16}$$

You model the problem with the damped eigenfrequency analysis for the beam, which is coupled with the thermal problem Equation 2-15.

When modeling in 2D, you use the plane stress approximation. Because the third stress component vanishes, you can replace Equation 2-16 by

$$Q_{\text{heat}} = -j\omega(\rho C_P \tilde{T} + T_0\alpha(\sigma_x + \sigma_y)) \tag{2-17}$$

In the eigenfrequency analysis, you use the temperature computer from Equation 2-15 as the strain temperature and set the strain reference temperature to zero, $T_{\text{ref}} = 0$. This is because the solution physically corresponds to thermoelastic oscillations of small amplitude—it is initialized to zero. However, T_0 in Equation 2-16 and Equation 2-17 is the actual temperature of the beam at rest.

Results and Discussion

Figure 2-21 and Figure 2-22 show the eigenmodes and temperature distribution corresponding to the found eigenvalue. Solved natural frequencies and Q values are given in Table 2-5. Reference data, one calculated with Equation 2-3 to Equation 2-5 and the others from measurements (see Ref. 1), are also given.

TABLE 2-5: COMPARISON OF NATURAL FREQUENCY AND Q VALUE.

SOURCE	F0 (MHZ)	Q
3D model	0.63 MHz	9151
2D model	0.63 MHz	10,170
Equation	0.63 MHz	10,260
Measurements (Ref. 1)	0.57 MHz	10,281

The Q value given by the 3D model appear to be roughly 10% smaller than the other estimates. One reason for this difference comes from the simplifying assumption that concerns both the Zener's equation (Equation 2-3) and the plane stress method. For example, the plane stress method assumes that the structure is very thin and that there are no stresses perpendicular to the plane. However, looking at the 3D model in more detail, you find that stresses and their spatial derivatives have components of equal magnitude in all three dimensions. The model also assumes that the beam was perfectly fixed at its ends. Physically, this cannot happen, and allowing more loose contact lowers the natural frequency and improves the Q value.

One factor that also affects the simulated Q values is the boundary condition for the thermal equation. This example uses thermal insulation on all boundaries, but you can assume that there is a flux of heat at least from both ends of the beam. If you simply assign a constant temperature ($T = 0$) to the beam ends, the Q value improves

considerably. The physically correct result should be somewhere between these two estimates.

A look at Figure 2-21 and Figure 2-22 shows a temperature distribution that appears to agree with the theory: the temperature is higher near the compressive strain and lower near the tensile strain.

Note, however, that you should not take the displayed temperature range (–4 K to 4 K) literally because the software normalizes the solution from the eigenfrequency solver.

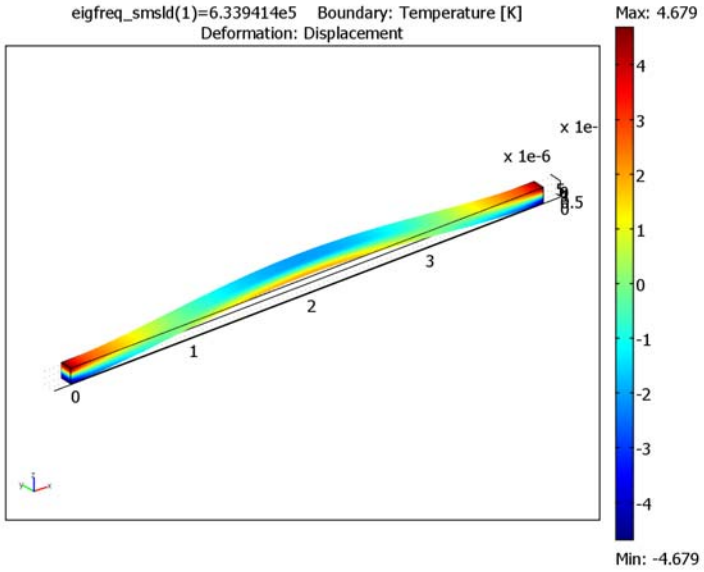


Figure 2-21: First eigenmode and temperature distribution of the 3D model.

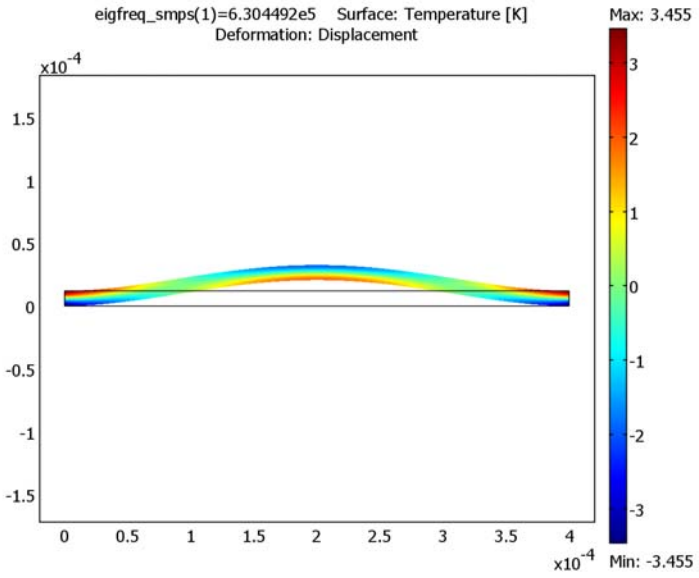


Figure 2-22: First eigenmode and temperature distribution of the 2D model.

Modeling in COMSOL Multiphysics

To create a model of thermoelastic damping with COMSOL Multiphysics requires two application modes. For the 3D model, use the Solid, Stress-Strain application mode from the MEMS Module and the steady-state Conduction application mode from the base package. In 2D, use the Plane Stress application mode from the MEMS Module with the same Conduction application mode as in 3D.

In this example you guide the eigenfrequency solver to find the eigenfrequency near the expected natural frequency (Equation 2-4). Alternatively, you can first solve the undamped eigenfrequency f_0 (select **Eigenfrequency analysis** in the **Solver Parameters** dialog box and solve only for the structural application mode). This approach is also valid for more complex geometries where you do not have an analytical expression for the estimated natural frequency.

This model, which consists of 2nd-order (structural) and 1st-order (thermal) eigenvalue problems, is numerically quite challenging. You can improve the results' accuracy by manually scaling the dependent variables. This is an approach that you can use more generally. Once you know the magnitudes of the dependent variables, go to

the **Advanced** page in the **Solver Parameters** dialog box and define manual scaling of the dependent variables.

For the 3D problem you can utilize its symmetry. The beam is truncated to 10 um in the width direction. Thus you get a smaller mesh size, but it also makes the problem easier to solve because the symmetry condition also prevents any flexural vibrations in this direction.

This example uses both rectangular and brick meshes. In 2D, first draw the geometry and use a mapped mesh to mesh it. In 3D, you utilize work planes by drawing a 2D view of the beam into the work plane. Then mesh it using the mapped mesh, and finally, a mesh extrusion creates the true 3D geometry.

In the damped eigenfrequency analysis, the resonator's quality factor Q is available as a predefined variable `Qfastor`. In the 3D analysis, you can use a predefined variable `Ent` for the elastic part of the entropy $S_{\text{elast.}}$ Use the explicit expression given in Equation 2-17 for 2D problem.

References

1. A. Duwel, R.N. Candler, T.W. Kenny, and M. Varghese, *Journal of Microelectromechanical Systems*, vol. 15, no. 6, pp. 1437–1445, 2006.

2. S. Gupta, *Estimation of Thermo-Elastic Dissipation in MEMS*, MSc. Thesis, Dept. Mechanical Engineering, Indian Institute of Science, Bangalore, July 2004.

3. T.V. Roszhart, "The Effect of Thermoelastic Internal Friction on the Q of Micromachined Silicon Resonators," *Tech. Dig. Solid-State Sens. Actuator Workshop*, Hilton Head, SC, 1990, pp. 13–16.

4. R. Lifshitz and K.L. Roukes, "Thermoelastic Damping in Micro- and Nanomechanical Systems," *Physical Review B*, vol. 61, no. 8, 15. Feb. 2000-II.

Model Library path:
`MEMS_Module/Actuator_Models/thermoelastic_damping_2d`

Model Library path:
`MEMS_Module/Actuator_Models/thermoelastic_damping_3d`

MODEL NAVIGATOR

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

2 Click **Multiphysics**.

3 From the list of application modes, select **MEMS Module>Structural Mechanics>Solid, Stress-Strain>Damped eigenfrequency analysis**.

4 Click **Add**.

5 From the list of application modes select **COMSOL Multiphysics>Heat Transfer>Conduction>Steady-state analysis**.

6 Click **Add**.

7 Click **OK**.

OPTIONS AND SETTINGS

Select **Options>Constants** and enter constants from the following table; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
E	157[GPa]	Young's modulus
rho	2330[kg/m^3]	Density
nu	0.3	Poisson's ratio
alpha	2.6e-6[1/K]	Thermal expansion coefficient
Cp	700[J/(kg*K)]	Specific heat capacity
k	90[W/(m*K)]	Thermal conductivity
T0	300[K]	Ambient and initial beam temperature
f0	4.730^2*sqrt(E/(rho*12))*12[um]/(2*pi*(400[um])^2)	Theoretical estimate for the natural frequency

The constant `f0` serves as an initial guess for the eigenfrequency solver.

GEOMETRY MODELING

1 Select **Draw>Work-Plane Settings**.

2 On the **Quick** page select the **z-x** check box.

3 Click **OK**. The 2D work plane becomes active.

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

5 In the **Width** edit field type `12e-6`, and in the **Height** edit field type `400e-6`.

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

MESH GENERATION

1 In the work plane select **Mesh>Mapped Mesh Parameters**.

2 In the **Subdomain** page select the first subdomain and click the **Boundary** tab.

3 Select Boundary 1.

4 Select the **Constrained edge element distribution** check box, then enter `25` in the **Number of edge elements** edit field.

5 Select Boundary 2.

6 Select the **Constrained edge element distribution** check box, then enter `4` in the **Number of edge elements** edit field.

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

8 Select **Mesh>Extrude Mesh**.

9 In the **Distance** edit field type `10e-6`.

10 Change to the **Mesh** page

11 In the **Number of element layers** edit field type `2`.

12 Click **OK**.

The 3D geometry should open automatically.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu select **1 Geom1: Solid, Stress-Strain (smsld)**.

2 Select **Physics>Subdomain Settings**.

3 Select Subdomain 1, and in the **Material** page enter settings according to the following table:

PROPERTY	VALUE
E	`E`
ν	`nu`
α	`alpha`
ρ	`rho`

4 Click the **Load** tab.

5 Select **Include thermal expansion** and type `T` for **Temp** and `0` for **Tempref**.

6 Change to the **Damping** page.

7 From the **Damping model** list select **No damping**.

8 Click **OK**.

9 From the **Multiphysics** menu select **2 Geom1: Heat Transfer by Conduction (ht)**.

10 Select **Physics>Subdomain Settings**.

11 See that Subdomain 1 is selected and in the **Material** page enter settings from the following table:

PROPERTY	VALUE
k (isotropic)	k
Q	`-jomega_smsld*(rho*Cp*T+T0*Ent_smsld)`

12 Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Geom1: Solid, Stress-Strain (smsld)**.

2 Select **Physics>Boundary Settings**.

3 Select Boundaries 1 and 6.

4 On the **Constraint** page, set **Constraint condition** to **Fixed**.

5 Select Boundary 2.

6 Set **Constraint condition** list to **Symmetry plane**.

7 Click **OK**.

8 From the **Multiphysics** menu, select **2 Geom1: Heat Transfer by Conduction (ht)**.

9 Select **Physics>Boundary Settings**.

10 Verify that **Thermal insulation** is the default value.

11 Click **OK**.

COMPUTING THE SOLUTION

1 Choose **Solve>Solver Parameters**.

2 Go to the **General** page.

3 Type `1` for **Desired number of eigenfrequencies**.

4 Type `f0` for **Search for eigenfrequencies around**.

5 Go to the **Advanced** page.

6 Locate the **Scaling of variables** area and choose **Manual** for **Type of scaling**.

7 In the **Manual scaling** edit field, type `u 1e-4 v 1e-4 w 1e-4 T 1`. Click **OK**.

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

The solver finds a solution with an eigenfrequency of approximately 63,394 Hz.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-21 follow these steps:

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

2 On the **General Page** verify that the **Boundary**, **Deformed shape**, and **Geometry edges** check boxes are selected and that all others are cleared.

3 Go to the **Boundary** page and select **Heat Transfer by Conduction (ht)>Temperature** from the **Predefined quantities** list.

4 Click **OK**.

You can see the eigenfrequency in the postprocessing plot. Use the **Global Data Display** dialog box to calculate the Q value:

1 Choose **Postprocessing>Data Display>Global**.

2 In the **Expression** edit field, type `Qfactor_smsld`.

3 Click **Apply**. You find the Q value in the message log.

Modeling Using the Graphical User Interface—2D Example

Start the model in the Model Navigator.

1 In the Model Navigator select **2D**.

2 Click **Multiphysics**.

3 From the list of application modes select **MEMS Module>Structural Mechanics>Plane Stress>Damped eigenfrequency analysis**.

4 Click **Add**.

5 From the list of application modes select **COMSOL Multiphysics>Heat Transfer>Conduction>Steady-state analysis**.

6 Click **Add**, then click **OK**.

OPTIONS AND SETTINGS

Choose **Options>Constants** and enter constants from the following table:

NAME	EXPRESSION	DESCRIPTION
E	157[GPa]	Young's modulus
rho	2330[kg/m^3]	Density
nu	0.3	Poisson's ratio
alpha	2.6e-6[1/K]	Thermal expansion coefficient
Cp	700[J/(kg*K)]	Specific heat capacity
k	90[W/(m*K)]	Thermal conductivity
T0	300[K]	Ambient and initial beam temperature
f0	4.730^2*sqrt(E/(rho*12))* 12[um]/(2*pi*(400[um])^2)	Theoretical estimate for the natural frequency

The constant `f0` serves as an initial guess for the eigenfrequency solver.

GEOMETRY MODELING

1. Shift-click the **Rectangle/Square** button on the Draw toolbar.
2. In the **Width** edit field type `400e-6`, and in the **Height** edit field type `12e-6`.
3. Click **OK**, then click the **Zoom Extents** button on the Main toolbar.

MESH GENERATION

1. In the work plane select **Mesh>Mapped Mesh Parameters**.
2. On the **Subdomain** page, select Subdomain 1.
3. Click the **Boundary** tab. Select Boundary 1.
4. Select the **Constrained edge element distribution** check box, then type `5` in the **Number of edge elements** edit field.
5. Select Boundary 2.
6. Select the **Constrained edge element distribution** check box, then type `25` in the **Number of edge elements** edit field.
7. Click **Remesh**, then click **OK**.

PHYSICS SETTINGS

Subdomain Settings—Plane Stress

1. From the **Multiphysics** menu, select **1 Plane Stress (smps)**.
2. Choose **Physics>Subdomain Settings**.

3 Select Subdomain 1. On the **Material** page, enter the following settings:

PROPERTY	VALUE
E	`E`
ν	`nu`
α	`alpha`
ρ	`rho`
thickness	`20e-6`

4 Click the **Load** tab.

5 Select the **Include thermal expansion** check box. Enter `T` for **Temp** and `0` for **Tempref**.

6 Change to the **Damping** page.

7 From the **Damping model** list, select **No damping**, then click **OK**.

Subdomain Settings—Heat Transfer by Conduction

1 From the **Multiphysics** menu, select **2 Heat Transfer by Conduction (ht)**.

2 Choose **Physics>Subdomain Settings**.

3 Verify that Subdomain 1 is selected, then on the **Physics** page enter settings according to the following table; when finished, click **OK**.

PROPERTY	VALUE
k (isotropic)	k
Q	`-jomega_smps*(rho*Cp*T+T0*alpha*(sx_smps+sy_smps))`

Boundary Conditions—Plane Stress

1 From the **Multiphysics** menu, select **1 Plane Stress (smps)**.

2 Choose **Physics>Boundary Settings**. Select Boundaries 1 and 4.

3 On the **Constraint** page, set **Constraint condition** to **Fixed**, then click **OK**.

Boundary Conditions—Heat Transfer by Conduction

1 From the **Multiphysics** menu, select **2 Heat Transfer by Conduction (ht)**.

2 Choose **Physics>Boundary Settings**.

3 Verify that **Thermal insulation** is the default value, then click **OK**.

COMPUTING THE SOLUTION

1 Choose **Solve>Solver Parameters**.

2 On the **General** page, enter 1 for **Desired number of eigenfrequencies**.

3 Enter `f0` for **Search for eigenfrequencies around**.

4 Go to the **Advanced** page.

5 Locate the **Scaling of variables** area and choose **Manual** for **Type of scaling**.

6 In the **Manual scaling** edit field, type `u 1e-4 v 1e-4 T 1`. Click **OK**.

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

The solver finds a solution with an eigenfrequency of approximately 63,045 Hz.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-22 follow the steps below:

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

2 On the **General** page, verify that the **Boundary**, **Deformed shape**, and **Geometry edges** check boxes are selected, and that all others are cleared.

3 On the **Surface** page, select **Heat Transfer by Conduction (ht)>Temperature** from the **Predefined quantities** list. Click **OK**.

You can see the eigenfrequency in the postprocessing plot. Use the **Global Data Display** dialog box to calculate the Q value:

1 Select **Postprocessing>Data Display>Global**.

2 In the **Expression** edit field type **Qfactor_smps**.

3 Click **Apply**. The Q value appears in the message log below the drawing area.

Thermomechanical Microvalve

Introduction

Active microvalves are common components in microfluidic systems (Ref. 1). In a thermomechanically actuated microvalve, an electric current generates the movement by resistively heating the actuator structure, thereby causing mechanical stress and deformation. This example shows how you can couple resistive heating to the temperature field and how an increase in temperature expands the solid structure and creates the necessary valve movement.

Model Definition

Consider a microvalve consisting of two silicon chips and a substrate as shown in Figure 2-23. The lower chip contains a cross-shaped actuator. Doped polysilicon heaters reside on the surfaces of the arms. The upper passive chip contains a valve seat with an orifice. The heated actuator structure expands, while the colder passive frame remains fixed. When the compressive stress accumulates to a critical value, the actuator buckles and the valve opens.

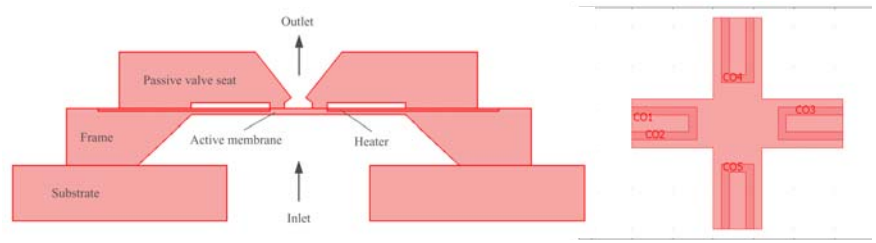


Figure 2-23: 2D cross-sectional view of a microvalve structure (left) and a top view of the arms (right).

At rest the valve is closed. When a voltage difference is applied across the ends of the heater elements, the resulting current resistively heats the doped polysilicon area. The heat conducts to the membrane, where it introduces stress and strain and finally causes the membrane to buckle, thereby opening the valve.

For analytical purposes, you can study an even more simplified structure. Consider a cantilever beam clamped rigidly at both ends as shown in Figure 2-24.

Figure 2-24: A simple cantilever-beam model. Both ends of the beam are tightly clamped into supporting frames.

In such a configuration, the central deflection, δ_c, of the silicon bridge is approximately given by

$$\delta_c = \frac{2}{\pi} L \sqrt{\alpha(\Delta T - \Delta T_{crit})}$$

where L is the beam length, α is the thermal expansion coefficient, and ΔT is the temperature difference between the membrane and the surrounding silicon frame (Ref. 2). You determine the critical buckling temperature difference, ΔT_{crit}, by substituting the strain generated by this temperature difference, $\varepsilon = \alpha \Delta T_{crit}$, into the equation of the critical-buckling strain $\varepsilon_{crit} = \pi^2 t^2/(3L^2)$, where t is the beam's thickness. The result reads

$$\Delta T_{crit} = \frac{\pi^2 t^2}{3\alpha L^2}.$$

For example, if a silicon bridge is 12 μm thick and 2600 μm long, and the thermal expansion coefficient is $2.6 \cdot 10^{-6}$/K, the critical temperature difference is 27 °C. A temperature difference of 200 °C then creates a deflection of 35 μm.

Modeling in COMSOL Multiphysics

This example models only the active cross-shaped actuator portion of the structure. It applies a potential difference to the ends of the heaters. Assuming that there are no external current sources and that the electric field is static, you can use the following equation to model the conductive surface:

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

Here σ_s is the surface conductivity and V is the electric potential. The surface conductivity is the reciprocal of the surface resistivity, $\sigma_s = 1/\rho_s$. You can also obtain it by multiplying the conductivity, σ, with the layer thickness, t_l, that is, $\sigma_s = t_l \sigma$. The

model uses the Conductive Media DC application mode's electric-shielding boundary condition to model the conductive layer.

Next calculate the resistive heat power generated in the layer per unit surface area, q, from the equation

$$q = t_1 \sigma \mathbf{E}_t \cdot \mathbf{E}_t = \sigma_s |\nabla_t V|^2$$

where ∇_t denotes the gradient in the directions tangential to the surface. The resistive heating couples to the Heat Transfer by Conduction application mode as an inward heat-flux term on the relevant boundaries. In the absence of internal heat sources, the equation for the temperature field, T, is analogous to the conductive media equation:

$$-\nabla \cdot (k \nabla T) = 0$$

Here k denotes the thermal conductivity. The model couples the temperature to the Plane Stress (in 2D) or Solid, Stress-Strain (in 3D) application mode's subdomain stress-load thermal expansion. Because the ends of the actuator arms are rigidly connected to the surrounding frame, the cross-shaped structure starts to deform.

Although the model geometry and the couplings of the application modes are rather simple, the meshing and solution require special techniques. The 2D model uses a mesh-mapping technique to generate a regular rectangular mesh. The 3D model increases the setting for the mesh scaling in the z direction from 1 to 10 to decrease the mesh size and the number of degrees of freedom. Depending on the amount of available memory on your computer, you can tune this value to increase or decrease the mesh size and thus change the solution accuracy.

Due to the problem's high degree of nonlinearity, this example solves the model using the parametric nonlinear solver; direct use of the nonlinear static solver can lead to solution errors.

The following tables show the dimensions and material parameters for the model:

STRUCTURE DIMENSION	MEASURE
Arm length	1000 μm
Arm width	600 μm
Structure height	12 μm
Cross-section area	600 μm x 600 μm

MATERIAL PROPERTY	VALUE
Material	Polysilicon
Young's modulus	160 GPa
Poisson's ratio	0.22
Coefficient of thermal expansion	$2.6 \cdot 10^{-6}$ 1/K
Density	2320 kg/m^3
Thermal conductivity	34 W/(m·K)
Heat capacity	678 J/(kg·K)
Sheet resistivity, heater layer	20 Ω
Doping-layer thickness	600 nm
Electric conductivity, membrane bulk	10^{-10} S/m

Note: The heat capacity drops out of the heat equation for stationary analyses and is given here for the sake of completeness only.

Results and Discussion

The following figures show the deformed shape and the deformation versus voltage both in 2D and 3D.

The 2D model gives values that agree well with the analytical result for a rigidly clamped cantilever beam: when the maximum deflection in the 2D model is 35 µm, the average temperature difference is 195 K compared to the analytical prediction of 200 K—a difference of only roughly 2.5%.

The 3D model, on the other hand, differs substantially from these results. Here, the maximum deformation 35 µm is reached for a voltage of 9.75 V with a corresponding average temperature difference of 364 K.

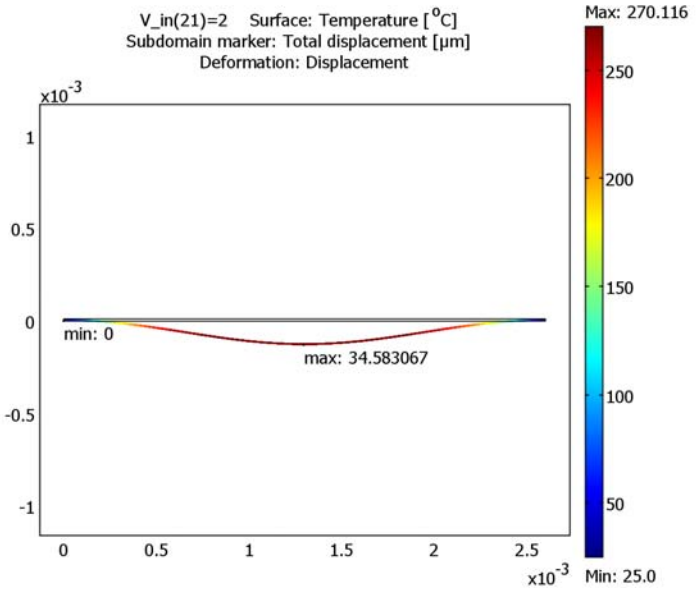


Figure 2-25: Deformed shape and temperature in 2D.

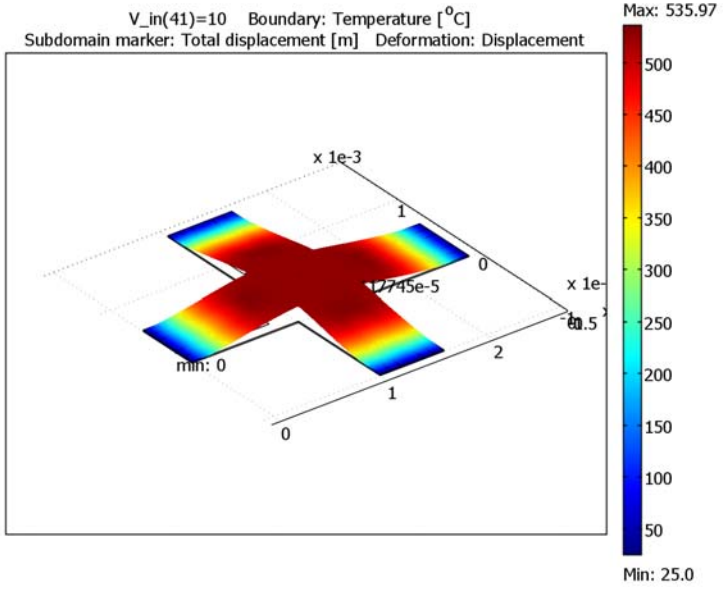


Figure 2-26: Deformed shape and temperature in 3D.

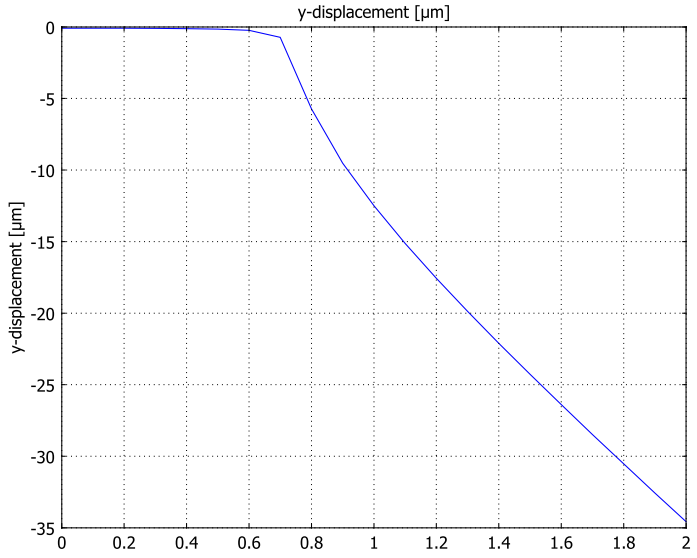


Figure 2-27: Deformation (y-displacement) versus voltage in 2D.

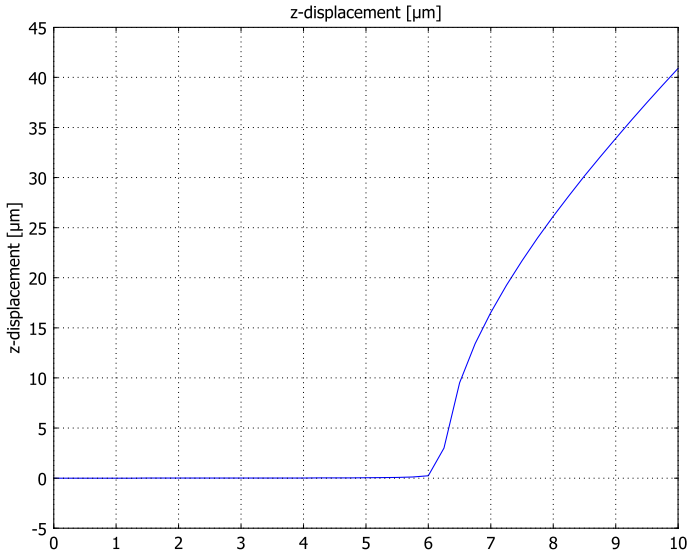


Figure 2-28: Deformation (z-displacement) versus voltage in 3D.

References

1. N.T. Nguyen and S.T. Werely, *Fundamentals and applications of microfluidics*, Arctech House, 2002, ch. 6. Microvalves, pp. 247–292.

2. T. Lisec et al. "Thermally driven microvalve with buckling behaviour for pneumatic applications," *Proc. MEMS'94*, 7th IEEE Intl Workshop Micro Electro Mechanical System, Oiso, Japan, 1994, p. 13.

Modeling Using the Graphical User Interface (2D)

Model Library path: `MEMS_Module/Actuator_Models/thermomechanical_valve_2d`

MODEL NAVIGATOR

1 In the **Model Navigator**, click the **New** tab. From the **Space dimension** list, select **2D**.

2 Click the **Multiphysics** button.

3 From the list of application modes, select **MEMS Module>Structural Mechanics>Plane Stress>Parametric analysis**, then click **Add**.

4 From the list of application modes, select **COMSOL Multiphysics>Heat Transfer>Conduction>Steady-state analysis**, then click **Add**.

5 From the list of application modes, select **MEMS Module>Electrostatics>Conductive Media DC**, then click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

Constants

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

2 Add the following constants (note that COMSOL Multiphysics automatically fills in the **Value** column); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
d	0.6[mm]	Bridge width
T_ref	25[degC]	Reference temperature
sigma_b	1e-10[S/m]	Electric conductivity, membrane bulk

NAME	EXPRESSION	DESCRIPTION
rho_s	20[ohm]	Surface resistivity
t_l	600[nm]	Heater-layer thickness
sigma_s	1/rho_s	Surface conductivity
sigma	sigma_s/t_l	Electric conductivity, heater layer
V_in	2[V]	Voltage

It is not strictly necessary to define `V_in` at this stage because you specify it later as the solver parameter. However, by defining `V_in` as a constant you avoid inconsistent-unit warnings, which occur when you enter an undefined constant in an edit field that expects input with a specific unit. It also allows you to try solving the problem directly using the stationary solver.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar and create the following rectangle; when done, click **OK**.

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	2600e-6	12e-6	Corner	0	0

2 Shift-click the Point button on the Draw toolbar and add these two points; when done, click **OK**.

NAME	X	Y
PT1	800e-6	12e-6
PT2	1800e-6	12e-6

3 Click the **Zoom Extents** button.

Initial geometry of the simplified thermomechanical microvalve's active element in 2D.

PHYSICS SETTINGS

Application Mode Properties—Plane Stress

1 From the **Multiphysics** menu, select **Plane stress (smps)**.

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

3 In the **Application Mode Properties** dialog box, set **Large deformation** to **On**.

4 Click **OK**.

Subdomain Settings—Plane Stress

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

2 In the **Subdomain selection** list, select **1**.

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

4 From the **Materials** tree, select **MEMS Material Properties>Semiconductors>Poly-Si**, then click **OK**.

5 In the **thickness** edit field, type `d`.

6 Click the **Load** tab. Select the **Include thermal expansion** check box, then specify settings according to the following table; when done, click **OK**.

PROPERTY	VALUE	DESCRIPTION
Temp	`T`	Strain temperature
Tempref	`T_ref`	Strain ref. temperature

Boundary Conditions—Plane Stress

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

2 On the indicated pages, specify these boundary conditions; when done, click **OK**.

SETTINGS	VALUE ON BOUNDARY			DESCRIPTION
	1, 6	2	OTHERS	
CONSTRAINT PAGE				
Constraint condition	Fixed	Free	Free	
LOAD PAGE				
F_y		`-0.01`		Edge load y dir.

Apply a downward load of 0.01 N/m along Boundary 2 to initiate buckling of the structure. You can easily verify that a value in the range of 0.001 N/m to 0.1 N/m has a negligible effect on the solution.

Subdomain Settings—Heat Transfer by Conduction

1 From the **Multiphysics** menu, select **Heat Transfer by Conduction (ht)**.

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

3 In the **Subdomain selection** list, select **1**.

4 From the **Library material** list, select **Poly-Si**, then click **OK**.

Boundary Conditions—Heat Transfer by Conduction

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

2 Enter the following values in the **Boundary Settings** dialog box; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 6	BOUNDARIES 3, 5	DESCRIPTION
Boundary condition	Temperature	Heat flux	
q_0		q	Inward heat flux
T_0	T_ref		Temperature

For Boundaries 2 and 4, leave the default thermal-insulation boundary condition.

Subdomain Settings—Conductive Media DC

1 From the **Multiphysics** menu, select **Conductive Media DC (emdc)**.

2 From the **Physics** menu choose **Subdomain Settings**.

3 From the **Subdomain selection** list or in the drawing area, select Subdomain 1.

4 In the σ **(isotropic)** edit field type `sigma_b`. (The solution is rather insensitive to this parameter value, as long as it is small but nonzero.)

5 Click **OK**.

Boundary Conditions—Conductive Media DC

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

2 In the **Boundary Settings** dialog box, enter these boundary conditions and values; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 2, 4, 6	BOUNDARIES 3, 5
Boundary condition	Electric insulation	Electric shielding
Conductivity		sigma
Thickness		t_l

Point Settings—Conductive Media DC

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

2 In the **Point Settings** dialog box, enter the following values; when done, click **OK**.

SETTINGS	POINTS 1, 5	POINTS 2, 6	POINTS 3, 4	DESCRIPTION
Q_{j0}	0			Point current source
V_0		0	V_in	Electric potential

Boundary Expressions—Conductive Media DC

1 From the **Options** menu, choose **Expressions>Boundary Expressions**.

2 Select Boundaries 3 and 5. Enter the following properties in the table's first row:

NAME	EXPRESSION
q	`sigma_s*(VTx^2+VTy^2)`

3 Click **OK**.

MESH GENERATION

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

2 Click the **Boundary** tab.

3 Enter these values for the boundaries:

SETTINGS	VALUE ON BOUNDARY			
	1	2	3	4
Constrained edge element distribution	Selected			
Number of edge elements	4	65	20	25

4 Click the **Remesh** button.

5 Click **OK**.

SOLVING THE MODEL

1 From the **Solve** menu, choose **Solver Parameters**.

2 On the **General** page, select **Parametric** from the **Analysis** list.

3 Set the **Parameter name** to `V_in` and the **Parameter values** to `0:0.1:2`.

4 Click the **Parametric** tab. From the **Predictor** list, select **Constant**. This change from the default linear prediction method is necessary to remain on the first deformation mode (with a single node) as the voltage is turned up.

5 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

Temperature Distribution and Deformed Shape

Follow the steps below to reproduce Figure 2-25 on page 126.

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

2 Click the **General** tab.

3 In the **Plot type** area, select the check boxes **Surface**, **Max/min marker**, **Deformed shape**, and **Geometry edges**.

4 Click the **Surface** tab.

5 On the **Surface Data** page, select **Heat-Transfer by Conduction (ht)>Temperature** from the **Predefined quantities** list. From the **Unit** list, select **°C** (or type `degC` in the edit field).

6 Click the **Max/Min** tab.

7 On the **Subdomain Data** page, select **Plane Stress (smps)>Total displacement** from the **Predefined quantities** list. From the **Unit** list, select **µm** (or type `um` in the edit field).

8 Click **OK**.

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

For comparison with theoretical values, calculate the difference between the average temperature in the active element and the surroundings.

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

2 Select Subdomain 1 and enter the **Expression** `(T-T_ref)/(2.6[mm]*12[um])`.

3 Click **OK**.

The average temperature difference value (roughly 194.8 K) appears in the message log at the bottom of the user interface.

Centerpoint Analysis

Follow the steps below to reproduce the plot in Figure 2-27 on page 127.

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

2 Click the **Point** tab.

3 From the **Predefined quantities** list inside the **y-axis data** area, select **Plane Stress (smps)>y-displacement**. From the **Unit** list, select **µm**.

4 In the edit fields for **x** and **y** inside the **Coordinates** area, type `1300e-6` and `12e-6`, respectively.

5 Click **OK**.

Model Library path: `MEMS_Module/Actuator_Models/thermomechanical_valve_3d`

MODEL NAVIGATOR

1 In the **Model Navigator** click the **New** tab, go to the **Space dimension** list, and select **3D**.

2 Click the **Multiphysics** button.

3 From the list of application modes select **MEMS Module>Structural Mechanics>Solid, Stress-Strain>Parametric analysis**, then click **Add**.

4 From the list of application modes select **COMSOL Multiphysics>Heat Transfer>Conduction>Steady-state analysis**, then click **Add**.

5 From the list of application modes select **MEMS Module>Conductive Media DC**, then click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

Constants

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

2 Add the following constants, (note that COMSOL Multiphysics automatically fills in the **Value** column); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
E	161[GPa]	Young's modulus
nu	0.33	Poisson's ratio
alpha	2.3e-6[1/K]	Thermal expansion coefficient
rho	2320[kg/m^3]	Density
d	0.6[mm]	Bridge width
T_ref	25[degC]	Reference temperature
k	34[W/(m*K)]	Thermal conductivity
sigma_b	1e-10[S/m]	Electric conductivity, membrane bulk
rho_s	20[ohm]	Surface resistivity

NAME	EXPRESSION	DESCRIPTION
t_l	600[nm]	Heater-layer thickness
sigma_s	1/rho_s	Surface conductivity
sigma	sigma_s/t_l	Conductivity
V_in	2[V]	Voltage

GEOMETRY MODELING

Work-Plane Settings

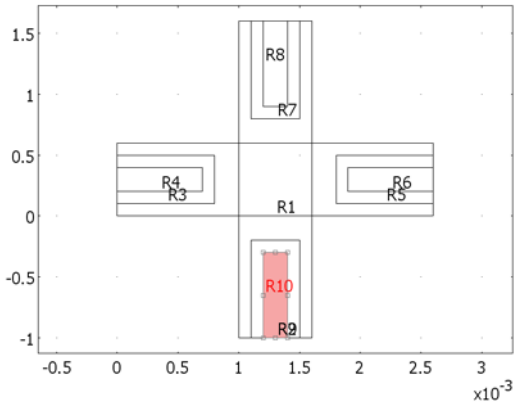
1 From the **Draw** menu, choose **Work-Plane Settings**.

2 Accept the default settings (an xy-plane at $z = 0$) by clicking **OK**.

Creating Objects

1 Shift-click the **Rectangle/Square** tool on the Draw toolbar and create ten rectangles; when done, click **OK**.

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	2600e-6	600e-6	Corner	-1300e-6	-300e-6
R2	600e-6	2600e-6	Corner	-300e-6	-1300e-6
R3	800e-6	400e-6	Corner	-1300e-6	-200e-6
R4	700e-6	200e-6	Corner	-1300e-6	-100e-6
R5	800e-6	400e-6	Corner	500e-6	-200e-6
R6	700e-6	200e-6	Corner	600e-6	-100e-6
R7	400e-6	800e-6	Corner	-200e-6	500e-6
R8	200e-6	700e-6	Corner	-100e-6	600e-6
R9	400e-6	800e-6	Corner	-200e-6	-1300e-6
R10	200e-6	700e-6	Corner	-100e-6	-1300e-6



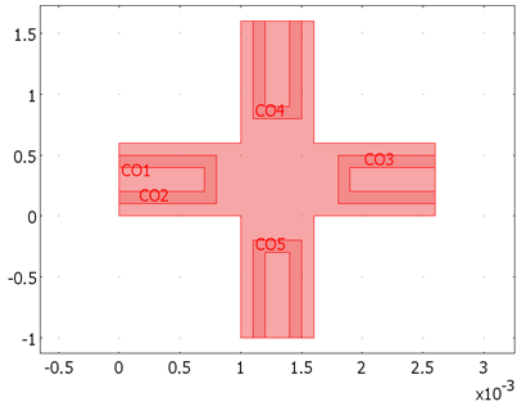
The rectangles that make up the geometry of the thermomechanical microvalve's active element in 3D.

2 From the **Draw** menu, choose **Create Composite Object**.

3 Clear the **Keep interior boundaries** check box.

4 In the **Set formula** edit field, enter these formulas to create composite objects; when done, click **OK**.

NAME	SET FORMULA
CO1	R1+R2
CO2	R3-R4
CO3	R5-R6
CO4	R7-R8
CO5	R9-R10



The composite objects that make up the geometry of the thermomechanical microvalve's active element in 3D.

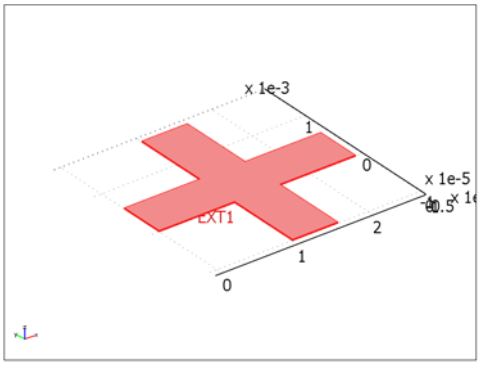
Extruding and Embedding into 3D

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

2 From the **Objects to extrude** list, select **CO1**.

3 Enter the following values in the **Extrude parameters** dialog box; when done, click **OK**.

NAME	VALUE
Distance	-12e-6
Scale x	1
Scale y	1
Displacement x	0
Displacement y	0
Twist (degrees)	0

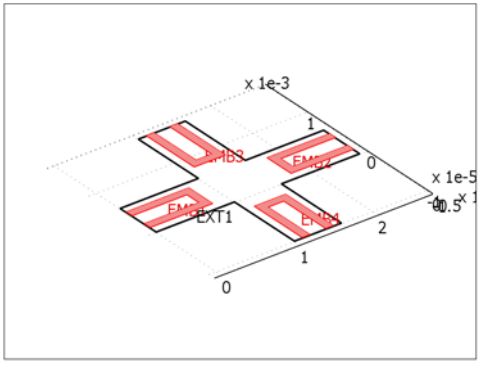


The extruded geometry of the thermomechanical microvalve's active element in 3D.

4 Click the **Geom2** tab at the top of the drawing area.

5 From the **Draw** menu, choose **Embed**.

6 In the **Objects to embed** list select **CO2**, **CO3**, **CO4**, and **CO5**; when done, click **OK**.



The actuator arms embedded in the overall geometry.

PHYSICS SETTINGS

Application Mode Properties—Plane Stress

1 From the **Multiphysics** menu, choose **Solid, Stress-Strain (smsld)**.

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

3 In the **Application Mode Properties** dialog box, change **Large deformation** to **On**.

4 Click **OK**.

Subdomain Settings—Plane Stress

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

2 In the **Subdomain selection** list, select **1**.

3 Enter settings according to the following table:

PROPERTY	VALUE	DESCRIPTION
E	`E`	Young's modulus
ν	`nu`	Poisson's ratio
α	`alpha`	Thermal expansion coeff.
ρ	`rho`	Density

4 Click the **Load** tab. Select the **Include thermal expansion** check box, then specify settings according to the following table; when done, click **OK**.

PROPERTY	VALUE	DESCRIPTION
Temp	`T`	Strain temperature
Tempref	`T_ref`	Strain ref. temperature

Boundary Conditions—Plane Stress

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

2 Select Boundaries 1, 9, 11, and 22. On the **Constraint** page, select **Fixed** from the **Constraint condition** list.

3 Click the **Load** tab. Select Boundary 3. In the $\mathbf{F_z}$ edit field, type `-1`.

As in the 2D case, you apply a small transverse load to simulate a perturbation that triggers buckling of the valve.

4 Click **OK**.

Subdomain Settings—Heat Transfer by Conduction

1 From the **Multiphysics** menu, choose **Heat Transfer by Conduction (ht)**.

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

3 In the **Subdomain selection** list, select **1**.

4 From the **Library material** list, select **Poly-Si**, then click **OK**.

Boundary Conditions—Heat Transfer by Conduction

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

2 Enter the following values in the **Boundary Settings** dialog box; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 9, 11, 22	BOUNDARIES 5, 12, 13, 20	DESCRIPTION
Boundary condition	Temperature	Heat flux	
q_0		q	Inward heat flux
T_0	T_ref		Temperature

At boundaries not mentioned in the table, the default thermal-insulation condition applies.

Subdomain Settings—Conductive Media DC

1 From the **Multiphysics** menu, choose **Conductive Media DC (emdc)**.

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

3 From the **Subdomain selection** list, select **1**.

4 In the σ **(isotropic)** edit field, type `sigma_b`.

5 Click **OK**.

Boundary Conditions—Conductive Media DC

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

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

SETTINGS	BOUNDARIES 1–4, 6–11, 14–19, 21, 22	BOUNDARIES 5, 12, 13, 20
Boundary condition	Electric insulation	Electric shielding
σ		sigma
d		t_l

Edge Settings—Conductive Media DC

1 From the **Physics** menu, choose **Equation System>Edge Settings**.

2 Enter the following values in the dialog box; when done, click **OK**.

SETTINGS	EDGES 10, 32, 46, 72	EDGES 6, 36, 44, 74	ALL OTHERS	DESCRIPTION
Q_{lj}			0	Line current source
V_0	0	V_in		Electric potential

Boundary Expressions

1 From the **Options** menu, choose **Expressions>Boundary Expressions**.

2 Add the following boundary expression; when done, click **OK**.

SETTINGS	BOUNDARIES 5, 12, 13, 20
q	sigma*t_l*(VTx^2+VTy^2+VTz^2)

MESH GENERATION

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

2 Click the **Advanced** tab.

3 In the **z-direction scale factor** edit field, type 10.

4 Click the **Remesh** button.

5 Click **OK**. The initialized mesh consists of roughly 2150 elements.

SOLVING THE MODEL

Solver Parameters

1 From the **Solve** menu, choose **Solver Parameters**.

2 From the **Analysis** list, select **Parametric**.

3 In the **Parameter name** edit field, type V_in.

4 In the **Parameter values** edit field, type 0:0.25:10.

5 Click **OK**.

Solving the Electric Potential

1 From the **Solve** menu, choose **Solver Manager**.

2 Click the **Initial Value** tab.

3 In the **Initial value** area, click the **Initial value expression** button.

4 In the **Values of variables not solved for and linearization point** area, click the **Zero** button.

5 Click the **Solve For** tab.

6 From the **Solve for variables** list, select **Conductive Media DC (emdc)**.

7 Click the **Solve** button.

Solving the Heat Transfer Problem

1 Click the **Initial Value** tab.

2 Click the **Store Solution** button.

3 Make sure that all the solutions are selected, then click **OK**.

4 In the **Values of variables not solved for and linearization point** area, click the **Stored solution** button.

5 From the **Parameter value** list, select **All**.

6 Click the **Solve For** tab.

7 From the **Solve for variables** list, select **Heat Transfer by Conduction (ht)**.

8 Click the **Solve** button.

Solving the Plane Stress Problem

1 Click the **Initial Value** tab.

2 Click the **Store Solution** button.

3 In the **Store Solution** dialog box, click **OK**.

4 Click the **Solve For** tab.

5 From the **Solve for variables** list, select **Solid, Stress-Strain (smsld)**.

6 Click the **Solve** button; the solution could take several minutes to compute.

7 Click **OK**.

POSTPROCESSING AND VISUALIZATION

Temperature Distribution and Deformed Shape

Follow the steps below to create Figure 2-26 on page 126.

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

2 Click the **General** tab.

3 In the **Plot type** area, select the check boxes **Boundary**, **Max/min marker**, **Deformed shape**, and **Geometry edges**. Clear all other check boxes.

4 Click the **Boundary** tab.

5 In the **Predefined quantities** list, select **Heat Transfer by Conduction (ht)>Temperature**.

6 In the **Unit** list, select **°C**.

7 Click the **Max/Min** tab.

8 From the **Predefined quantities** list on the **Subdomain Data** page, select **Solid, Stress-Strain (smsld)>Total displacement**. From the **Unit** list, select **μm**.

9 Click **OK**.

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

Next, calculate the difference between the average temperature in the active element and the surroundings.

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

2 Select Subdomain 1 and enter the **Expression** `(T-T_ref)/3.312e-11[m^3]`. The denominator is the actuator's volume. This value is available on the **Subdomain** page of the **Geometric Properties** dialog box that you open from the **Postprocessing** menu.

3 In the **Solution to use** area, select **9.75** from the **Parameter value** list.

4 Click **OK**.

The average temperature difference value (roughly 364 K) appears in the message log at the bottom of the user interface.

Cross-Section Analysis

Follow the steps below to create Figure 2-28 on page 127.

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

2 Click the **Point** tab.

3 From the **Predefined quantities** list inside the **y-axis data** area, select **Solid, Stress-Strain (smsld)>z-displacement**. From the **Unit** list, select **μm**.

4 Click **OK**.

3

MEMS Sensor Models

This chapter highlights models that describe different types of sensors in MEMS devices. The accelerometer example shows modeling in both 2D and 3D. An example of a pressure sensor describes a device that measures static pressures in the range from zero up to atmospheric pressure. Another model uses the Material Library to simulate thermal expansion in a MEMS device that could be part of a microgyroscope.

Squeezed-Film Gas Damping in an Accelerometer

Micromechanical structures that use capacitance to measure another parameter such as acceleration typically have a very narrow gap between their electrodes. The gap usually contains gas, which damps the movements of the mechanical parts. This model of a microsystem accelerometer shows how to couple squeezed-film gas damping, which you model with the linearized Reynolds equation, to displacements in the sensor.

Introduction

Squeezed-film gas damping is a critical aspect of many MEMS transducers and actuators. An example of a typical microsystem component where gas-damping properties are important is the accelerometer common in vehicle motion-control and safety systems.

In accelerometers, inertia produces a motion that the device detects. A typical structure connects a large proof mass, with dimensions typically in millimeters, to surrounding structures with elastic beams. This combination forms a mechanical oscillator with a specific resonance frequency. However, in accurate motion-detection applications these resonances are unwanted, and the device damps the movements to produce smooth time-step and frequency responses. Such a device can usually achieve suitable damping with a low gas pressure (100 Pa–1000 Pa) which, considering the dimensions of the device, lead to rarefied gas effect in the system.

A narrow gap formed by two solid horizontal plates restricts the displacement of the gas perpendicular to the surfaces. When the sensor squeezes the gap, the gas flows out from its edges. The narrow pathway restricts the flow, which causes gas pressure to increase, which decelerates the plates' movement.

You can model the pressure distribution in the narrow gap with the *modified Reynold's equation*

$$\nabla \cdot (h^3 Q_{\mathrm{ch}} p \nabla p_{\mathrm{F}}) = 12\eta\left(\frac{dp_{\mathrm{F}}}{dt}h + p\frac{dh}{dt}\right)$$

where p_{F} denotes the gas film pressure variation, $p = p_{\mathrm{A}} + p_{\mathrm{F}}$ is the total fluid pressure consisting of the initial/ambient pressure and the variation, $h = h_0 + \Delta h$ is the gap

height consisting of the initial gap and the deformation in the normal direction of the boundary, and η is the fluid viscosity at normal conditions. The term Q_{ch} denotes the relative flow rate function that accounts for the rarefied gas effects. Veijola and others (Ref. 2) have used a simple equation for the relative flow coefficient

$$Q_{\mathrm{ch}} = 1 + 9.638(\sigma_P K_n)^{1.159}$$

which is valid for $0 \le K_n \le 880$. The Knudsen number is the ratio between the gas' mean free path, λ, and the gap height, h:

$$K_n = \lambda / h$$

and the coefficient σ_P is calculated from the tangential momentum accommodation coefficient, α_v:

$$\sigma_P = \frac{2 - \alpha_v}{\alpha_v}(1.016 - 0.1211(1 - \alpha_v)) .$$

The mean free path at a pressure p comes from

$$\lambda = (p_0 \lambda_0)/p$$

where λ_0 is the mean free path at the reference pressure p_0.

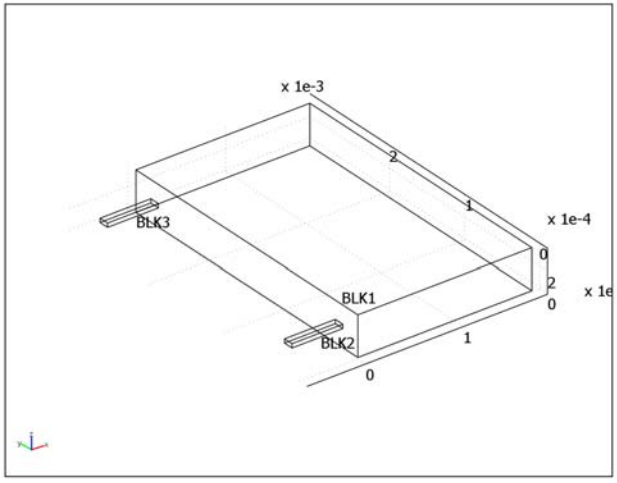
Another way to tune the damping is to perforate the structure with holes. By adding a term related to the gas flow through the holes, it is also possible to use the Reynolds equation for perforated plates. For more information about this approach see Ref. 3.

Model Definition

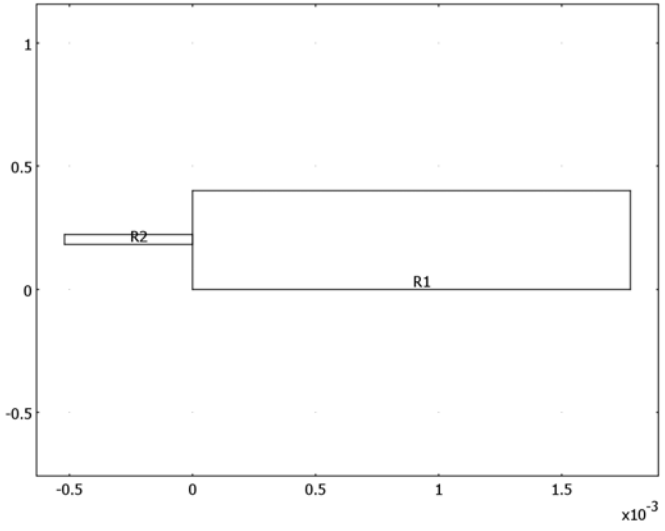
This example models the solid moving parts in the accelerometer using the Solid, Stress-Strain application mode in 3D and using the Plane Strain application mode in 2D. This model solves the squeezed-film air damping on the lower and upper surfaces using the Film Damping application mode. The model constrains the film pressure, p_F, to 0 at the edges of the boundary.

The following two figures show the accelerometer geometry in 3D and in 2D. The model consists of two thin silicon cantilever beams and a silicon proof mass. The cantilever beams are fixed to the surrounding structures at one end. The proof mass reacts to inertial forces and bends the cantilevers. The external acceleration, a, acts in the z direction and causes a body volume force $F_z = \rho_{\mathrm{solid}}\, a$.

In 2D the two cantilevers are lumped as one structure whose thickness equals the sum of the two cantilevers. Consequently, the model has two domains with different thicknesses at the connecting boundary. Thus you should be prudent when inspecting stress levels near this area.



Model geometry in 3D.



Model geometry in 2D.

The following tables list the structures' dimensions as well as pertinent material and gas properties used to calculate the effective viscosity:

PARAMETER	CANTILEVERS	PROOF MASS	GAP
Length	520 μm	1780 μm	1780 μm
Height	40 μm	400 μm	3.95 μm
Width	100 μm	2960 μm	2960 μm

PARAMETER	VALUE
Structure material	Silicon
Young's modulus	131 GPa
Poisson's ratio	0.27
Density	2330 kg/m^3
Viscosity of the gas	22.6·10^{-6} Ns/m^2
λ_0	70 nm
p_0	101.325 kPa

Results and Discussion

Figure 3-1 shows the pressure distribution on the surface of the proof mass after 4 ms of simulation. The ambient pressure, p_A, in this case is 300 Pa, and the acceleration switches on at the beginning of the simulation. The acceleration's magnitude is half that due to gravity, g. In this figure, the maximum displacement at the tip of the proof mass is roughly 0.4 μm, or 0.1% of its thickness.

Figure 3-2 shows the total displacement of the proof mass tip as a function of time for ambient pressures of 3 Pa, 30 Pa, and 300 Pa. As ambient pressure increases, the film damping at the upper and lower surfaces increases through the increase in the gas' effective viscosity and density. This increased damping results in a substantial decrease in oscillation with increasing pressure. At 300 Pa, there is no apparent oscillations, and the proof mass seems asymptotically to reach the value of 0.2 μm in total displacement.

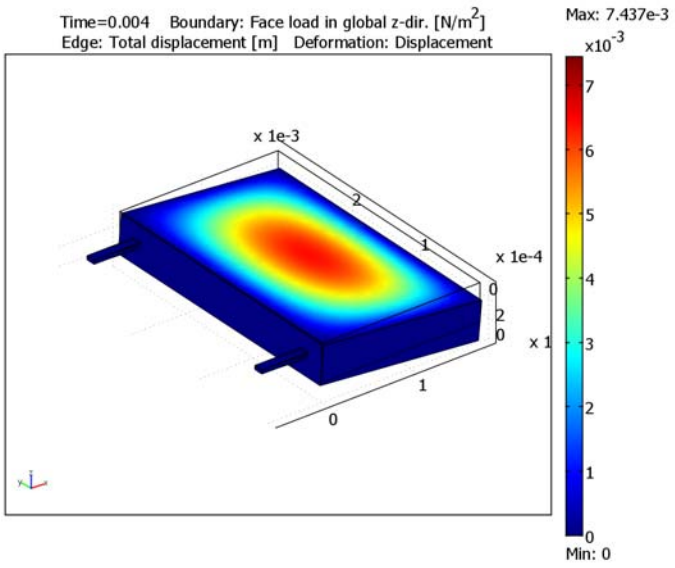


Figure 3-1: A load on the face of the proof mass in the z direction leads to a deformation.

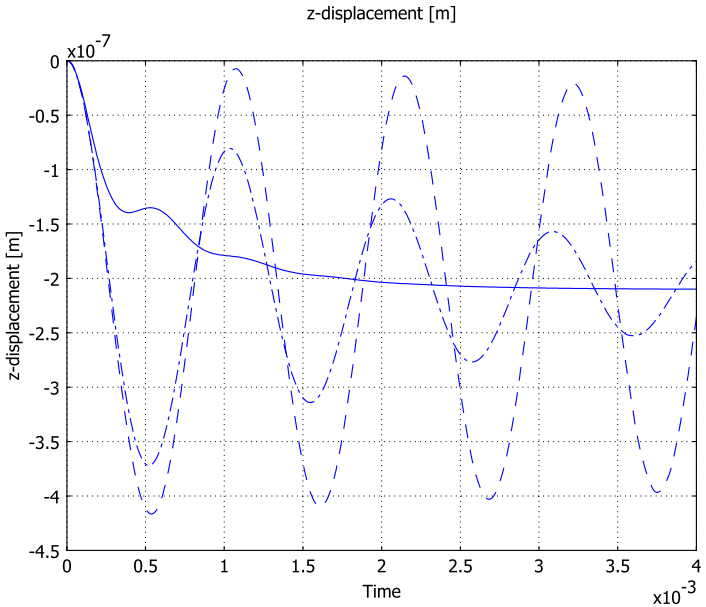


Figure 3-2: Plot of the displacement of the proof mass tip at ambient pressures of 3 Pa (dashed line), 30 Pa (dashed-dotted line), and 300 Pa (solid line).

References

1. J.B. Starr, "Squeeze-film damping in solid-state accelerometers," *Technical Digest IEEE Solid-State Sensor and Actuator Workshop*, 1990, p. 47.

2. T. Veijola, H. Kuisma, J. Lahdenperä, and T. Ryhänen, "Equivalent-circuit model of the squeezed gas film in a silicon accelerometer," *Sensors and Actuators*, A 48, pp. 239–248, 1995.

3. M. Bao, H. Yang, Y. Sun, and P.J. French, "Modified Reynolds' equation and analytical analysis of squeeze-film air damping of perforated structures," *J. Micromech. Microeng.*, vol. 13, pp. 795–800, 2003.

Modeling Using the Graphical User Interface (2D)

Model Library path: `MEMS_Module/Sensor_Models/accelerometer_2d`

Use the following instructions to create the 2D version of the accelerometer model.

MODEL NAVIGATOR

1. Open the **Model Navigator**, from the **Space dimension** list select **2D**.
2. In the list of application modes select **MEMS Module>Structural Mechanics> Plane Strain with Film Damping>Transient analysis**.
3. Click **OK**.

OPTIONS AND SETTINGS

1. From the **Options** menu choose **Constants**.
2. In the **Constants** dialog box enter names, expressions, and descriptions (optional) for the following constants; when done click **OK**.

NAME	EXPRESSION	DESCRIPTION
accel	9.81[m/s^2]/2	Applied acceleration
P_A	300[Pa]	Ambient gas pressure

GEOMETRY MODELING

1 Open the **Rectangle** dialog box either by Shift-clicking the **Rectangle/Square** button on the Draw toolbar or by going to the **Draw** menu and choosing **Specify Objects>Rectangle**. Create these two rectangles:

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	1780e-6	400e-6	Corner	0	0
R2	520e-6	40e-6	Corner	-520e-6	180e-6

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

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu choose the **Plane Strain (smpn)** application mode.

2 From the **Physics** menu choose **Subdomain Settings**.

3 Enter the following values in the **Subdomain Settings** dialog box:

QUANTITY	VALUE IN SUBDOMAIN		DESCRIPTION
	1	2	
MATERIAL PAGE			
Library material	Silicon		Click the **Load** button, go to **Materials>Basic Material Properties** and select **Silicon**
E	131e9[Pa]		Young's modulus
ν	0.27		Poisson's ratio
α	4.15e-6[1/K]		Coefficient of thermal expansion
ρ	2330[kg/m^3]		Density
thickness	200e-6	2960e-6	Thickness
LOAD PAGE			
F_x	0		Body load (force/volume), x dir.
F_y	-rho_smpn*accel		Body load (force/volume), y dir.
DAMPING PAGE			
Damping model	No damping		

4 While still on the **Load** page, click the **Body load is defined as force/volume using the thickness** option button for both subdomains.

5 Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu verify that you the **Plane Strain (smpn)** application mode is still selected.

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

3 Select Boundary 1, and on the **Constraint** page select **Fixed** from the **Constraint condition** list.

4 Click the **Groups** tab, and in the **Name** edit field (under the **Group selection** list) type **Fixed**; then press Enter.

5 Click the **Boundaries** tab.

6 Select Boundaries 5 and 8. From the **Group** list select **Film damping** (click the **Load** tab to see the predefined loads)

7 Click **OK**.

8 From the **Multiphysics** menu choose the **Film Damping (mmfd)** application mode.

9 From the **Physics** menu choose **Boundary Settings**.

10 From the **Boundaries** list select 5 and 8, and from the **Group list** select **Film damping**.

11 In the **Settings** page enter the following boundary settings (some of them are correct initially); when done, click **OK**.

QUANTITY	VALUE ON BOUNDARY 5, 8
dx,dy	`u v`
h_0	`3.95e-6`
P_A	`P_A`
λ_0	`70e-9`
$p_{\lambda, 0}$	`101325`
η	`22.6e-6`
α_v	`1`
Q_{ch}	`Model 1.`
Use perforation effects	No

Point Settings

The default point setting, which sets the film pressure to zero, is sufficient for this model.

COUPLING VARIABLES

To observe the total damping force, create two integration coupling variables with these steps:

1. From the **Options** menu select **Integration Coupling Varaibles>Boundary Variables**.
2. In the dialog that opens define coupling variables (each variable on a separate row) according to the following table; when done, click **OK**.

BOUNDARY	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
5	`force_bot`	`-ny*pf*thickness_smpn`	4	yes
8	`force_top`	`-ny*pf*thickness_smpn`	4	yes

MESH GENERATION

1. From the **Mesh** menu select **Free Mesh Parameters**.
2. Keep the **Predefined mesh sizes** selection **Normal**, then click the **Custom mesh size** button.
3. Set **Resolution of narrow regions** to 2.
4. Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

1. From the **Solve** menu choose **Solver Parameters**.
2. Keep the time-dependent analysis and solver, and make the following changes in the **Solver Parameters** dialog box; when done, click **OK**:

PARAMETER	VALUE
Analysis	Transient
Auto select solver	yes
GENERAL PAGE	
Times	`0:1e-5:4e-3`
TIME STEPPING PAGE	
Time steps taken by the solver	Intermediate

3. Click the **Solve** button on the Main toolbar to start the analysis.

POSTPROCESSING AND VISUALIZATION

1. From the **Postprocessing** menu choose **Plot Parameters**.
2. Click the **Surface** tab.

3 In the **Surface data** area choose **Plane Strain>Total displacement** from the **Predefined quantities** list.

4 Click the **Arrow** tab and select the **Arrow plot** check box.

5 In the **Plot arrows on** list select **Boundaries**. Click the **Boundary Data** tab and select **Film Damping>Pressure load** from the **Predefined quantities** list.

6 Click the **Deform** tab and select the **Deformed shape plot** check box.

7 Click **OK**.

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

9 Select the **Point** page and from the **Point selection** list select Point 7.

10 Select **Plane Strain>y-displacement** from the **Predefined quantities** list.

11 Click **Apply**.

12 Type `force_bot` in the **Expression** edit field.

13 Click **OK**.

If you want to compare the step responses in the same figure window for different pressures, open the **Constants** dialog box and change the value for p_A to `3[Pa]` or `300[Pa]`. Then click the **Solve** button again, and when the solution is ready, open the **Domain Plot Parameters** dialog box. Go to the **General** page and select the **Keep current plot** check box. Following this procedure plots both step responses in the same graph when you click **OK** or **Apply**.

You might also want to animate the step response. To do so:

1 Open the **Plot Parameters** dialog box and click the **Animate** tab.

2 Select **AVI** or **QuickTime** from the **File type** list.

3 Click the **Start Animation** button.

Modeling Using the Graphical User Interface (3D)

Model Library path: `MEMS_Module/Sensor_Models/accelerometer_3d`

Use the following instructions to create the 3D version of the accelerometer model.

MODEL NAVIGATOR

1 Open the **Model Navigator** and select **3D** from the **Space dimension** list.

2 Select the application mode **MEMS Module>Structural Mechanics>Solid, Stress-Strain with Film Damping>Transient analysis**.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the **Constants** dialog box enter these variable names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
accel	9.81[m/s^2]/2	Applied acceleration
P_A	300[Pa]	Ambient gas pressure

GEOMETRY MODELING

1 Open the **Block** dialog box; to do so either go to the **Draw** menu and choose **Block**, or Shift-click the **Block** button on the Draw toolbar on the left side of the user interface.

2 Create these three solid blocks:

NAME	LENGTH			AXIS BASE POINT		
	X	Y	Z	X	Y	Z
BLK1	1780e-6	2960e-6	400e-6	0	0	0
BLK2	520e-6	100e-6	40e-6	-520e-6	200e-6	180e-6
BLK3	520e-6	100e-6	40e-6	-520e-6	2660e-6	180e-6

3 Click the **Zoom Extents** button.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu select the **Solid, Stress-Strain (smsld)** application mode.

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

3 Enter the following subdomain settings values; when done, click **OK**.

QUANTITY	VALUE IN SUBDOMAIN 1–3	DESCRIPTION
MATERIAL PAGE		
Library material	**Silicon**	Click the **Load** button, go to **Materials>Basic Material Properties** and select **Silicon**

QUANTITY	VALUE IN SUBDOMAIN 1–3	DESCRIPTION
E	131e9[N/m^2]	Young's modulus
ν	0.27	Poisson's ratio
α	4.15e-6[1/K]	Coefficient of thermal expansion
ρ	2330[kg/m^3]	Density
LOAD PAGE		
Coordinate system	Global coordinate system	
F_x	0	Body load (force/volume) x dir.
F_y	0	Body load (force/volume) y dir.
F_z	-rho_smsld*accel	Body load (force/volume) z dir.
DAMPING PAGE		
Damping model	No damping	

Boundary Conditions

1. Verify on the **Multiphysics** menu that the **Solid, Stress-Strain (smsld)** application mode is still selected.
2. From the **Physics** menu select **Boundary Settings**.
3. Select Boundaries 1 and 6.
4. On the **Constraint** page select **Fixed** from the **Constraint condition** list.
5. Click the **Group** tab and type **Fixed** in the **Name** edit field, then press Enter.
6. Click the **Boundaries** tab.
7. Select Boundaries 13 and 14, and from the **Group** list select **Film damping**; notice the predefined load on the **Load** page. Click **OK**.
8. From the **Multiphysics** menu select the **Film Damping (mmfd)** application mode.
9. From the **Physics** menu select **Boundary Settings**.
10. Select Boundaries 13 and 14.
11. In the **Group** list select **Film damping**, then enter the settings from the following table (some are correct by default); when done, click **OK**.

QUANTITY	VALUE ON BOUNDARY 13, 14
dx,dy,dz	u v w
h_0	3.95e-6

QUANTITY	VALUE ON BOUNDARY 13, 14
p_A	P_A
λ_0	70e-9
$p_{\lambda, 0}$	101325
η	22.6e-6
α_v	1
Q_{ch}	Model 1.
Use perforation effects	No

Edge Settings

The default edge setting, which sets the film pressure to zero, applies to this model.

COUPLING VARIABLES

To observe the total damping force, create two integration coupling variables according to the following steps.

1. From the **Options** menu select **Integration Coupling Varaibles>Boundary Variables**.
2. In the dialog box that opens, define coupling variables according to the following tables (one coupling variable per row); when done, click **OK**.

BOUNDARY	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
13	force_bot	-nz*pf	4	yes
14	force_top	-nz*pf	4	yes

MESH GENERATION

1. From the **Mesh** menu select **Free Mesh Parameters**.
2. In the **Predefined mesh sizes** list choose **Coarse**.
3. Click **Remesh**.
4. Click **OK**.

COMPUTING THE SOLUTION

1. From the **Solve** menu select **Solver Parameters**.

2 Keep the time dependent analysis and solver, but otherwise make the following changes in the **Solver Parameters** dialog box; when done, click **OK**:

PARAMETER	VALUE
Analysis	Transient
Auto select solver	yes
GENERAL PAGE	
Times	`0:1e-5:4e-3`
TIME STEPPING PAGE	
Times to store in output	Specified times
Time steps taken by the solver	Intermediate

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

POSTPROCESSING AND VISUALIZATION

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

2 In the **Plot type** area clear the **Slice** check box.

3 Click the **Boundary** tab.

4 Select the **Boundary plot** check box.

5 In the **Boundary data** area go to the **Predefined quantities** list and choose **Face load in global z dir**.

6 Click the **Edge** tab.

7 Select the **Edge plot** check box.

8 Click the **Uniform color** option button.

9 Click the **Color** button and select black from the color palette. Click **OK**.

10 Click the **Deform** tab.

11 Select the **Deformed shape** check box.

12 Click **OK**.

Also plot the z-displacement at the bottom corner and the damping force at the bottom versus time:

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

2 Select the **Point** page.

3 From the **Point selection** list choose Point 21.

4 Select **Solid, Stress-Strain>z-displacement** from the **Predefined quantities** list.

5 Click **Apply**.

6 Type **force_bot** in the **Expression** edit field.

7 Click **OK**.

If you want to compare the step responses in same figure for different pressures, go to the **Constant** dialog box and change the value for p_a to `3[Pa]` or `300[Pa]`; then click the **Solve** button again. When the solution is ready and you want to plot both step responses in the same graph, open the **Domain Plot Parameters** dialog box, click the **General** tab, and select the **Keep current plot** check box.

You might also want to animate the step response. To do so:

1 Open the **Plot Parameters** dialog box and click the **Animate** tab.

2 In the **File type** list select your preference of **AVI** or **QuickTime**.

3 Click the **Start Animation** button.

Estimating the Q Factor of a MEMS Gyroscope

A particularly simple type of MEMS gyroscope is a 2-DOF vibrational system with a single proof mass. The complete system with proof mass, support structure, drive and sense units can be fabricated in one piece out of polysilicon. High sensitivity and low power consumption are important design goals. Both are affected by a number of possible dissipative processes where vibrational energy is turned into heat inside the structure or in interaction with its surroundings.

This model focuses on the slide film damping due to air viscosity in the thin air layer between the gyroscope's proof mass and the substrate. The Q factor obtained from this analysis is therefore an upper bound for the considered design. All other processes contribute to the damping work to further decrease the Q factor. Therefore, if the slide film damping can be assumed to be the dominating dissipative process in the system, optimizing the Q value obtained from this simplified model will be a good starting point for improving the design.

The model is inspired by Ref. 1.

Introduction

The working principle of a vibrational gyroscope is surprisingly simple. A proof mass is suspended above a surface in such a way that its first two vibrational modes are orthogonal and tangential to the surface. If one of the modes, from now on referred to as the ***drive mode***, is excited using for example a comb drive unit, any rotation about an out-of-plane axis will induce Coriolis forces, which transfer energy to the other, orthogonal, mode. This induced excitation of the ***sense mode*** can be detected by

measuring capacitance between the proof mass and a pair of sense electrodes. See Figure 3-3.

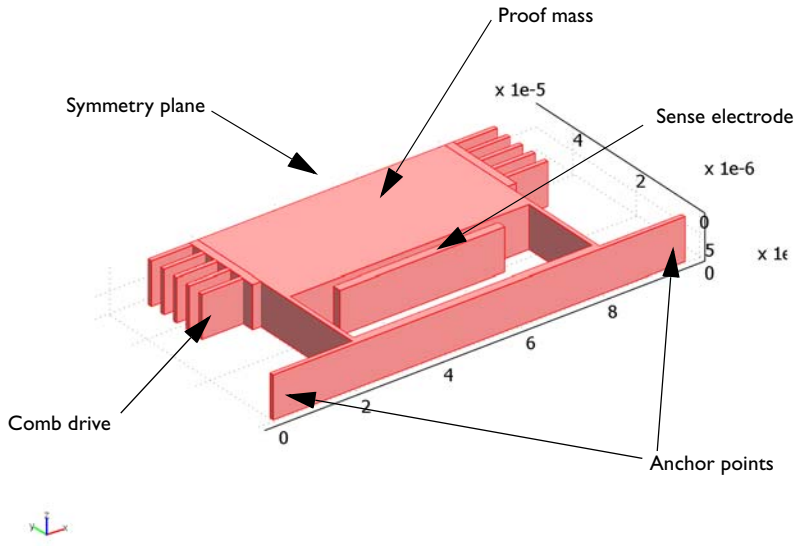


Figure 3-3: Schematic drawing of one half of a generic 2-DOF gyroscope.

Model Definition

To model the vibration in the drive direction, you only need to include one half of the real structure in the geometry. The symmetry boundary condition on the mirror plane saves computation time and memory but also removes any modes oscillating in the sense direction. Therefore, the coupling between the modes cannot be studied and the sense electrodes are excluded from the model.

To simplify further, the model does not include the details of the comb drive. It is assumed that the drive is working in its region of linear response so that the unit can be replaced by a corresponding driving force. Considering the comb drive to act like a stack of idealized plate capacitors leads to the following expression for the total force acting on the drive assembly (Ref. 1):

$$F_{\mathrm{cd}} = 4\frac{\varepsilon_0 z_0 N}{y_0} V_{\mathrm{DC}} V_{\mathrm{AC}} \tag{3-1}$$

Here $\varepsilon_0 = 8.854$ pF/m is the permittivity of free space, $z_0 = 10$ µm the height of the fingers, $y_0 = 4$ µm the distance between neighboring fingers, $N = 10$ the number of fingers, $V_{DC} = 30$ V the bias voltage, and finally $V_{AC} = 2$ V the applied driving voltage.

As mentioned above, all damping processes except slide-film damping between the proof mass and the substrate are excluded from the model. Internal viscous damping in the polysilicon structure can be assumed to be small, as well as thermo-elastic damping in the supporting beams. The slide-film and squeeze-film damping in the comb drives may be considered in a refined model.

This particular gyroscope is intended for use under atmospheric conditions. The 2 µm thick gas film between the proof mass and the substrate is therefore assumed to contain air at atmospheric pressure. The following parameters are relevant for describing the film behavior under these conditions:

SYMBOL	VALUE	DESCRIPTION
h_0	2 µm	Film thickness
p_A	1 atm	Ambient pressure
λ_0	70 nm	Mean free path at 1 atm
η	$18 \cdot 10^{-6}$ Pa·s	Dynamic viscosity

The Q factor is a measure of the ratio between stored energy and energy lost per cycle in a free oscillation. Two possible definitions are

$$Q = \frac{2\pi W_0}{\Delta W} = \frac{\omega_0}{2\delta}$$

where W_0 is the stored vibrational energy, ΔW is the energy lost per cycle, ω_0 is the natural angular frequency, and δ is the damping factor (vibrations decay exponentially with δt). When considering steady-state driven oscillations, the Q factor is commonly defined as the resonance frequency divided by the bandwidth

$$Q = \frac{\omega_0}{\Delta\omega}$$

where the bandwidth $\Delta\omega$ is in turn defined as the half-power width of the spectrum.

To evaluate the Q factor as the ratio between frequency and bandwidth you can, for example, run a frequency sweep with high resolution close to the resonant frequency. Then a standard eigenvalue analysis is a natural starting point. Once you know the eigenfrequency, you can add the slide-film damping and switch to a frequency response analysis for frequencies in the immediate vicinity of the resonance.

It is, however, more efficient and accurate to extract the Q factor using the equivalent definition

$$Q = \frac{\omega_0}{2\delta} = \left|\frac{\text{imag}(\lambda)}{2\,\text{real}(\lambda)}\right|$$

where λ is a complex eigenvalue. The last part of this example illustrates how COMSOL Multiphysics' eigenvalue solver can be applied directly on a model set up for frequency response analysis.

The relation between eigenvalue λ and a complex frequency *f* is

$$\lambda = i\omega = 2\pi i f \;\Leftrightarrow\; f = \frac{\lambda}{2\pi i}$$

where ω is the angular frequency. This expression for the frequency can be inserted directly into the frequency response equations. The eigenvalue solver provides the damped eigenvalue in one step when the system of equations is a quadratic polynomial in the angular frequency, otherwise a few steps of fix-point iteration is usually enough to reach convergence.

Results and Discussion

The drive direction resonance is found to be close to 433 kHz. Since the mesh resolution is rather low, the eigenfrequency may depend somewhat on the details of the mesh. Running a frequency sweep of a ±1 kHz interval around the obtained resonance frequency and plotting the square of the proof mass velocity gives you

Figure 3-4. Carefully measuring the half-height width of the peak leads to an estimated $Q \approx 8000$.

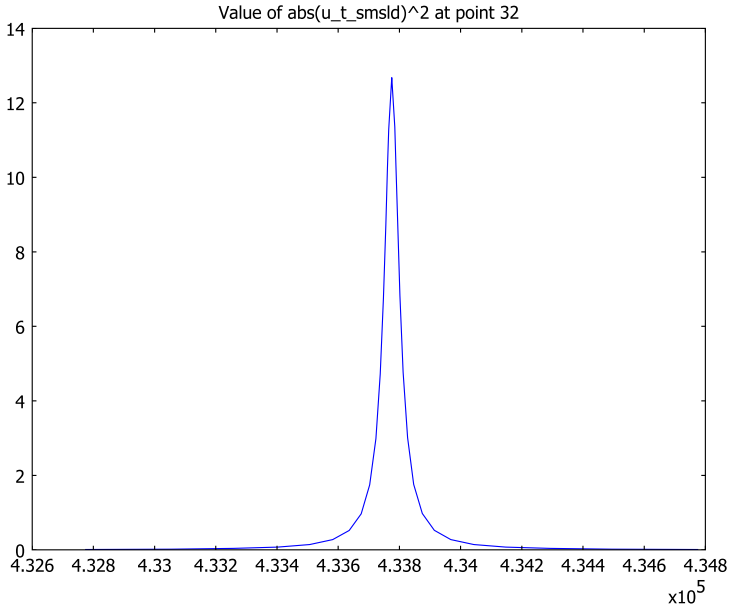


Figure 3-4: The drive mode resonance peak is very sharp despite the added slide-film damping. The Q value obtained from measuring the width at half power is therefore not very accurate.

The Q value obtained from measuring the bandwidth agrees well with the value given by the simple formula (Ref. 2)

$$Q = \frac{\omega m h_0}{\eta A} \tag{3-2}$$

Inserting the angular frequency at resonance $\omega = 2.73 \cdot 10^6$ rad/s, proof mass $m = 3.9 \cdot 10^{-11}$ kg, gap height $h_0 = 2$ µm, dynamic viscosity $\eta = 18 \cdot 10^{-6}$ Pa·s, and slide film area $A = 1.68 \cdot 10^{-9}$ m^2, gives an estimated $Q = 7030$. This formula does not account for the breakdown of the continuum assumption at small scales, and will therefore underestimate the Q value.

Using the eigenvalue solver to extract the desired value instead gives $Q = 7524$, which is also well in agreement with both the previous estimates. In fact, considering the many simplifications in the present model, the value obtained from Equation 3-2 is for most practical purposes good enough. When other dissipative processes are added, or

the geometry is made more complex, the numerical modeling technique illustrated here will be justified, though.

References

1. C. Acar, *Robust Micromachined Vibratory Gyroscopes*, Ph.D. thesis, Univ. of California, Irvine, 2004

2. M. Bao, *Analysis and Design Principles of MEMS Devices*, ch. 3, Elsevier, 2005.

Modeling in COMSOL Multiphysics

The Solid, Stress-Strain with Film Damping predefined Multiphysics coupling by default solves for both the structural displacements and the pressure in the air film between the proof mass and the substrate. The tangential velocity $\mathbf{u}_T$ given by Navier's equation in the solid are inserted into the modified Reynolds equation describing the film pressure, p_F, on the slide-film boundary:

$$\nabla_T \cdot (h_0{}^3 Q_{\mathrm{ch}} p \nabla_T p_F - 6\eta h_0 \mathbf{u}_T) = 12 j\omega\eta h_0 p_F$$

Here, the gap width h_0, relative flow rate function Q_{ch}, and viscosity η are taken to be constant, and ∇_T represents differentiation in the tangential direction. The slide film in return applies a stress

$$F = -\eta \frac{\mathbf{u}_T}{h_0(1 + 2K_{\mathrm{s}})} - \frac{h_0 \nabla_T p_F}{2}$$

on the structure, where K_{s} is the scaled Knudsen number. In the present situation, where the sliding surfaces are parallel, the contribution from the pressure in the second term is very small. Therefore, you can actually save some computation time without sacrificing much accuracy by simply switching off the film pressure variable during solving.

As a first step, the undamped vibrational modes of the gyroscope are found with only the Solid, Stress-Strain application mode active. Adding slide-film damping does not change the natural frequency perceptibly, so when measuring the half-power width of the resonance peak, you can safely restrict the frequency sweep to a very narrow band around the first pure structural eigenfrequency. Finally, the eigenvalue solver lets you find the same result in a more convenient way.

Model Library path: `MEMS_Module/Sensor_Models/mems_gyroscope`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Select **3D** from the **Space dimension** list.

2 Expand the predefined Multiphysics node **MEMS Module>Structural Mechanics>Solid, Stress-Strain with Film Damping** and select **Frequency response analysis**.

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

OPTIONS AND SETTINGS

1 Open the **Constants** dialog box from the **Options** menu, and enter the following constants.

NAME	EXPRESSION	DESCRIPTION
e0	8.854e-12[F/m]	permittivity of free space
z0	10e-6[m]	structure thickness
y0	4e-6[m]	distance between fingers
N	10	number of comb fingers
V_dc	30[V]	bias voltage
V_ac	2[V]	drive voltage
F_cd	4*e0*z0*N*V_dc*V_ac/y0	comb drive force
A_cd	40e-6*10e-6[m^2]	comb drive area

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

GEOMETRY MODELING

1 The somewhat idealized geometry is built entirely from blocks. First, use the **Block** button on the Draw toolbar repeatedly to create four blocks with the following dimensions and positions:

LENGTH			AXIS BASE POINT		
X	Y	Z	X	Y	Z
100e-6	50e-6	10e-6	0	0	0
20e-6	49e-6	10e-6	0	1e-6	0
20e-6	49e-6	10e-6	80e-6	1e-6	0
58e-6	20e-6	10e-6	21e-6	2e-6	0

2 Press Ctrl+A to select all objects and click the **Difference** button on the Main toolbar.

3 Add two more blocks to represent the simplified comb drives:

LENGTH			AXIS BASE POINT		
X	Y	Z	X	Y	Z
2e-6	20e-6	10e-6	18e-6	30e-6	0
2e-6	20e-6	10e-6	80e-6	30e-6	0

4 Click the **Zoom Extents** button on the main toolbar to fit the geometry to your screen.

PHYSICS SETTINGS

Subdomain Settings

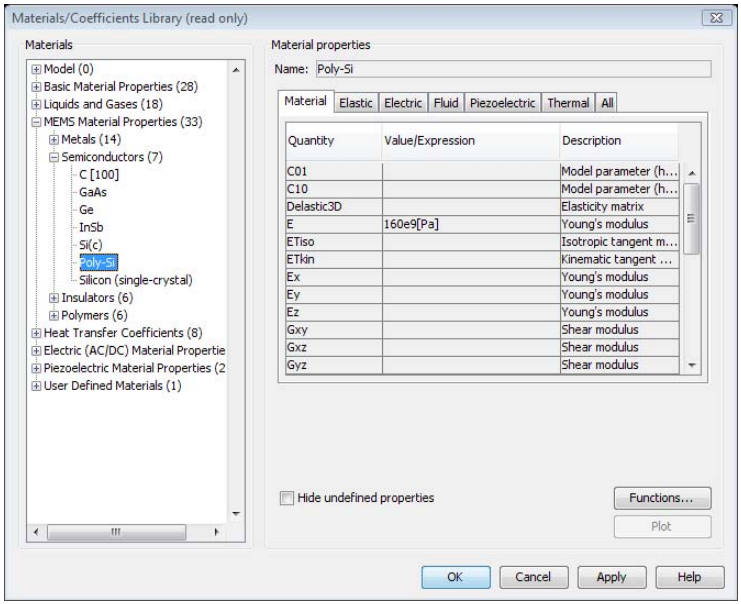
The gyroscope structure is made entirely of polycrystalline silicon, which shows negligible internal viscous damping at these scales. Poly-Si is a standard material that can be found in the MEMS Material Library.

1 Select the **Solid, Stress-Strain** application mode from the **Model Tree**.

2 Open the **Subdomain Settings** dialog box by clicking in the **Model Tree** or choosing **Subdomain Settings** from the **Physics** menu.

3 Select all three subdomains in the list and click the **Load** button.

4 In the **Materials/Coefficients Library**, select **MEMS Material Properties>Semiconductors>Poly-Si**.



5 Click **OK** to close the dialog box and return to **Subdomain Settings**.

6 Click the **Damping** tab and disable structural damping by selecting **No damping** from the **Damping model** drop-down list.

Cubic Lagrange elements can be used to somewhat compensate for the fact that it is difficult to create a mesh with more than one element across the thickness of the thin support beams. In fact, third-order elements in general give considerably better accuracy in relation to the number of degrees of freedom when applied to bending of thin structures compared to the default second-order elements.

7 Click the **Element** tab, then choose **Lagrange - Cubic** from the **Predefined elements** list.

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

Boundary Conditions—Solid, Stress-Strain

The first step in the analysis is to find the frequency of the drive-direction resonance. For that purpose, it is enough to solve the pure, undamped structural eigenvalue problem. The Film Damping application mode is by default disabled on all boundaries. Therefore, it is enough, for now, to set appropriate constraints on the structure.

1 Open the **Boundary Settings** dialog box for the **Solid, Stress-Strain** application mode.

2 Select Boundaries 1 and 26, which represent anchor points, and select **Fixed** from the **Constraint condition** list.

3 Select Boundaries 10, 13, and 24 (the mirror plane boundaries) and set the **Constraint condition** to **Symmetry plane**.

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

MESH GENERATION

1 While still in Boundary mode, select the top surface Boundaries 4, 9, and 23 and click the **Interactive Meshing** button on the Mesh toolbar.

2 Then click the **Decrease Mesh Size** button once to decrease the mesh size from Normal to Fine.

3 Mesh the selected surfaces by clicking the **Mesh Selected (Free)** button.

4 Choose **Swept Mesh Parameters** from the **Mesh** menu.

5 Select all subdomains in the **Subdomain selection** list and select the **Manual specification of element layers** check box.

6 Enter 1 in the **Number of element layers** edit field.

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

8 To create the final mesh, click the **Mesh Remaining (Swept)** button on the Mesh toolbar.

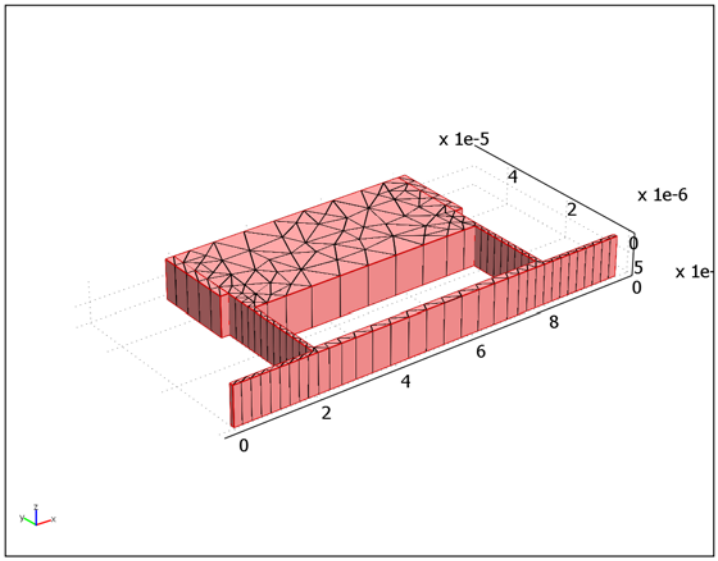


Figure 3-5: The swept mesh is rather coarse, but the use of cubic shape functions ensures that the accuracy is sufficient.

COMPUTING THE SOLUTION

As a preliminary step, before evaluating the Q factor, use the eigenvalue solver to find the first few resonance frequencies of the structure.

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

2 Select **Eigenfrequency** from the **Analysis** list, then click **OK**.

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

POSTPROCESSING AND VISUALIZATION

The default plot shows the von Mises stress on a number of cross sections. A deform plot makes it easier to classify the different eigenmodes.

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

2 In the **Plot type** frame, clear the **Slice** check box and select the **Boundary** and **Deformed shape** check boxes.

3 Click **OK** to display the shape of the first eigenmode.

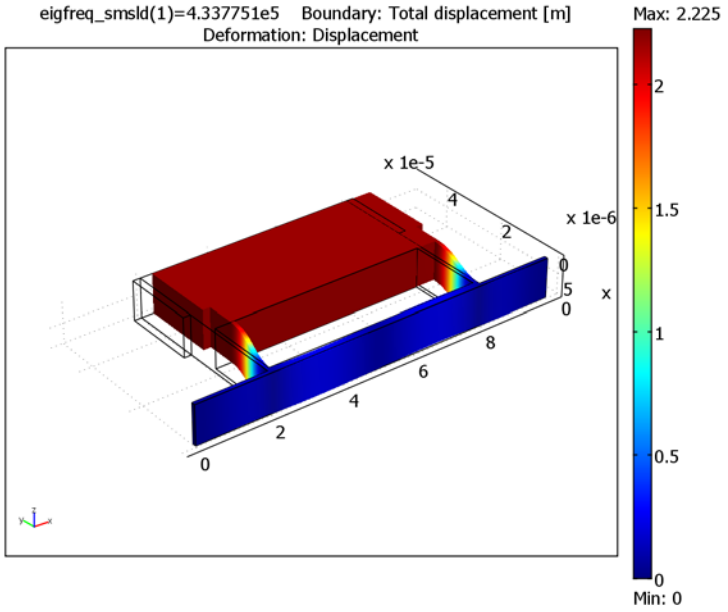


Figure 3-6: The first eigenmode shows the proof mass oscillating in the drive direction with a frequency of about 433 kHz.Due to the limited mesh resolution, the exact frequency obtained might vary slightly.

PHYSICS SETTINGS

Now, knowing the resonance frequency of the drive mode, it is time to apply the comb drive forcing according to Equation 3-1 and activate the slide-film damping.

Boundary Conditions—Solid, Stress-Strain

1 Open the **Boundary Settings** dialog box for the Solid, Stress-Strain application mode again.

2 On the **Load** page, select Boundaries 6 and 25. Apply the driving force on these boundaries by entering the distributed load `F_cd/A_cd` in the $\mathbf{F_x}$ edit field.

3 Select the lower surface of the model, consisting of Boundaries 3, 8, and 22, and choose **Film damping** from the **Group** list.

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

Boundary Conditions—Film Damping

1 Locate **Geom1>Film Damping>Boundary Settings** in the **Model Tree** and double-click the node.

2 Make sure the slide-film boundaries (Boundaries 3, 8, and 22) are still selected and choose **Film damping** from the **Group** list.

3 Change the **Gas film settings** according to the following table:

PROPERTY	VALUE
Damping type	Slide film
h_0	`2e-6[m]`
p_A	`1[atm]`
λ_0	`70[nm]`
$\mathbf{p}_{\lambda, 0}$	`1[atm]`
η	`18e-6[Pa*s]`
Q_{ch}	Slip

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

Edge Settings—Film Damping

1 Open the **Edge Settings** dialog box, either from the **Physics** menu or by clicking in the **Model Tree**.

2 Select Edges 15, 24, and 49, which are part of the symmetry plane, and choose **Closed/Symmetry** as **End condition**.

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

COMPUTING THE SOLUTION

Above, the eigenvalue solver was used to calculate the resonance frequency of the drive mode. Next, apply the parametric solver to obtain the frequency response of the damped model for frequencies in the immediate neighborhood of the known resonance. With a clever choice of frequency steps, you can resolve the resonance peak accurately without having to use a short sampling interval everywhere. For example using

```
sort([433775 433775-logspace(1,3,15) 433775+logspace(1,3,15)])
```

gives you a sorted frequency list, as expected by the solver, which resolves the neighborhood of 433775 Hz.

The damping in the model is rather weak, with an estimated Q factor close to 8000. The expected band width of the resonance peak is then less than 100 Hz, which is less than the errors caused by the rather coarse mesh. Small differences between meshes created on different hardware platforms can potentially move the peak more than its

bandwidth. Therefore it may be necessary to modify the suggested parameter list to reflect the actual resonance frequency found in the first solution step.

Solver Settings

1. Open the **Solver Parameters** dialog box.
2. Select **Frequency response** from the **Analysis type** list, which both modifies the implementation of the structural equations and switches to the **Parametric** solver.

   Note that the Film Damping application mode is already set to the Frequency response analysis type because it was started in that mode. The **Analysis type** list in the **Solver Parameters** dialog box only affects the *ruling application mode*, which in this case is the Solid, Stress-Strain application mode.
3. Enter `freq` as **Parameter name**. This defines the variable freq, which will be used below.
4. In the **Parameter values** edit field, enter

   `sort([433775 433775-logspace(1,3,15) 433775+logspace(1,3,15)])`.
5. Click **OK** to close the **Solver Parameters** dialog box.

Scalar Variables

Both application modes are now set to the Frequency response analysis type, which means that they describe harmonic motion at a fixed frequency. You must specify this frequency for both modes:

1. Choose **Scalar Variables** from the **Physics** menu.
2. In the **Application Scalar Variables** dialog box, set both variables described as **Excitation frequency** to `freq[Hz]`.
3. Click **OK** to accept the changes and close the dialog box.

Probe Plot

When working with the parametric solver, it is often convenient to set up a probe plot that lets you check your results as they are produced. In this model, the quantity of interest is the vibrational energy at steady state for each frequency. Looking at the shape of the drive mode, it is obvious that the vibrational energy will be very nearly proportional to the square of the proof mass's peak velocity, which is constant throughout the proof mass.

1. Choose **Probe Plot Parameters** from the **Postprocessing** menu.
2. In the dialog box, click **New**.
3. Select **Point probe** from the **Plot type** list, then click **OK** to create the new probe plot.

4 Select Point 32 and change the **Expression** field to `abs(u_t_smsld)^2`.

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

Solving the Model

Click the **Solve** button on the Main toolbar to compute the frequency sweep.

As the sweep progresses, the probe plot appears in the **Progress** window, showing a distinct peak in the vibrational energy curve. When the solving stage finishes, the resulting plot is automatically copied to a separate figure window. The curve should be similar to that in Figure 3-4 on page 165.

POSTPROCESSING AND VISUALIZATION

The Q factor can be estimated directly from the probe plot by measuring the width of the resonance peak at half its maximum value and dividing the resonance frequency by the measured bandwidth. This, however, gives you a very rough estimate.

It is possible to use the **Point Evaluation** dialog box to manually look for the frequencies that give values for the squared velocity at Point 32 close to half the peak value. Using some back-of-the-envelope interpolation you can conclude that the Q factor must lie somewhere close to 8000, not far from what is predicted by Equation 3-2. This result serves to verify that the frequency response model is likely to be correct. With a working frequency response model and knowledge about what the drive mode looks like, you can proceed to the final step.

COMPUTING THE SOLUTION

The slide-film damping application mode does not explicitly support the eigenvalue analysis type to calculate damped eigenvalue solutions. Instead, you can do an eigenvalue analysis of the equations solved above for frequency response just by switching solver and rewriting the frequency in terms of the eigenvalue variable `lambda`.

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

2 Select **Eigenvalue** from the **Solver** list, then click **OK**.

3 Choose **Scalar Variables** from the **Physics** menu.

4 In the **Application Scalar Variables** dialog box, set the **Excitation frequency** for both application modes to `lambda/(2*pi*i)`.

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

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

POSTPROCESSING AND VISUALIZATION

Solving a damped eigenvalue problem like this gives you a number of complex eigenvalues which do not necessarily show up in the same order as for the lossless model. Your first task is therefore to locate the drive mode. If the displayed plot does not already look like Figure 3-6 on page 172, do the following:

1. Open the **Plot Parameters** dialog box, by choosing it from the **Postprocessing** menu or clicking the corresponding button on the Main toolbar.
2. Because $\lambda = 2\pi if$, search the **Eigenvalue** list on the **General** page for an eigenvalue with imaginary part close to $2.7 \cdot 10^6$. There should be two, one with positive and one with negative imaginary part.
3. Click **Apply** and check the plot to verify that you have indeed found the drive mode.
4. Click **OK** or **Cancel** to close the dialog box.

   Finally, proceed to evaluate the Q factor as half the ratio between imaginary and real part of the eigenvalue:

5. Choose **Data Display>Global** from the **Post** menu.
6. Enter `abs(imag(lambda)/real(lambda)/2)` in the **Expression** field and select the drive mode from the **Eigenvalue** list.
7. Click **OK** to close the dialog box and display the final result in the message log.

Piezoresistive Elevator Button

Introduction

This is a simplified model of a design of a piezoresistive in-wall elevator button described in a patent application submitted by C.J. Slabinski and R.B. Leach (Ref. 5). The elevator button is designed with the following requirements in mind:

- durability with respect to high temperatures
- capability of producing signals that can be easily used in digital signal processing
- reliability, even when subjected to high loads

With respect to each of these requested characteristics, piezoresistive devices are superior to piezoelectrical ones. To make the device resistant against fire and heat, the button assembly includes parts of materials that are unresponsive to heat, such as clay or brick.

Piezoresistive materials change their resisitivity when subjected to mechanical stresses. This model concentrates on piezoresistivity in silicon-type materials, which is the most important group for practical applications. Although the effect is also observed in metals with crystal structures different from silicon, the piezoresistive effect is more than an order of magnitude higher in silicon than in metals (Ref. 1).

Note: This Model requires the MEMS module and the AC/DC Module.

Figure 3-7 shows the simplified elevator-button design that you use in this model.

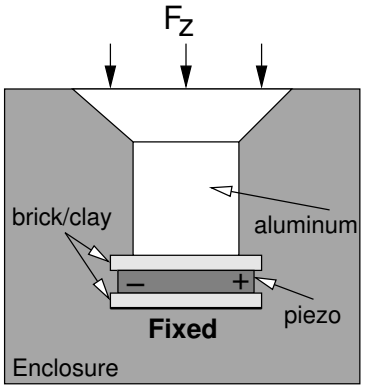


Figure 3-7: Schematic elevator button design.

The button is embedded in an enclosure formed by the elevator control panel. Its operation is modeled by a force, F_z, which acts on the button's upper boundary. The upper part of the button, composed of a conical and a cylindrical part, is made of aluminum. The conical shape ensures that the inner button parts are protected if the button is subjected to high impacts.

Furthermore, as mentioned in the introduction, it is vital that the button functions perfectly even at high ambient temperatures, such as in the event of fire. To shield the piezoresitive silicon layer, an adhesive, made of clay or brick, is attached to the resisitive layer's upper and lower sides.

To implement the button in COMSOL Multiphysics, you need two application modes:

- Solid, Stress-Strain, active in the whole geometry of the device
- Electric Currents, which is only active in the sensing resistor domain

To measure the change in the resistivity, a fixed voltage of 1 V is applied across the silicon layer. The integral of the current density over one of the resistor's contacts gives the ohmic resistance via Ohm's law, $U = RI$.

PIEZORESISTIVITY FOR AN ANISOTROPIC CRYSTAL

Below follows a short outline of the piezoresistive relations (Ref. 1). For a 3-dimensional anisotropic crystal, the electric field is related to the current-density

field by a 3-by-3 resistivity tensor. In piezo crystals, the nine components always reduce to six values arranged in a symmetric tensor:

$$\begin{bmatrix} E_1 \\ E_1 \\ E_1 \end{bmatrix} = \begin{bmatrix} \rho_1 & \rho_6 & \rho_5 \\ \rho_6 & \rho_2 & \rho_4 \\ \rho_5 & \rho_4 & \rho_3 \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ I_3 \end{bmatrix} \tag{3-3}$$

For the cubic silicon lattice—with axes aligned with the <100> axes—ρ_1, ρ_2, and ρ_3 define the dependence of the electric field on the current along the same orthogonal directions; the other components are the cross terms.

The six resistivity components depend on the normal and shear stresses in the material (Ref. 2). Under stress-free conditions and with Cartesian coordinates aligned with the material <100> axes, the normal resistivity components are equal, and the cross terms are zero. Thus, under these conditions, the resistivity tensor is isotropic:

$$\rho_{3\text{-by-}3} = \rho_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3-4}$$

The relative changes in the resistivity can be written as a product of the structural stresses, σ, and the piezoresistive stress coefficients, Π. In Voigt notation, this reads:

$$\frac{1}{\rho_0} \begin{bmatrix} \Delta\rho_1 \\ \Delta\rho_2 \\ \Delta\rho_3 \\ \Delta\rho_4 \\ \Delta\rho_5 \\ \Delta\rho_6 \end{bmatrix} = \begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{12} & \pi_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{44} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{bmatrix} \tag{3-5}$$

The following table lists the correspondences between the element indices or positions in Equation 3-5 and the tensor components along the spatial coordinate axes:

Π MATRIX		RESISTIVITY		SHEAR STRESS		Π MATRIX
RC	*xy*	*i*	*xy*	*i*	*xy*	RC
12	xy	ρ_6	ρ_{xy}	τ_3	τ_{xy}	66
13	xz	ρ_5	ρ_{xz}	τ_2	τ_{xz}	55
23	yz	ρ_4	ρ_{yz}	τ_1	τ_{yz}	44

Here, “R” and “C” stand for row and column position, respectively.

When modeling electric currents in conductive media, conductivity is used instead of resistivity. The anisotropic conductivity matrix corresponding to the resistivity matrix results from a simple inversion of the resistivity matrix.

Coordinate Transformations

To get a nice representation of the material parameters, it is common in piezoelectricity and piezoresistivity to rotate the coordinate system by 45° around the z-axis, so that the coordinate system aligns with the <110> directions for the crystal axes. The drawback of this representation is that the Cartesian axes (for which the stresses are defined) are aligned along the material <100> axes, in contrast to the representation used in structural mechanics (standard global coordinate system). Therefore, a local coordinate system is introduced for computing the resisitivity coefficients.

When you create and use a local coordinate system in COMSOL Multiphysics, you get an orthogonal 3-by-3 transformation matrix T, whose components appear as `coord`*`n`*`_T`*`ij`* variables in the equations. This matrix represents a transformation from local to global coordinates. The transformation of stresses from global to local coordinates is

$$\sigma_l = T^{\mathrm{T}} \begin{bmatrix} \sigma_x & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_y & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_z \end{bmatrix} T$$

Use these stress components in the local representation to calculate the resistivity matrix, and then transform the resistivity matrix to global coordinates using the inverse transformation

$$\rho_g = T \begin{bmatrix} \rho_1 & \rho_6 & \rho_5 \\ \rho_6 & \rho_2 & \rho_4 \\ \rho_5 & \rho_4 & \rho_3 \end{bmatrix} T^{\mathrm{T}} = T \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{bmatrix} T^{\mathrm{T}}$$

Finally, invert this matrix and use the conductivity values in the conductive-media equation.

MATERIAL PROPERTIES

Table 3-1 lists the elastic properties for the materials used in the different button components. For aluminum and brick, you can use the basic material properties library included with COMSOL Multiphysics, whereas you enter the properties for the piezo

element manually. The thermal expansion coefficients, α, are included in the table to simplify generalizing the model to take heat effects into account.

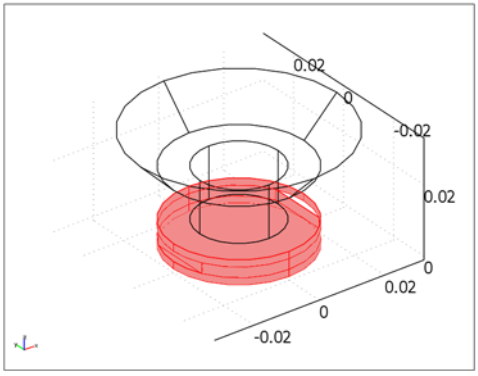
TABLE 3-1: ELASTIC MATERIAL PROPERTIES

PROPERTY	ALUMINUM	BRICK	PIEZO ELEMENT	DESCRIPTION
E (GPa)	70	17	169	Young's modulus
ν	0.33	0.3	0.278	Poisson's ratio
ρ (kg/m^3)	2700	2000	7850	Density
α (1/K)	$23 \cdot 10^{-6}$	$6 \cdot 10^{-6}$	$12 \cdot 10^{-6}$	Thermal expansion coefficient

BOUNDARY CONDITIONS

Solid, Stress-Strain—Constraints

Apply roller constraints to the boundaries highlighted in the figure below. Consider all other boundaries to be unconstrained.



Boundaries for which roller constraints apply.

Solid, Stress-Strain—Loads

On the top button surface, apply a homogeneous downward pressure of 1 kPa, corresponding to a total force of roughly 2.8 N.

Electric Currents

Apply a voltage of 1 V between the electrodes. All other boundaries are electrically insulating.

Results

Figure 3-8 displays the displacement of the boundary when full pressure is applied to the top button surface. The very small displacement values show that the button does not need to move for a signal to be generated.

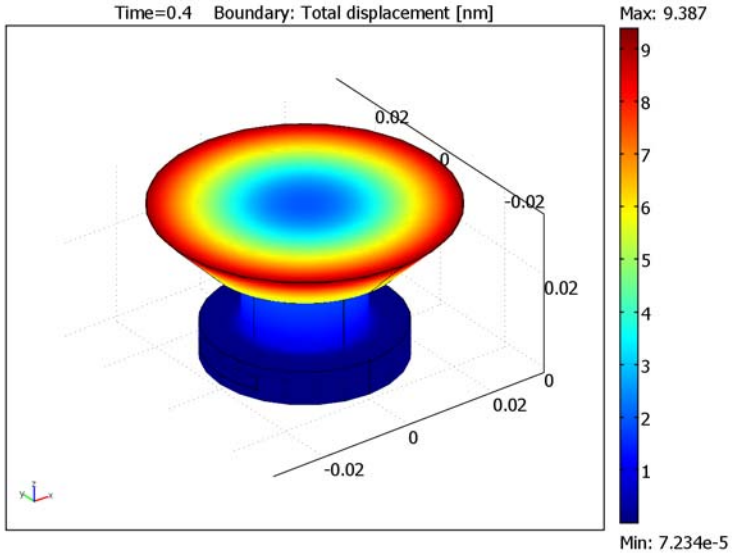


Figure 3-8: Total displacement of the button's boundary surfaces when a uniform downward pressure is applied on the top surface. The values of the displacement are so small that button movement is imperceptible.

Figure 3-9 shows the applied force and the current response as functions of time.

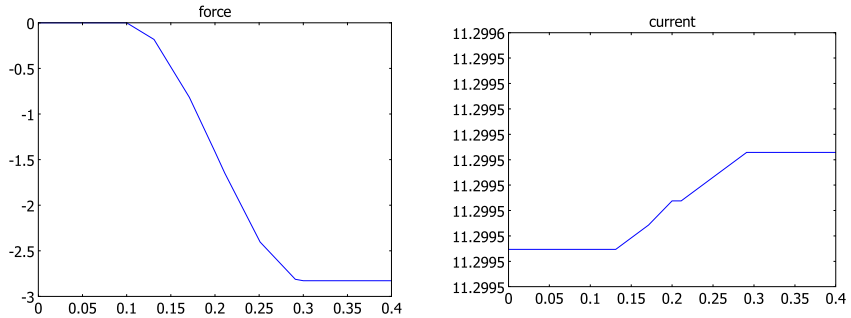


Figure 3-9: Applied force (left) and current response (right) as functions of time.

Because of the very small amplitude of the current signal, it is useful to plot $I - I_0$, where I_0 denotes the current in the absence of a load. Figure 3-10 shows this quantity as a function of time.

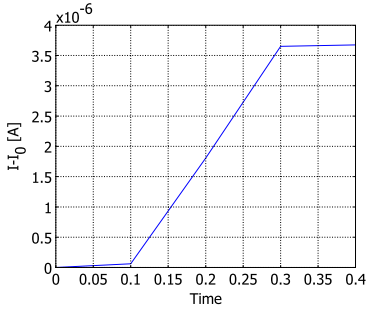


Figure 3-10: Differential current response.

From Figure 3-10 and the plot in the right panel of Figure 3-9 you can read off a signal-to-bias ratio of less than 10^{-6}. To allow the signal to be detected, the noise level needs to be even smaller than this. Thus, the simplified model of this example merely illustrates a possible application of piezoresistivity. The design must be refined and accompanied by the appropriate electronic circuitry to be technically viable.

References

1. *The MEMS Handbook*, ch. 16.4.2.5. Piezoresistivity in Silicon.

2. *The MEMS Handbook*, ch. 25.2. Piezoresistive Pressure Sensors.

3. COMSOL Model Database, id 724. Modeling Piezoresistivity.

4. C.S. Smith, "Piezoresistance Effect in Germanium and Silicon," *Phys. Rev.*, vol. 94, pp. 42–49, 1954.

5. C.J. Slabinski and R.B. Leach, United States Patent, patent no. 5,040,640, patent date Aug. 20, 1991.

Model Library path: `MEMS_Module/Sensor_Models/elevator_button`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 From the **Space dimension** list, select **3D**.

2 Select the application mode **MEMS Module>Solid, Stress-Strain>Quasi-static analysis**.

3 Click **Multiphysics**, then click **Add**.

4 Select the **AC/DC Module>Quasi-Statics, Electric>Electric Currents>Transient analysis** application mode

5 Click **Add**, then click **OK**.

OPTIONS AND SETTINGS

Constants

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

2 On separate rows in the dialog-box table, enter the resistivity and piezoresistive stress tensor components listed in the following table. Alternatively, click the **Import Variables From File** button, browse to the folder `MEMS_Module/Sensor_Models` in the Model Library root directory, select the file `elevator_button_const.txt`, and click **Open**.

NAME	EXPRESSION	DESCRIPTION
rho0	180e-6[ohm*m]	Resistivity of the unstressed material
p11	6.6e-11[1/Pa]	Piezoresistive stress coefficient component
p12	-1.1e-11[1/Pa]	Piezoresistive stress coefficient component
p44	138.1e-11[1/Pa]	Piezoresistive stress coefficient component
P11, P22, P33	p11	Piezoresistive stress coefficient matrix component

NAME	EXPRESSION	DESCRIPTION
P12, P13, P21, P23, P31, P32	p12	Piezoresistive stress coefficient matrix component
P44, P55, P66	p44	Piezoresistive stress coefficient matrix component

Coordinate Systems

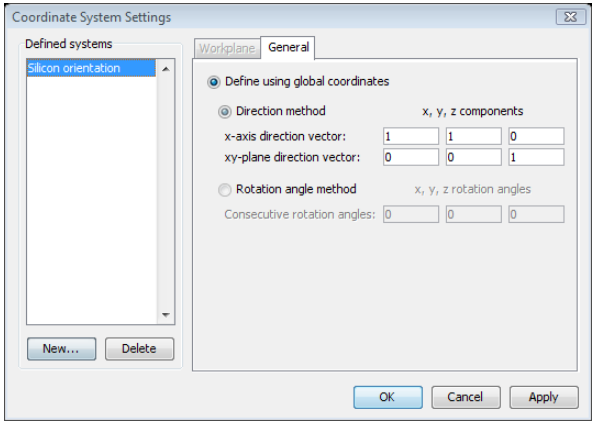
Because the piezoresistive coefficients are given in local coordinates, you must transform them to the standard global coordinate system used in the Solid, Stress-Strain application mode. Define the local coordinate system as follows:

1 From the **Options** menu, choose **Coordinate Systems**.

2 Click the **New** button. In the **Name** edit field, type `Silicon orientation`, then click **OK**.

3 Back in the **Coordinate System Settings** dialog box, enter the following settings on the **General** page:

SETTINGS	X	Y	Z
x-axis direction vector	1	1	0
xy-plane direction vector	0	0	1



4 Click **OK**.

Scalar Expressions

Next, add the stress-dependent resistivity and conductivity components in local and global coordinates defined in Table 3-2 through Table 3-5. You can either enter them

manually in the **Scalar Expressions** dialog box or, more conveniently, load them directly from a data file included with the MEMS Module.

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

2 Enter the stress, resistivity, and conductivity components listed in the following tables or (preferably) click the **Import Variables From File** button, browse to the folder `MEMS_Module/Sensor_Models` in the Model Library root directory, select the file `elevator_button_expr.txt`, and click **Open**.

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

TABLE 3-2: MATERIAL STRESS IN LOCAL COORDINATES

NAME	EXPRESSION
sxl	sxl_smsld
syl	syl_smsld
szl	szl_smsld
sxzl	sxzl_smsld
syzl	syzl_smsld
sxyl	sxyl_smsld

TABLE 3-3: RELATIVE RESISTIVITY (RHO/RHO0) IN LOCAL COORDINATES

NAME	EXPRESSION
rhol11	1+P11*sxl+P12*syl+P13*szl
rhol22	1+P21*sxl+P22*syl+P23*szl
rhol33	1+P31*sxl+P32*syl+P33*szl
rhol23	P44*syzl
rhol13	P55*sxzl
rhol12	P66*sxyl

TABLE 3-4: RELATIVE RESISTIVITY IN GLOBAL COORDINATES

NAME	EXPRESSION
rho11	coord1_T11*(rhol11*coord1_T11+rhol12*coord1_T12+ rhol13*coord1_T13)+coord1_T12*(rhol12*coord1_T11+ rhol22*coord1_T12+rhol23*coord1_T13)+coord1_T13* (rhol13*coord1_T11+rhol23*coord1_T12+rhol33*coord1_T13)
rho22	coord1_T21*(rhol11*coord1_T21+rhol12*coord1_T22+ rhol13*coord1_T23)+coord1_T22*(rhol12*coord1_T21+ rhol22*coord1_T22+rhol23*coord1_T23)+coord1_T23* (rhol13*coord1_T21+rhol23*coord1_T22+rhol33*coord1_T23)

TABLE 3-4: RELATIVE RESISTIVITY IN GLOBAL COORDINATES

NAME	EXPRESSION
rho33	coord1_T31*(rho11*coord1_T31+rho12*coord1_T32+ rho13*coord1_T33)+coord1_T32*(rho12*coord1_T31+ rho22*coord1_T32+rho23*coord1_T33)+coord1_T33* (rho13*coord1_T31+rho23*coord1_T32+rho33*coord1_T33)
rho12	coord1_T11*(rho11*coord1_T21+rho12*coord1_T22+ rho13*coord1_T23)+coord1_T12*(rho12*coord1_T21+ rho22*coord1_T22+rho23*coord1_T23)+coord1_T13* (rho13*coord1_T21+rho23*coord1_T22+rho33*coord1_T23)
rho23	coord1_T21*(rho11*coord1_T31+rho12*coord1_T32+ rho13*coord1_T33)+coord1_T22*(rho12*coord1_T31+ rho22*coord1_T32+rho23*coord1_T33)+coord1_T23* (rho13*coord1_T31+rho23*coord1_T32+rho33*coord1_T33)
rho13	coord1_T11*(rho11*coord1_T31+rho12*coord1_T32+ rho13*coord1_T33)+coord1_T12*(rho12*coord1_T31+ rho22*coord1_T32+rho23*coord1_T33)+coord1_T13* (rho13*coord1_T31+rho23*coord1_T32+rho33*coord1_T33)

TABLE 3-5: CONDUCTIVITY

NAME	EXPRESSION
det_rho	rho11*rho22*rho33+2*rho12*rho23*rho13-rho13^2*rho22- rho12^2*rho33-rho11*rho23^2
sigma11	(rho22*rho33-rho23^2)/(rho0*det_rho)
sigma22	(rho11*rho33-rho13^2)/(rho0*det_rho)
sigma33	(rho11*rho22-rho12^2)/(rho0*det_rho)
sigma12	(rho13*rho23-rho12*rho33)/(rho0*det_rho)
sigma13	(rho12*rho23-rho13*rho22)/(rho0*det_rho)
sigma23	(rho12*rho13-rho11*rho23)/(rho0*det_rho)

GEOMETRY MODELING

1 Click the **Cylinder** button on the Draw toolbar. Create a cylinder with **Radius** `0.02`, **Height** `0.002`, and the **Axis base point** at (`0`, `0`, `0`). Click **OK** to close the dialog box.

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

3 Repeat this procedure for three more cylinders with the following values:

NAME	RADIUS	HEIGHT	AXIS BASE POINT
CYL2	`2e-2`	`3e-3`	`(0,0,2e-3)`

NAME	RADIUS	HEIGHT	AXIS BASE POINT
CYL3	2e-2	2e-3	(0,0,5e-3)
CYL4	12e-3	15e-3	(0,0,7e-3)

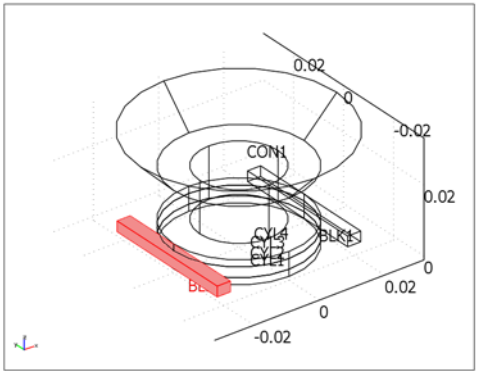
4 Click the **Cone** button on the Draw toolbar and specify the following parameters:

PARAMETER	VALUE
Axis base point	(0,0,3.2e-2)
Radius	3e-2
Height	1e-2
Semi-angle	45
Axis direction vector	(0,0,-1)

5 Click the **Block** button on the Draw toolbar. In the **Base** area, click **Center**. Set the **Axis base point** to (0.02, 0, 0.0035) and the **Length** to (0.004, 0.04, 0.003). Click **OK** to close the dialog box and create the block BLK1.

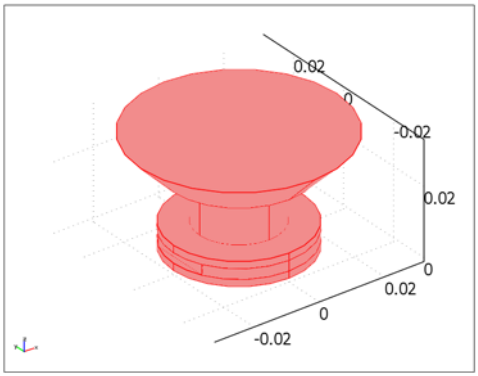
6 Select BLK1 and create a second block, BLK2, by pressing first Ctrl+C and then Ctrl+V. In the **Paste** dialog box, to specify the **Displacements** (-0.04, 0, 0). Click **OK**.

The geometry in the drawing area should now look like that in the following figure.



7 From the **Draw** menu, choose **Create Composite Object**. In the **Set formula** edit field, enter the expression CYL1+CYL2+CYL3+CYL4+CON1-BLK1-BLK2. Click **OK**.

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



PHYSICS SETTINGS

Subdomain Settings—Solid, Stress-Strain

1 From the **Multiphysics** menu, select **1 Solid, Stress-Strain (smsld)**.

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

3 Select Subdomains 1 and 5, then click the **Load** button in the **Material settings** area.

4 From the **Basic Material Properties** library, select **Aluminum**, then click **OK**.

5 Select Subdomains 2 and 3, then click the **Load** button.

6 From the **Basic Material Properties** library, select **Brick**, then click **OK**.

7 Select Subdomain 4 and specify settings according to the following table:

PROPERTY	VALUE
Coordinate system	Silicon orientation
E	169e9
ν	0.278
α	12e-6
ρ	7850

8 Click **OK**.

Boundary Conditions—Solid, Stress-Strain

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

2 On the **Constraint** page, specify the following constraint condition:

SETTINGS	BOUNDARIES 4–6, 8, 9, 13, 14, 17, 23–25, 28–30, 32
Constraint condition	Roller

The boundaries not listed above are free, which is the default constraint condition.

3 Go to the **Load** page and select Boundary 3.

4 In the $\mathbf{F_z}$ edit field, type `-1[kPa]*flc1hs(t[1/s]-0.2,0.1)`.

5 Click **OK**.

Subdomain Settings—Electric Currents

1 From the **Multiphysics** menu, choose **2 Electric Currents (emqvw)**.

2 Select Subdomains 1–3 and 5. Clear the **Active in this domain** check box.

3 Select Subdomain 4. In the σ edit field type `sigma11 sigma12 sigma22 sigma13 sigma23 sigma33`. The editable pop-up window displays the components' positions in the anisotropic, symmetric electric conductivity tensor.

4 Click **OK**.

Boundary Conditions—Electric Currents

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

2 Select the **Interior boundaries** check box.

3 Select all boundaries and set the boundary condition to **Electric insulation**.

4 Select Boundary 13. From the **Boundary condition** list, choose **Electric potential**. In the $\mathbf{V_0}$ edit field, type `1`.

5 Select Boundary 32. From the **Boundary condition** list, choose **Ground**.

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

Integration Coupling Variables

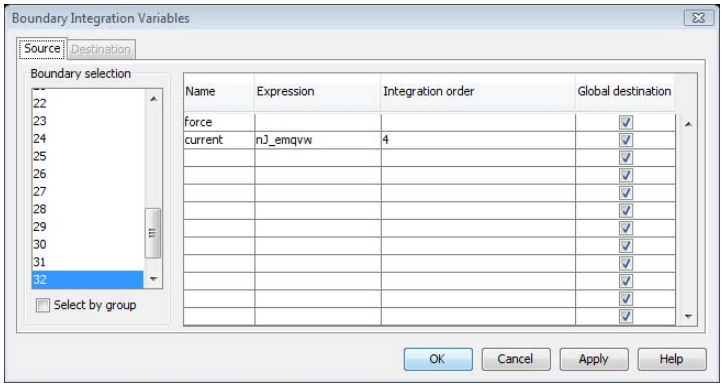
To have a probe plot for the developing of the electric current and the applied load on the top surface, define two boundary integration variables.

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

2 Define the following integration variables by first selecting the boundary, and then entering the name and expression on the first available row in the dialog box table.

BOUNDARY	NAME	EXPRESSION
3	force	Fzg_smsld
32	current	nJ_emqvw

In the **Integration order** and **Global destination** columns, leave the default settings.



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

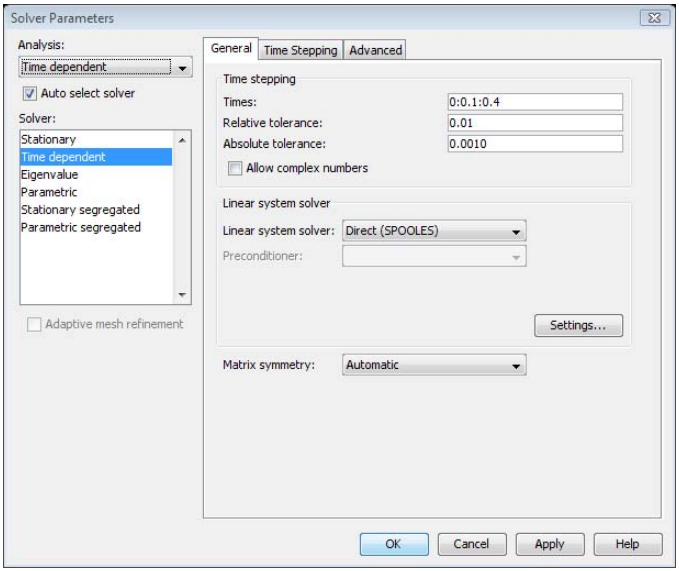
MESH GENERATION

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

COMPUTING THE SOLUTION

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

2 On the **General** page, type `0:0.1:0.4` in the **Times** edit field. Also, verify that the **Linear system solver** is set to **Direct (SPOOLES)**.



3 From the **Postprocessing** menu, choose **Probe Plot Parameters**.

4 In the **Probe Plot Parameters** dialog box, click the **New** button.

5 From the **Plot type** list, select **global**. In the **Plot name** edit field, type `force`.

6 Click **OK**.

7 In the **Expression to plot** area, the integration coupling variable `force` in the **Expression** edit field.

8 In the same fashion, define a probe plot with the label **current** for the integration coupling variable with the same name.

9 Click **OK** to close the **Probe Plot Parameters** dialog box.

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

POSTPROCESSING AND VISUALIZATION

To reproduce the plot of the boundary displacement field displayed in Figure 3-8, follow these steps:

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

2 On the **General** page, clear the **Slice** check box and select the **Boundary** check box in the **Plot type** area.

3 Click the **Boundary** tab and verify that **disp_smsld** is selected from the **Predefined quantities** list. From the **Unit** list, select **nm**.

4 Click **OK** to close the dialog box and generate the plot.

5 Click the **Scene Light** button on the Camera toolbar.

Reproduce the plot in Figure 3-10 with these instructions:

1 From the **Postprocessing** menu, choose **Global Variables Plot**.

2 In the **Expression** edit field, type `current-with(1,current)`.

3 Click the **Add Entered Expression** button.

4 Click the **Axis/Title** button.

5 Click the right option buttons for **Title** and **Second axis label**.

6 In the **Second axis label** edit field, type `I-I<sub>0</sub> [A]`.

7 From the **Plot in** list, select **New figure**.

8 Click **OK**.

Capacitive Pressure Sensor

Introduction

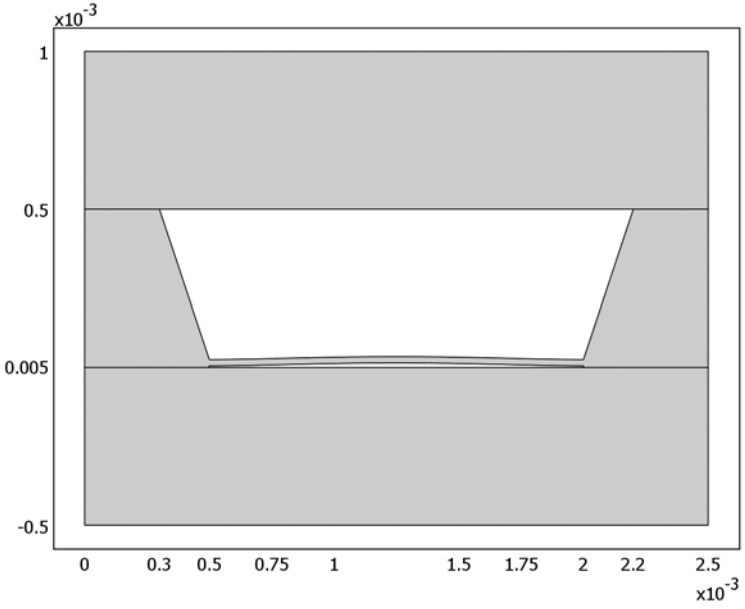
The basic structure of a pressure sensor consists of two cavities separated by a thin membrane. One cavity contains the reference pressure (possibly a vacuum), and the other connects to the measurable pressure. When that pressure changes, the membrane deforms by a magnitude that depends on several things: the amount of pressure, the material's mechanical properties, and the structure's shape.

Any initial stresses in the material also affect the deformation. Therefore, the manufacturing process and the selected materials directly affect sensor operation. In some structures the membrane and cavities are engraved onto silicon and sealed with layers of glass. Because the materials are bonded together at a high temperature, cooling them down to the sensor's normal operating temperature produces undesirable stresses in the material that affect device performance.

A common way to detect membrane deformation is by measuring capacitance. The surface of the deforming membrane and the opposite side of one of the cavities are coated with metal. Thus they form a capacitor whose value depends on the distance of the plates and on the system's geometry.

The sensor in this example measures static pressures of a magnitude from zero to atmospheric pressure. The model first computes the initial stresses from device construction; then it accounts for the structure's mechanical deformation resulting from an applied pressure. It finally calculates the sensor's capacitance for the deformed shape from the electric field.

Being in 2D, this model describes a different geometry from a true 3D sensor. Often the deforming membrane is a circular or rectangular diaphragm fixed at all boundaries. But when you view this structure in 2D, a bridge type structure results, which is fixed only at the two edges. The following figure illustrates the model's deformed geometry.



2D view of a pressure sensor.

Model Definition

MODEL GEOMETRY

From that diagram you can see that the model consists of three layers. The active silicon structure sits between two blocks of glass. The following list provides descriptions of the different structures in the sensor:

- Top and bottom layers
  - Rectangular
  - Material: Glass, HOYA, SD-2
  - Width: 2.5 mm
  - Height: 0.5 mm

- Middle layer
  - Complex structure: a rectangle in which cavities needed for sensor operation are engraved
  - Material: Silicon
  - Width: 2.5 mm
  - Height: 0.5 mm
  - Membrane width: 1.5 mm
  - Membrane height: 20 μm
- Cavity with a vacuum
  - Symmetric trapezoid at the upper boundary of the middle layer
  - Material: Vacuum
  - Width at the top: 1.9 mm
  - Width at the bottom: 1.5 mm
  - Height: 0.475 mm
- Cavity with ambient pressure
  - Rectangular
  - Material: Air
  - Width: 1.5 mm
  - Height: 5 μm
- Capacitance measurement
  - Done with two metal plates at the top and bottom of the cavity with ambient pressure
  - Top plate potential: 1 V
  - Bottom plate potential: Ground
  - Plate width: 1.0 mm

The thickness of all parts is 2.5 mm.

The structure is fixed at two points but is otherwise allowed to deform freely. The lower left corner is fixed in the x and y directions but can rotate. The lower right corner is fixed in the y direction but can rotate and move in the x direction.

STRESS AND DEFORMATION

During manufacturing, the sensor is bonded together in a vacuum and at a high temperature and is then cooled down. Therefore, during this process no external forces act on the sensor's boundaries, but internal stresses appear because the two materials have different coefficients of thermal expansion. This process also produces a vacuum in the upper cavity, and it serves as the reference pressure.

During normal operation, the sensor is fixed on a solid surface, and ambient pressure pushes on all outer boundaries. The temperature also changes, which produces extra stresses due to thermal expansion.

For a linear elastic material, the stress-strain relationship including the initial stress (σ_0), initial strain (ε_0), and thermal effects (ε_{th}), is

$$\sigma = D\varepsilon_{\text{el}} = D(\varepsilon - \varepsilon_{\text{th}} - \varepsilon_0) + \sigma_0$$

where D is the elasticity matrix, and vectors give the normal and shear values of the stresses and strains.

Initially only thermal expansion is active, and it comes from the relationship

$$\varepsilon_{\text{th}} = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{bmatrix} = \alpha_{\text{vec}}(T - T_{\text{ref}}),$$

where α_{vec} are the coefficients of thermal expansion, T is the ambient temperature, and T_{ref} is the reference temperature. The manufacturing stage produces the initial stress for normal operation, where further thermal expansion takes place. This model assumes that after manufacturing the sensor is close to its initial geometry and thus the initial strain is zero.

For calculating large deformations, strain values come from the Green strains as

$$\frac{\gamma_{ij}}{2} = \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i} \cdot \frac{\partial u_k}{\partial x_j}\right).$$

For the case of large deformations, the model solves the problem using the principle of virtual work, which states that the sum of virtual work from internal strain is equal to work from external loads.

CAPACITANCE

For computing sensor capacitance, the model solves for the electric field in the deformed geometry or frame, which is defined by the Moving Mesh (ALE) application mode.

To calculate the capacitance, a port boundary condition is used. It calculates the capacitance from the energy of the electric field with the equation

$$C = \frac{2}{U^2} \int_{\Omega_d} W_e d\Omega_d$$

where U is the potential difference between the plates ($U = 1$ for the port boundary condition) and W_e is the electric energy density. The area Ω_d corresponds to the narrow air gap in the sensor.

Results and Discussion

Figure 3-11 shows the results after the bonding phase, where bonding took place at 400 °C and the sensor is then cooled down to 22 °C. In the image the x- and y-axes have different scales, and the structural deformation is scaled by 20.

It appears that the membrane slightly pulls towards the larger cavity even though there are no applied loads. Stresses appear near the boundaries of the different materials and in the silicon membrane, which is narrower than other parts of the sensor. The maximum appears at the lower left corner of the smaller cavity.

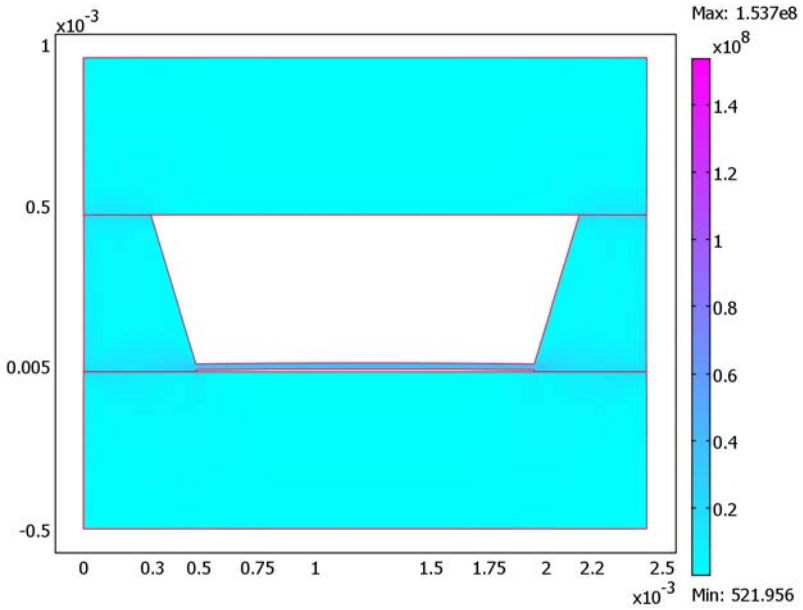


Figure 3-11: Initial stresses of the materials in the pressure sensor.

Figure 3-12 shows the results when the sensor is in operation: it is exposed to a pressure of one atmosphere at 15 °C. The figure is arbitrarily scaled and is focused on the left half of the lower cavity. The membrane deforms toward the vacuum with maximum deformation at the middle. Maximum stresses appear at the upper corners of the lower cavity where the membrane attaches to the silicon boundaries.

The streamlines show the electric field in the lower cavity. The lines are vertical between the two electrodes. Some field lines appear outside of the electrode region,

but the field strength is very small there (dark blue color).

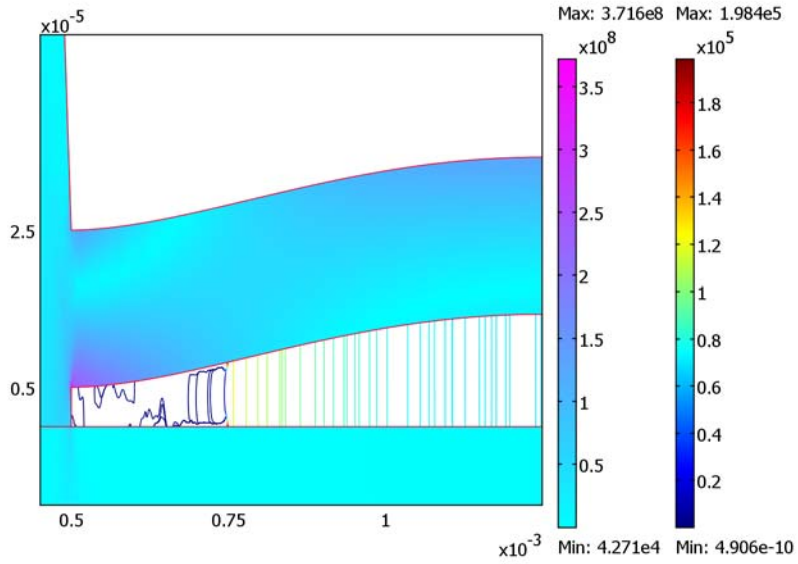


Figure 3-12: Sensor deformation, stresses (left color bar: von Mises Stress) and electric field (right colorbar: Electric field strength) when exposed to ambient pressure.

Figure 3-13 show the capacitance values computed from the electric field for four conditions as described in Table . Conditions A and B have the same ambient temperature but a higher bonding temperature. In Condition C all temperature values are the same so no stresses or deformations arise from thermal effects. For Condition D, thermal deformation does result from the ambient temperature.

You can also compare the computed capacitance values to those for a plate capacitor with a plate size of 1 mm times unity and a gap of 5 µm when not deformed. The capacitance for this plate capacitor is $C = \varepsilon_0 A/d = 1.771 \cdot 10^{-9}$ F; the corresponding value from the COMSOL Multiphysics model is $1.7760763 \cdot 10^{-9}$ F computed with settings for Condition C and zero pressure.

TABLE 3-6: TEMPERATURE CONDITIONS FOR COMPUTING THE CAPACITANCE VALUES

TEMPERATURE	A	B	C	D
High bonding (°C)	400	200	22	22
Low bonding (°C)	22	22	22	22
Ambient (°C)	15	15	22	-18

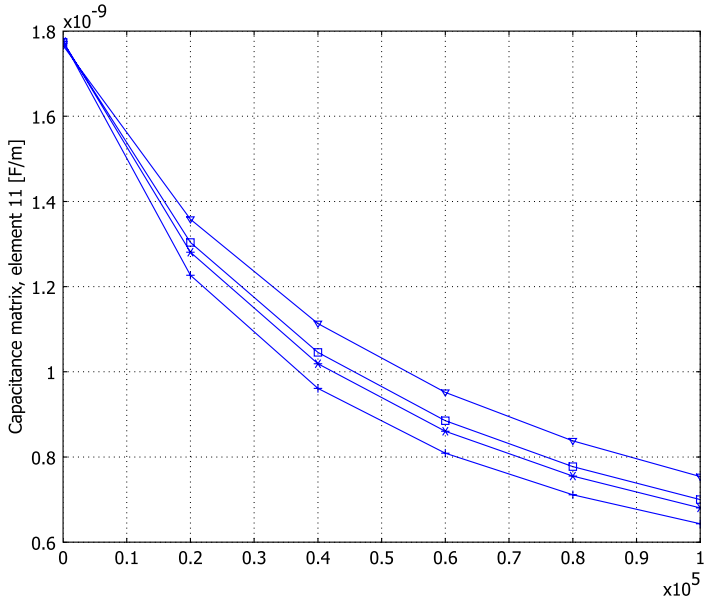


*Figure 3-13: Computed capacitance vs. ambient pressure for different temperature conditions: Condition A, triangles; Condition B, squares; Condition C, +; Condition D, *.*

Modeling in COMSOL Multiphysics

In COMSOL Multiphysics you solve this problem using four application modes: two Plane Stress application modes, one Moving Mesh (ALE) application mode, and one Electrostatics application mode. The latter two are defined in a frame to allow the mesh to move.

Because the structure's deformation can be large, you must use a large deformation analysis for both Plane Stress application modes.

You solve for the mesh movement and the electric field only in the small air gap where the ambient pressure is applied to the sensor. The mesh movement follows the structural deformation on the model's parts.

The solution process takes place in four steps:

1 The first Plane Stress application mode represents the sensor's fabrication, and it computes the initial stresses that result from thermal expansion. This is solved with the static solver.

2 The second Plane Stress application mode solves the deformation and stresses that result when the sensor is exposed to ambient temperature and pressure. It uses the initial stresses and deformation from the first plane stress application mode. This is solved with a parametric solver for different values of ambient pressure.

3 Using a parametric solver you solve the ALE mesh for each ambient pressure.

4 Finally, using a parametric solver you solve the electric field for each ambient pressure.

Several constants define the different manufacturing and ambient conditions. The following table contain descriptions and default values for them. For temperature values the model uses the normal temperature $T_0 = 273.15$ K. If you want to use static analysis to solve for single solutions, you can define a constant `P_ambient`. It is not needed for the parametric analysis.

CONSTANT	VALUE	UNIT	DESCRIPTION
`T_bondingH`	`400+T0`	K	High bonding temperature
`T_bondingL`	`22+T0`	K	Low bonding temperature
`T_ambient`	`15+T0`	K	Ambient temperature
`P_ambient`	`101e3`	Pa	Ambient pressure

Model Library path: `MEMS_Module/Sensor_Models/pressure_sensor_2d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, go to the **New** page, and select **2D** from the **Space dimension** list.

2 Click the **Multiphysics** button.

3 From the list of application modes select **MEMS Module>Structural Mechanics>Plane Stress>Static analysis**. Add it to the model two times by clicking the **Add** button twice. Note that COMSOL Multiphysics adds both to a 2D geometry it labels **Geom1 (2D)**.

4 In the **Multiphysics** area on the right select **Plane Stress (smps)**.

5 Click the **Application Mode Properties** button, find the **Large deformation** list, and select **On**. Click **OK**.

6 In the **Multiphysics** area select **Plane Stress (smps2)**.

7 Click the **Application Mode Properties** button, find the **Large deformation** list, and select **On**. Click **OK**.

8 In the **Multiphysics** area select **COMSOL Multiphysics>Deformed Mesh>Moving Mesh (ALE)>Static analysis**. Click **Add**.

9 From the list of application modes select **MEMS Module>Electrostatics>Electrostatics**. Click **Add**. Note that this application mode appears under **Frame (ale)**.

10 In the **Multiphysics** area select **Electrostatics (emes)** and click the **Application Mode Properties** button. In the **Weak Constraints** list select **On** and in the **Constraint type** list choose **Non-ideal**.

11 Find the **Ruling application mode** list at the bottom of the dialog box and select **Moving Mesh (ALE) (ale)**.

12 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the dialog box that opens, go to the **Axis** page and clear the **Axis equal** check box. Then define axis settings according to the following table:

x min	-1e-3
x max	3e-3
y min	-1e-3
y max	2e-3

3 Go to the **Grid** page and clear the **Auto** check box. Then define axis settings according to the following table. When complete, click **OK**.

x spacing	0.5e-3
Extra x	0.3e-3 0.75e-3 1.75e-3 2.2e-3
y spacing	0.5e-3
Extra y	5e-6 25e-6

4 From the **Options** menu select **Constants**. In the resulting dialog box enter the following names and expressions (you can change these values to model different bonding and ambient conditions). When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
T0	273.15[K]	Normal temperature
T_bondingH	T0 + 400[K]	High bonding temperature
T_bondingL	T0 + 22[K]	Low bonding temperature
T_ambient	T0 + 15[K]	Ambient temperature

5 From the **Options** menu select **Materials/Coefficients Library**. In the resulting dialog box select **Model** and then click **New**.

6 Go to the **Name** edit field and enter `Glass HOYA`, then in the **Material properties** area set these parameter values; when done, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
E	86.667e9	Young's modulus
nu	0.244	Poisson ratio
rho	2600	Density
alpha	3.41e-6	Thermal expansion

GEOMETRY MODELING

1 Draw four rectangles as given in the following table. To do so, go to the Draw toolbar and Shift-click the **Rectangle/Square** button; alternatively, from the Main menu choose **Draw>Specify Objects>Rectangle**.

NAME	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	2.5e-3	0.5e-3	Corner	0	-0.5e-3
R2	2.5e-3	0.5e-3	Corner	0	0
R3	2.5e-3	0.5e-3	Corner	0	0.5e-3
R4	1.5e-3	5e-6	Corner	0.5e-3	0

2 Create the composite object CO1, which consists of the points in the following table. To do so, go to the Draw toolbar, click the **Line** button, and left-click through the points in sequence. Finish the geometry by right-clicking on the drawing area.

Alternatively, go to the Draw toolbar and Shift-click the **Line** button. In the resulting dialog box go to the **Style** list and select **Closed polyline (solid)**. In the **Name** edit field, verify that the name is **CO1**; if not, enter it. Then enter the coordinates (all four x

values go on one line separated by spaces; the same holds for the *y* values). When finished, click **OK**.

COORDINATE	
X	Y
0.3e-3	0.5e-3
0.5e-3	25e-6
2.0e-3	25e-6
2.2e-3	0.5e-3

3 Create a composite object of objects **R2** and **C01**. On the Draw toolbar select the **Create Composite Object** button, go to the **Set formula** edit field and enter `R2-C01`, then click **OK**.

4 Draw four points on the coordinates given on the following table. To do so, successively select the **Point** button from the Draw toolbar and click the grid points. Alternatively, from the Draw toolbar shift-click the **Point** button four times, each time entering a coordinate pair.

NAME	COORDINATES	
	X	Y
PT1	7.5e-4	5e-6
PT2	1.75e-3	5e-6
PT3	7.5e-4	0
PT4	1.75e-3	0

PHYSICS SETTINGS

Subdomain Settings

You supply material parameters separately for each application mode. Furthermore, here you define in which subdomain the model solves each application mode.

Specify the subdomain settings for the **Plane Stress (smps)** application mode as follows:

1 From the Main menu choose **Multiphysics>Plane Stress (smps)**.

2 Choose the menu item **Physics>Subdomain Settings**.

3 Go to the **Material** page.

4 Select Subdomain 4 and clear the **Active in this domain** check box.

5 Select Subdomains 1 and 3.

6 Click **Load**, then from the **Materials** list select **Geom1>Glass HOYA (mat1)**. Click **OK**.

7 Go to the **thickness** edit field and enter `2.5[mm]`.

8 Select Subdomain 2.

9 Click **Load**. From the **Materials** list select **Basic Material Properties>Silicon**, then click **OK**.

10 Go to the **thickness** edit field and enter `2.5[mm]`.

11 To enable thermal stresses first select Subdomains 1, 2, and 3.

12 Click the **Load** tab. Select the **Include thermal expansion** check box. Go to the **Temp** edit field and enter `T_bondingL`, then go to the **Tempref** edit field and enter `T_bondingH`.

13 Click **OK**.

Specify the subdomain settings for the **Plane Stress (smps2)** application mode as follows:

1 From the Main menu select **Multiphysics>Plane Stress (smps2)**.

2 Choose the menu item **Physics>Subdomain Settings**.

3 Set the material parameters for Subdomains 1, 2, and 3, and deactivate subdomain 4 following the same procedures as for the first Plane Stress application mode in the previous list (Steps 3 to 10). Note, though, that you can select materials directly from the **Library material** list on the **Material** page.

4 To include initial stresses and further thermal stresses first select Subdomains 1, 2, and 3.

5 Click the **Load** tab. Select the **Include thermal expansion** check box. Go to the **Temp** edit field and enter `T_ambient`, then go to the **Tempref** edit field and enter `T_bondingL`.

6 Click the **Initial Stress and Strain** tab. Select the **Include initial stress** check box. Enter values for σ_{xi} (`sX_smps`), for σ_{yi} (`sY_smps`), for σ_{zi} (`sZ_smps`), and for σ_{xyi} (`sXY_smps`).

7 Click **OK**.

Specify the subdomain settings for the **Moving Mesh (ALE) (ale)** application mode as follows:

1 From the Main menu select **Multiphysics>Moving Mesh (ALE) (ale)**.

2 Choose the menu item **Physics>Subdomain Settings**.

3 Select Subdomains 1, 2, and 3 and select the **Physics induced displacement** check box.

4 Enter `u2` and `v2` in the **dx** and **dy** edit fields, respectively.

5 Select Subdomain 4.

6 See that the **Free displacement** option button is selected.

7 Click **OK**.

When configuring the Electrostatics application mode, use material parameters corresponding to air.

1 From the Main menu select **Multiphysics>Electrostatics (emes)**.

2 Choose the menu item **Physics>Subdomain Settings**.

3 Select Subdomains 1, 2, and 3 and clear the **Active in this domain** check box.

4 Leave parameter values for Subdomain 4 at their initial values (that is, the constitutive relationship is $D = \varepsilon_0 \varepsilon_r E$ with $\varepsilon_r = 1$ and ρ is 0). Check the **Init** page to verify that the setup has initialized V to zero.

5 Click **OK**.

Boundary Conditions

The manufacturing process applies no loads or constraints on the boundaries. Thus you do not need to set any boundary conditions for **Plane Stress (smps)** because, by default, there are not any loads or constraints. Define boundary conditions for the other application modes according to the following steps:

1 Select **Multiphysics>Plane Stress (smps2)** and open the **Physics>Boundary Settings** dialog box.

2 Select Boundary 2, and on the **Constraint** page set **Constraint condition** to **Fixed**.

3 Go to the **Load** page and select all boundaries

4 Click the **Edge load is defined as force/area using the thickness** button.

5 Select **Tangent and normal coord. sys. (t,n)** from the **Coordinate system** list.

6 See that **Ft** is zero for all boundaries.

7 Set the **Fn** values as follows:

SETTINGS	BOUNDARIES 10, 12, 15, 17	BOUNDARIES 1, 3, 5, 7, 11, 14, 16, 18, 22–24	BOUNDARIES 8, 9, 13, 20
F_n	P_ambient	-P_ambient	0

8 Click **OK**, then click **Update symbols** on the Visualization/Selection toolbar to see that all boundary forces point towards the sensor.

9 Select **Multiphysics>Moving Mesh (ALE) (ale)** and then **Physics>Boundary Settings**.

10 Select all active boundaries, that is, Boundaries 10–12 and 14–18.

11 Select the **dx** and **dy** check boxes and type `u2` and `v`, respectively, in the corresponding edit fields.

12 Click **OK**.

13 Select **Multiphysics>Electrostatics (emes)** and then **Physics>Boundary Settings**.

14 Define boundary settings for the active boundaries as in the following table. Note that you define the port settings on the separate **Port** page; when done click **OK**.

SETTINGS	BOUNDARIES 10–12, 16–18	BOUNDARY 14	BOUNDARY 15
Boundary condition	Zero charge/Symmetry	Ground	Port
Port number			1
Use port as input			Selected
Input property			Forced voltage

Point Settings

1 Select **Multiphysics>Plane Stress (smps)** and then **Physics>Point Settings**.

2 Make sure the **Standard notation** button is selected. Then define point constraints according to the following table. Check also that **Global coordinate system** is selected in the **Coordinate system** list; when done, click **OK**.

SETTINGS	POINT 1	POINT 17
R_x	0	(not selected)
R_y	0	0

MESH GENERATION

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

2 On the **Global** page find the **Maximum element size** edit field and enter `0.5e-4`.

3 Select the **Subdomain** page.

4 Select Subdomain 4, then go to the **Maximum element size** edit field and enter `1e-6`.

5 Select the **Advanced** page.

6 In the **x-direction scale factor** edit field enter `0.2`.

7 Click **Remesh** to initialize the mesh.

8 Click **OK**.

COMPUTING THE SOLUTION

The following steps use a static solver to first solve the bonding phase and the parametric solver to solve the sensor operation for different pressures.

To make it easier to test the model with different temperature settings, use solver scripting. Before proceeding with the steps below, go to the **Solver Manager** dialog box, click the **Script** tab, select **Automatically add commands when solving**, and then close the **Solver Manager** dialog box. Next perform the steps below, and finally clear the **Automatically add commands when solving** check box. Later on you can return to the **Script** page of the **Solver Manager**, select the **Solve using a script** check box, and click the **Solve** button. The script automatically performs all the steps needed for the solution.

1. From the **Solve** menu select **Solver Parameters**.
2. On the **General** page verify that the **Analysis** list has the selection **Static** and that the **Solver** list has the selection **Stationary**. Click **OK**.
3. From the **Solve** menu choose the **Solver Manager**; alternately, click the **Solver Manager** button on the Main toolbar.
4. On the **Initial Value** page the default values are correct (**Initial value: Initial value expression evaluated using current solution**; **Value of variables not solved for and linearization point**: **Use setting from Initial value frame**).
5. Click the **Solve For** tab. Select **Plane Stress (smps)** and then click **Solve**.
6. Keeping the **Solver Manager** open, select **Solver Parameters** from the **Solve** menu.
7. On the **General** page select **Parametric** from the **Solver** list.
8. In the **Parameter name** field type `P_ambient`.
9. In the **Parameter values** list type `0 1e4:1e4:1e5`. Click **OK**.
10. Go back to the **Solver Manager**.
11. Click the **Initial Value** tab. In the **Value of variables not solved for and linearization point** area click the **Current solution** button.
12. Click the **Solve For** tab. Select **Plane Stress (smps2)** and then click **Solve**.
13. On the **Initial Value** page find the **Value of variables not solved for and linearization point** area. Verify that the **Parameter value** list is active and has the selection **All**.
14. On the **Solve For** page select the **Moving Mesh (ALE) (ale)** application mode. Click **Solve**.
15. Select the **Electrostatics (emes)** application mode. Click **Solve**.
16. Click **OK** to close the **Solver Manager**.

POSTPROCESSING AND VISUALIZATION

Bonding Phase

Use following steps to create Figure 3-11 on page 199:

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

2 Go to the **General** page.

3 On the **Plot type** area verify that only the **Surface**, **Boundary** and **Deformed shape** check boxes are selected. See that the **Frame** list shows **Frame (ref)**.

4 Examine the **Parameter value** list. Any solution is fine because there is only one solution, that for the first step.

5 Click the **Surface** tab. From the **Predefined quantities** list select **von Mises stress (smps)**.

6 Go to the **Surface color** area, and in the **Colormap** list select **Cool**.

7 Go to the **Boundary** page. Any selection in the **Predefined quantities** list is fine.

8 In the **Boundary color area** select **Uniform color**; then click the **Color** button, select red, and click **OK**.

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

Response to Ambient Pressure

Use following steps to create Figure 3-12 on page 200:

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

2 On the **General** page go to the **Plot type** area and make sure that only the **Surface**, **Boundary**, and **Streamline** check boxes are selected.

3 Verify that the **Frame** list shows **Frame (ale)**.

4 From the **Parameter value** list select the solution you want to plot

5 Move to the **Surface** page, go to the **Predefined quantities** list and select **Plane Stress (smps2)>von Mises stress**. In the **Colormap** list select **cool**.

6 On the **Boundary** page use the same settings given in Steps 7 and 8 in the previous postprocessing section.

7 Go to the **Streamline** page. Under **Streamline Data** set the **Predefined quantities** list to **Electric field (emes)**.

8 On the **Start Points** tab, set the **Number of start points** to 100.

9 Click the **Line Color** tab, then click the **Use expression** button, and click the **Color Expression** button.

10 In the dialog box that opens, set the **Predefined quantities** list to **Electrostatics (emes)>Electric field, norm**, then click **OK**.

11 Click the **Advanced** button and select **Normalize vector field**, then click **OK**.

12 Click **OK**.

Capacitance

To compute the capacitance, perform the following steps:

1. From the **Postprocessing** menu choose **Data Display>Global**.
2. From the **Predefined quantities** list, select **Electrostatics (emes)>Capacitance matrix, element 11**.
3. From the **Parameter value** list select the solution you want to plot.
4. Click **OK**.

You find the result in the message log at the bottom of the main window. The model calculates a capacitance of approximately 1.77 nF for zero pressure.

You can also plot the capacitance:

1. From the **Postprocessing** menu choose **Domain Plot Parameters**.
2. Click the **Point** tab.
3. In the **Expression to evaluate** edit field type `C11_emes`.
4. Select any point.
5. Click **OK**.

SAW Gas Sensor

Introduction

A surface acoustic wave (SAW) is an acoustic wave propagating along the surface of a solid material. Its amplitude decays rapidly, often exponentially, with the depth of the material. SAWs are featured in many kinds of electronic components, including filters, oscillators, and sensors. SAW devices typically use electrodes on a piezoelectric material to convert an electric signal to a SAW, and back again.

In this model, you investigate the resonance frequencies of a SAW gas sensor. The sensor consists of an interdigitated transducer (IDT) etched onto a piezoelectric $LiNbO_3$ (lithium niobate) substrate and covered with a thin polyisobutylene (PIB) film. The mass of the PIB film increases as PIB selectively adsorbs CH_2Cl_2 (dichloromethane, DCM) in air. This causes a shift in resonance to a slightly lower frequency.

Model Definition

Figure 3-14 shows a conceptual view of the gas sensor in this model. IDTs used in SAW devices may have hundreds of identical electrodes, and each electrode can be about 100 times longer than it is wide. You can therefore neglect the edge effects and reduce the model geometry to the periodic unit cell shown in Figure 3-15. The height of this cell does not have to extend all the way to the bottom of the substrate but only a few wavelengths down, so that the SAW has almost died out at the lower boundary. In the model, this boundary is fixed to a zero displacement.

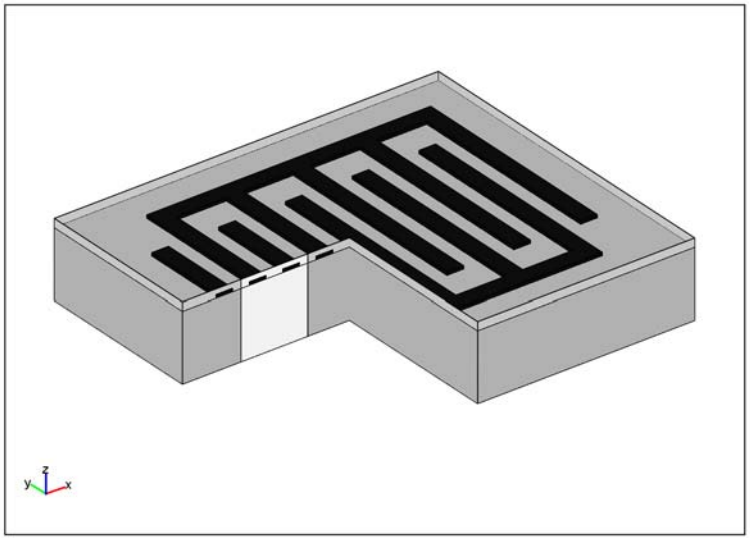


Figure 3-14: Conceptual view of the SAW gas sensor, showing the IDT electrodes (in black), the thin PIB film (light gray), and the $LiNbO_3$ substrate (dark gray). For the sake of clarity, the dimensions are not to scale and the IDT has fewer electrodes than in common devices. A slice of the geometry is removed to reveal the modeled unit cell (in white).

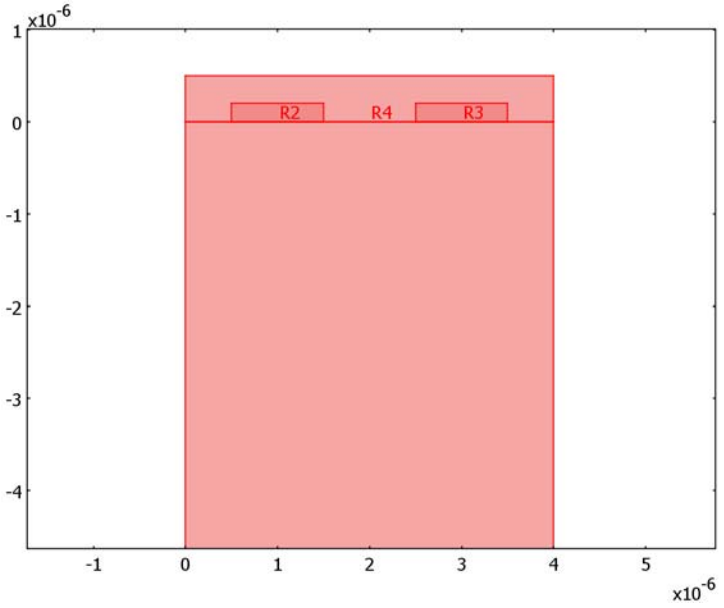


Figure 3-15: The modeled geometry of the model. A 500 nm PIB film covers two 1 μm-wide electrodes on top of the $LiNbO_3$ substrate. The substrate subdomain continues below the lower frame of the picture and has a total height of 22 μm. In the first version of the model, the substrate is the only active subdomain.

You set up the model in the Piezo Plane Strain application mode, which requires the out-of-plane strain component to be zero. This should be a valid assumption, considering that the SAW is generated in the model plane and that the sensor is thick in the out-of-plane direction.

The first version of the model deals only with free SAW propagation in the $LiNbO_3$ substrate, without any applied electric field. In order to find the velocity of the wave, we use periodic boundary conditions to dictate that the voltage and the displacements be the same along both vertical boundaries of the geometry. This implies that the wavelength will be an integer fraction of the width of the geometry. The lowest SAW eigenmode has its wavelength equal to the width of the geometry, 4 μm. The eigenfrequency of this mode multiplied by 4 μm hence gives the velocity of the wave.

In a second version of the model, the aluminum IDT electrodes and the PIB film are added. This causes the lowest SAW mode to split up in two eigensolutions, the lowest one representing a series resonance, where propagating waves interfere constructively

and the other one a parallel ("anti-") resonance, where they interfere destructively. These two frequencies constitute the edges of the stopband, within which no waves can propagate through the IDT.

The adsorption of DCM gas is represented as a slight increase of the density of the PIB film. In the third and final version of the model, the sensor is exposed to 100 ppm of DCM in air at atmospheric pressure and room temperature. The "partial density" of DCM in the PIB film is then calculated as

$$\rho_{\mathrm{DCM,PIB}} = KMc\,,$$

where $K = 10^{1.4821}$ (Ref. 1) is the air/PIB partition coefficient for DCM, M is its molar mass, and

$$c = 100 \cdot 10^{-6} \cdot p/(RT)$$

is its concentration in air.

The substrate used in the simulation is YZ-cut $LiNbO_3$ with properties cited in Ref. 2. The density of the PIB film is from Ref. 1. The Poisson's ratio is taken to be 0.48, which corresponds to a rather rubbery material. The Young's modulus is set to 10 GPa. Even at the comparatively high frequencies considered in this model, this is likely an overestimation. However, a much lower value would result in a multitude of eigenmodes located inside the film. While those may be important to consider in designing a SAW sensor, the focus in this model is on the SAW modes. Also, any effects of the DCM adsorption on other material properties than the density are neglected.

Results

Figure 3-16 shows the SAW as it propagates along the surface of the piezoelectric substrate. The frequency corresponding to a 4 μm wavelength computes to 870 MHz, giving a phase velocity of 3479 m/s.

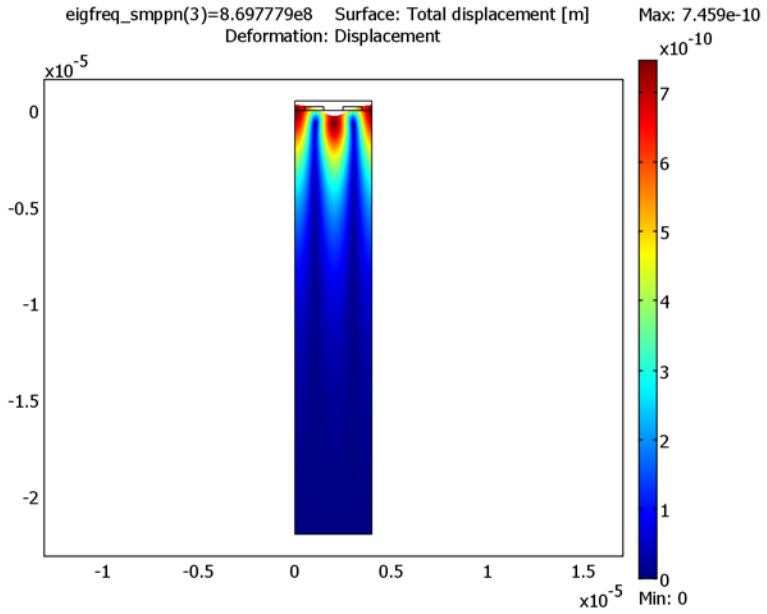


Figure 3-16: Deformed shape plot of a freely propagating SAW in the substrate. The color scale shows the magnitude of the displacements.

In the full model with the periodic IDT and the thin film included, the resonance and anti-resonance frequencies evaluate to 841 MHz and 850 MHz, respectively. Figure 3-17 and Figure 3-18 show the electric potential distribution characteristics for these solutions.

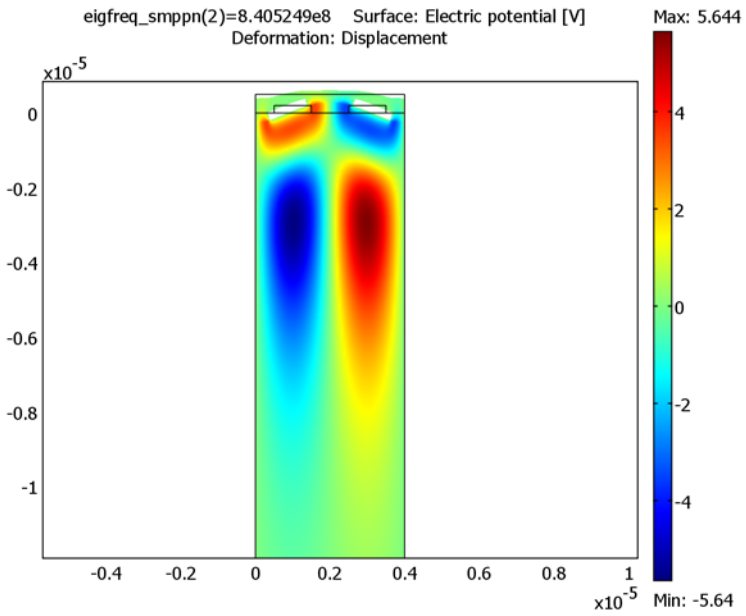


Figure 3-17: Electric potential distribution and deformations at resonance, 841 MHz. The potential is symmetric with respect to the center of each electrode.

Exposing the sensor to a 100 ppm concentration of DCM in air leads to a resonance frequency shift of 227 Hz downwards. This is computed by evaluating the resonance frequency before and after increasing the density of adsorbed DCM to that of the PIB domain.

Note that the computational mesh is identical in both these solutions. This implies that the relative error of the frequency shift is similar to that of the resonance frequency itself. Thus the shift is accurately evaluated despite being a few magnitudes smaller than the absolute error of the resonance frequency.

In a real setup, the drift is often measured by mixing the signal from a sensor exposed to a gas with a reference signal from one protected from the gas. The beat frequency then gives the shift.

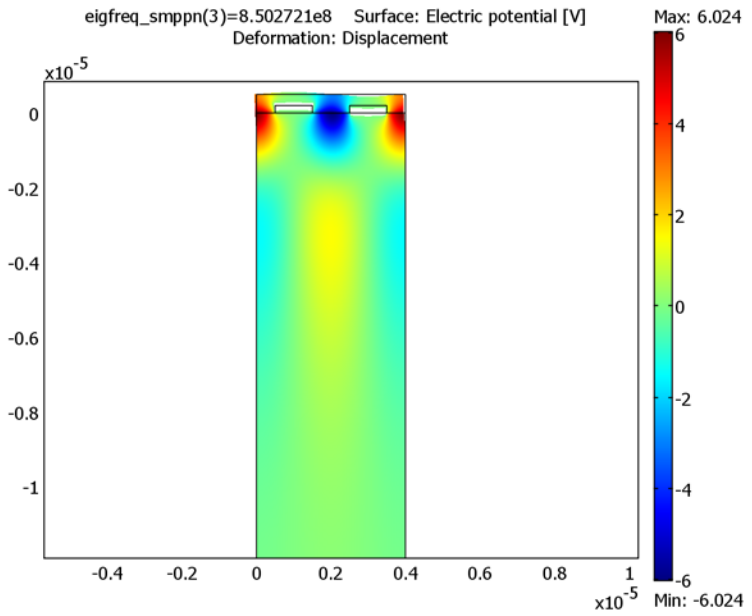


Figure 3-18: Electric potential distribution and deformations at antiresonance, 851 MHz. The potential is antisymmetric with respect to the center of the electrodes.

References

1. K. Ho and others, "Development of a Surface Acoustic Wave Sensor for In-Situ Monitoring of Volatile Organic Compounds", *Sensor*s vol. 3, pp. 236–247, 2003.

2. Ahmadi and others, "Characterization of multi- and single-layer structure SAW sensor [gas sensor]", *Sensors 2004, Proceedings of IEEE*, vol. 3, pp. 1129–1132, 2004.

Model Library path: `MEMS_Module/Sensor_Models/SAW_gas_sensor`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator** and click the **New** tab.

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

3 In the list of application modes select **MEMS Module>Structural Mechanics>Piezo Plane Strain>Eigenfrequency analysis**.

4 Click **OK**.

GEOMETRY MODELING

1 Create the following rectangles by repeatedly using **Draw>Specify Objects>Rectangle**:

WIDTH	HEIGHT	BASES: CORNER X	BASE: CORNER Y
4	22	0	-22
1	0.2	0.5	0
1	0.2	2.5	0
4	0.5	0	0

2 Select all objects and choose **Draw>Modify>Scale**. In the dialog box that appears, enter `1e-6` for both scale factors; then click **OK**.

3 Click the **Zoom Extents** button on the Main toolbar to zoom in on the now micron-sized geometry.

OPTIONS AND SETTINGS

1 Choose **Options>Constants**.

2 Define the following constant names, expressions, and (optionally) descriptions:

NAME	EXPRESSION	DESCRIPTION
p	101.325[kPa]	Air pressure
T	25[degC]	Air temperature
R	8.3145[Pa*m^3/(K*mol)]	Gas constant
c_DCM_air	100e-6*p/(R*T)	DCM concentration in air
M_DCM	84.93[g/mol]	Molar mass of DCM
K	10^1.4821	PIB/air partition constant for DCM
rho_DCM_PIB	K*M_DCM*c_DCM_air	Mass concentration of DCM in PIB
rho_PIB	0.918[g/cm^3]	Density of PIB
E_PIB	10[GPa]	Young's modulus of PIB
nu_PIB	0.48	Poisson's ratio of PIB
eps_PIB	2.2	Relative permittivity of PIB

3 Click **OK**.

PHYSICS SETTINGS

In the first version of the model, you compute the velocity for SAW propagation in a homogenous, electrically insulated $LiNbO_3$ substrate. The supplied material data are with reference to the *xy*-plane.

Subdomain Settings

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

2 Select Subdomains 2–4 and clear the **Active in this domain** check box.

3 Select Subdomain 1 and select **Material orientation: xy plane**.

4 Click the **Edit** button associated with $\mathbf{c_E}$ and enter the following values into the **Elasticity matrix** dialog box; when finished, click **OK**.

$$\begin{bmatrix} 2.424e11 & 0.752e11 & 0.752e11 & 0 & 0 & 0 \\ & 2.03e11 & 0.573e11 & 0 & 0.085e11 & 0 \\ & & 2.03e11 & 0 & -0.085e11 & 0 \\ & & & 0.752e11 & 0 & 0.085e11 \\ & & & & 0.595e11 & 0 \\ & & & & & 0.595e11 \end{bmatrix}$$

5 Click the **Edit** button associated with **e** and enter the following values into the **Coupling matrix** dialog box; when finished, click **OK**.

$$\begin{bmatrix} 1.33 & 0.23 & 0.23 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2.5 & 0 & 3.7 \\ 0 & -2.5 & 2.5 & 0 & 3.7 & 0 \end{bmatrix}$$

6 Click the **Edit** button associated with ε_{rS} and enter the following values into the **Relative permittivity** dialog box; when finished, click **OK**.

$$\begin{bmatrix} 28.7 & 0 & 0 \\ & 85.2 & 0 \\ & & 85.2 \end{bmatrix}$$

7 Enter 4647 in the **Density** edit field.

8 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

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

2 Select Boundary 2 and set the **Constraint condition** to **Fixed**.

3 Select all exterior boundaries (1, 2, 4, 7, 10, 12, 15, 16).

4 On the **Electric BC** page, set the **Boundary condition** to **Zero charge/Symmetry**.

5 Click **OK**.

6 Choose **Physics>Periodic Conditions>Periodic Boundary Conditions**.

7 On the **Source** tab, select Boundary 1 and enter `u` in the first **Expression** edit field.

8 On the **Destination** page, check Boundary 16 and enter `u` in the **Expression** edit field.

9 On the **Source Vertices** page, select Vertex 1 and click the right double-arrow. Then select Vertex 2 and click the right double-arrow.

10 On the **Destination Vertices** page, select Vertex 12 and click the right double-arrow, then Vertex 13 and the right double-arrow.

11 Define the expressions `v` and `V` in a similar fashion, starting by entering them in the **Expression** edit field on the **Source** page, on rows 2 and 3 respectively.

12 Click **OK** to close the **Periodic Boundary Conditions** dialog box.

MESH GENERATION

1 Choose **Mesh>Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, choose **Extremely fine**.

3 On the **Subdomain** page, select all subdomains and set the **Method** to **Quad**.

4 On the **Boundary** page, select the upper boundaries of the substrate (4, 7, 10, 12, 15) and enter `0.05e-6` for the **Maximum element size**.

5 Click **Remesh**, then click **OK**. When done, a zoom-in on the upper part of the geometry should look like Figure 3-19.

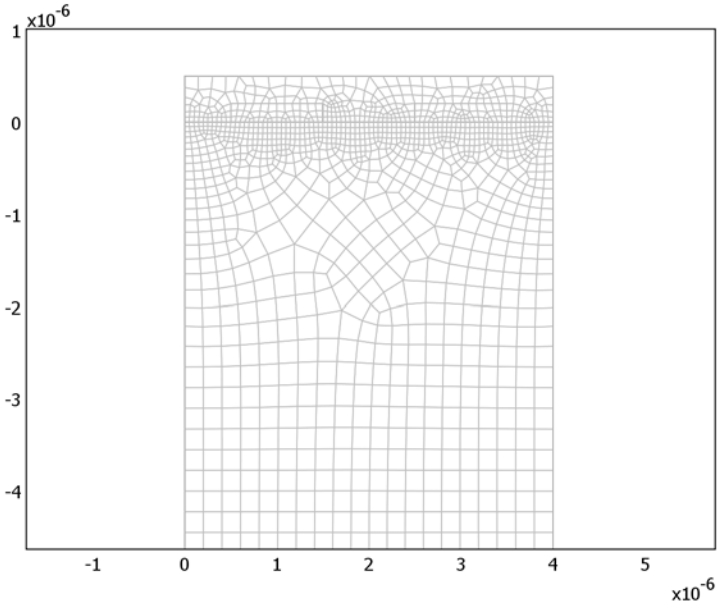


Figure 3-19: The meshed geometry.

COMPUTING THE SOLUTION

1. From the **Solve** menu, open the **Solver Parameters** dialog box.
2. Enter `850e6` in the **Search for eigenfrequencies around** edit field, then click **OK**.
3. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The solver returns 6 eigensolutions with eigenfrequencies in the vicinity of 850 MHz. At 869.8 MHz, two of them are—within the numerical accuracy—the same. These show the shape and the frequency for a SAW with wavelength equal to the width of the geometry.

1. Open the **Plot Parameters** dialog box from the **Postprocessing** menu.
2. On the **General** page, select one of the eigenfrequencies equal to 869.8 MHz.
3. On the **Deform** page, select the **Deformed shape plot** check box. Clear the **Auto** check box and enter `400` in the **Scale factor** edit field.

4 Click **OK** to close the dialog box and see a plot of the total displacement. If you want to, you can repeat the procedure with the other solution to verify that they are the same, only shifted by 90 degrees. One of the solutions will look like Figure 3-16.

5 To evaluate the velocity, choose **Postprocessing>Data Display>Global**.

6 Enter `eigfreq_smppn*4e-6[m]` in the **Expression** edit field.

7 In the **Eigenfrequency** list, select one of the 869.8 MHz eigenfrequencies.

8 Click **OK** to see the value of the velocity in the message log. It evaluates to approximately 3479 m/s.

This concludes the first part of the model. Proceed to find out how the electrodes and the PIB film affect the behavior of the SAW.

Sensor without Gas Exposure

Subdomain Settings

1 Open the **Subdomain Settings** dialog box and select Subdomains 2–4.

2 Select the **Active in this domain** check box.

3 Select **Material model: Decoupled, isotropic**.

4 Select only Subdomain 2.

5 On the **Structural** page, enter `E_PIB` for the **Young's modulus**, `nu_PIB` for the **Poisson's ratio**, and `rho_PIB` for the **Density**.

6 On the **Electrical** page, select the **Enable electrical equation** check box and enter `eps_PIB` for the relative permittivity.

7 Select Subdomains 3 and 4 and click the **Load** button.

8 In the **Materials/Coefficients Library** dialog box, select **Basic Material Properties>Aluminum** and click **OK**.

9 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

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

2 Select the **Interior boundaries** check box.

3 Select Boundaries 6-9 and 11-14. On the **Electric BC** page, set the condition to **Electric potential**. Keep the default zero potential.

4 Select Boundaries 3, 5, and 17, and set the condition to **Zero charge/symmetry**.

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

Note: The eigenfrequencies and hence the stopband do not depend on the values of the potentials. In fact, for linear eigenfrequency problems, they are automatically set to zero at the electrodes, regardless of the applied value. You can solve the corresponding driven problem by switching to a frequency response analysis and applying different potentials to the electrodes.

6 Choose **Physics>Periodic Conditions>Periodic Boundary Conditions**.

7 On the **Source** page, select Boundary 3. Enter `u` in the first **Expression** edit field and `v` in the row below, and `V` in the third row.

8 On the **Destination** page, select **Constraint name: pconstr1**, check Boundary 17, and enter `u` in the **Expression** field.

9 Still on the **Destination** page, select **Constraint name: pconstr2**, check Boundary 17, and enter `v` in the **Expression** field.

10 Finally, select **Constraint name: pconstr3**, check Boundary 17, and enter `V` in the **Expression** field.

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

You have now established the periodicity in the PIB film.

COMPUTING THE SOLUTION

Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

If you are still using the manual scaling of the deformations from the previous exercise, the plot that appears after solving will look rather distorted. Proceed as follows to find the SAW modes and use more suitable plot parameters:

1 Open the **Plot Parameters** dialog box from the **Postprocessing** menu.

2 On the **General** page, select the 850 MHz eigenfrequency.

3 On the **Deform** page, enter `40` in the **Scale factor** edit field.

4 Click **Apply** to view a plot of the total displacement at anti-resonance.

5 On the **General** page, select the 841 MHz eigenfrequency and click **Apply** to see the deformations at resonance. This plot should look like Figure 3-20.

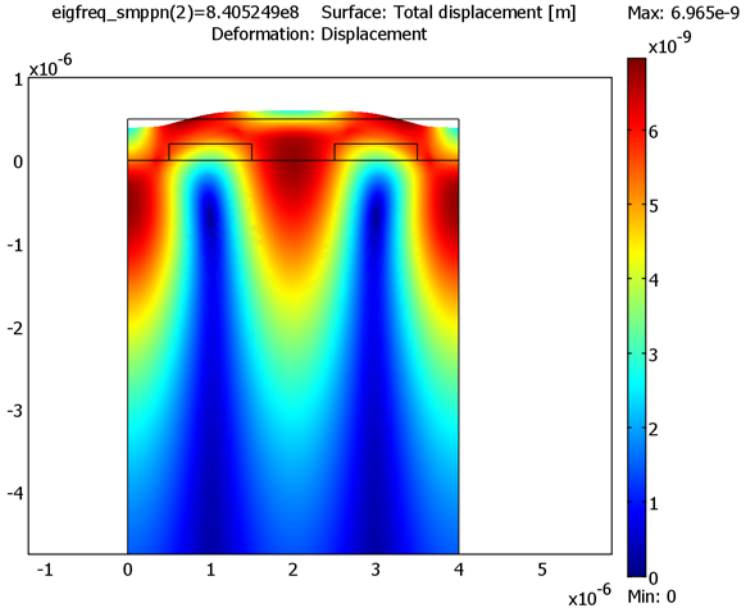


Figure 3-20: Deformations at resonance.

A plot of the electric potential shows a qualitative difference between the two solutions.

6 On the **Surface** page, select **Piezo Plane Strain (smppn)>Electric potential** from the **Predefined quantities** list.

7 Click **Apply** to see the potential distribution at resonance, as shown in Figure 3-17 on page 217. Notice that it is symmetric with respect to each individual electrode.

8 On the **General** page, select the 850 MHz eigenfrequency and click **OK** to see the potential distribution at anti-resonance, as in Figure 3-18 on page 218. This time, it is antisymmetric.

Sensor with Gas Exposure

In the final version of this model, you will expose the sensor to DCM gas. The eigenfrequencies are expected to shift by a very small amount. In order to see the shift, you need to include more digits in the output.

1 Choose **Postprocessing>Data Display>Global**.

2 Enter the expression `eigfreq_smppn` and select the 841 MHz eigenfrequency.

3 Select the **Display result in full precision** check box, then click **OK**.

The message log now shows all computed digits of the eigenfrequency.

Subdomain Settings

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

2 Select Subdomain 2. On the **Structural** tab, change the **Density** so that it reads `rho_PIB+rho_DCM_PIB`.

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

COMPUTING THE SOLUTION

Click the **Solve** button.

POSTPROCESSING AND VISUALIZATION

1 Choose **Postprocessing>Data Display>Global**.

2 Make sure that the expression still says `eigfreq_smppn` and select the 841 MHz eigenfrequency.

3 Click **OK**.

The first 6 digits of the eigenfrequency are the same as before. Subtracting the new value from the previous value (which is most easily done by copying and pasting the results from the message log) shows that the eigenfrequency with gas exposure is lower by 227 Hz.

Thermal Expansion in a MEMS Device Using the Material Library

The purpose of this model is to exemplify the use of the Material Library in COMSOL Multiphysics. This library contains more than 20,000 property functions for 2500 materials. The larger part of these properties are mechanical and thermal properties for solid materials given as functions of temperature. You need the Material Library to build the model.

Introduction

Thermal expansion is a common method used in the microscale to displace a part of a component, for example in an actuator. In this example model the opposite is required; that is, there should be a minimum of thermal expansion. Such a device could be included in a microgyroscope or any other sensor for acceleration or positioning.

Model Definition

Figure 3-21 below shows the model geometry:

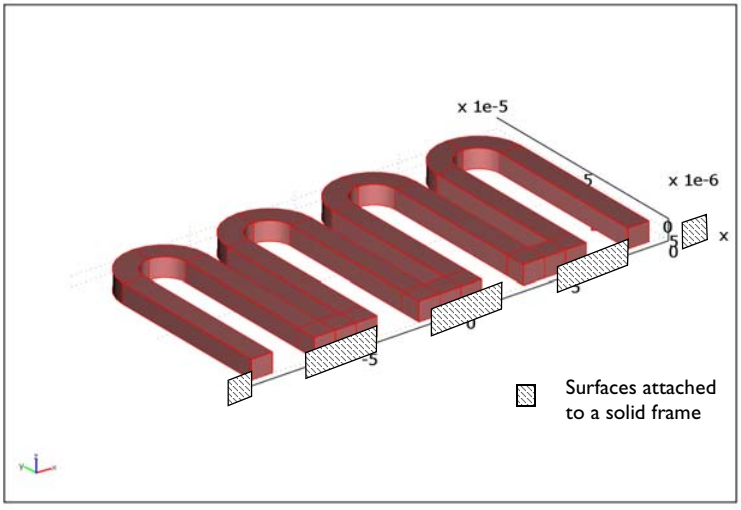


Figure 3-21: Geometry of the device.

The model consists of two sets of physics:

- A thermal balance with a heat source in the device, originating from Joule heating (ohmic heating). Air cooling is applied on the boundaries except at the position where the device is attached to a solid frame, where an insulation condition is set.
- A force balance for the structural analysis with a volume load caused by thermal expansions. The device is fixed at the positions where it is attached to a solid frame (see Figure 3-21).

The device is made of the copper-beryllium alloy UNS C17500.

The thermal balance consists of a balance of flux at steady state. The heat flux is given by conduction only. The heat source is a constant heat source of $1 \cdot 10^8$ W/m^3. The air cooling at the boundaries is expressed using a constant heat transfer coefficient of 10 W/m^2 and an ambient temperature of 298 K.

The stress and strains are well within the elastic region for the material. The expression for thermal expansion requires a strain reference temperature for the copper-beryllium alloy, which in this case is 293 K.

All other thermal and mechanical properties are obtained from the Material Library.

Results and Discussion

The following figure shows the temperature distribution in the device. The heat source increases the temperature to 323 K from an ambient temperature of 298 K. The temperature varies less than 1/100 of a degree in the device. The displacements vary

accordingly, and the model shows that it is possible to study the device using only one unit cell, for example, 1/2 of a U-shaped section.

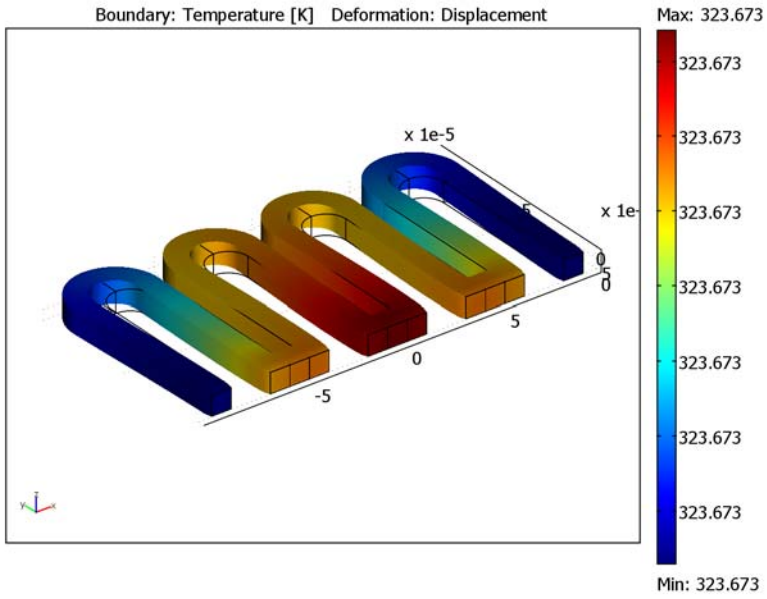


Figure 3-22: Temperature and displacement of the device. The edges of the original geometry are shown in black. The deformed shape is exaggerated by a factor of almost 200.

The following figure (Figure 3-23) shows the displacement of a curve that follows the top inner edges of the device from left to right. It is clear from Figure 3-23 that the displacement follows a repetitive pattern along the length of the device. This also

supports the hypothesis that 1/2 of a U-shaped section is enough to represent the behavior of the device.

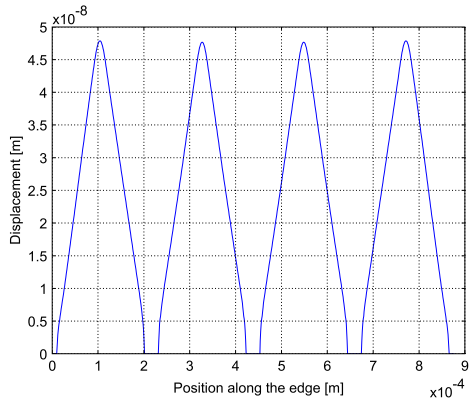


Figure 3-23: The displacement along the inner edge of the device shows a repetitive pattern, which means that a model of half of the u-shaped structure is enough to study the effects of thermal expansion on the device.

Model Library path: `MEMS_Module/Sensor_Models/thermal_expansion`

Modeling Using the Graphical User Interface

1 Open the **Model Navigator**.

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

3 Select **MEMS Module>Thermal-Structural Interactions>Solid, Stress-Strain with Thermal Expansion>Static analysis**.

4 Click **OK**.

GEOMETRY MODELING

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

2 Click the **x-y** plane option button if it is not already selected.

3 Click **OK**.

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

5 Enter `-1.3e-4` in the **x min** edit field, `1.3e-4` in the **x max** edit field, `-0.3e-4` in the **y min** edit field, and `1.3e-4` in the **y max** edit field.

6 Click the **Grid** tab.

7 Clear the **Auto** box.

8 Enter `1e-5` in the **x spacing** and `1e-5` in the **y spacing** edit fields, respectively.

9 Click **OK**.

Next, draw a projection of the 3D geometry and then extrude it to create a 3D object:

1 From the **Draw** menu, select **Specify Objects>Rectangle**.

2 Type `1e-5` in the **Width** and `8e-5` in the **Height** edit fields, respectively.

3 Type `-1e-4` in the **x** edit field in the **Position** area using the **Corner** option in the **Base** list.

4 Click **OK**.

5 Click the **2nd Degree Bezier Curve** tool button.

6 Click the coordinates (-9e-5, 8e-5), (-9e-5, 9e-5), and (-8e-5, 9e-5) to create an arc.

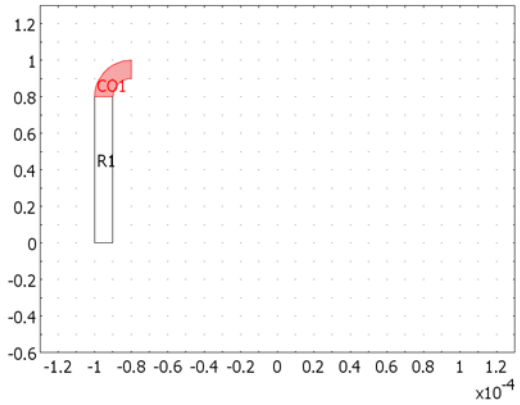
7 Click the **Line** tool button.

8 Click the coordinate (-8e-5, 1e-4).

9 Click the **2nd Degree Bezier Curve** tool button.

10 Click the coordinates (-1e-4, 1e-4) and (-1e-4, 8e-5).

11 Click the right mouse button to form a composite object with the shape of an elbow.

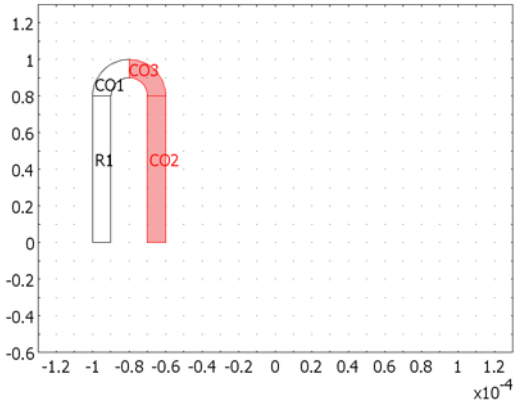


12 Press Ctrl+A to select all objects.

13 Click the **Mirror** tool button.

14 Enter `-8e-5` in the **x** edit field in the **Point on line** row in the **Paste** dialog box. Make sure that the normal vector to the line has the default values (1, 0).

15 Click **OK**.



16 Press Ctrl+A to select and Ctrl+C to copy all objects.

17 Press Ctrl+V to paste all objects.

18 Enter `5e-5` in the **x** edit field for **Displacements** in the **Paste** dialog box.

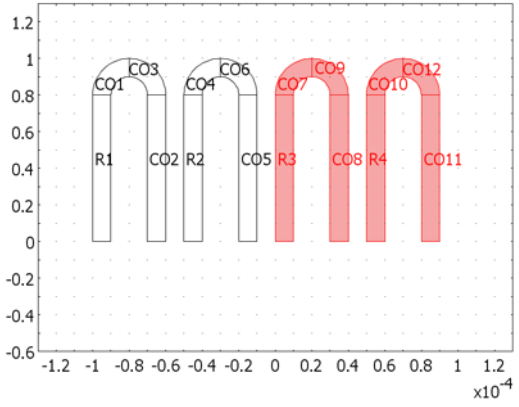
19 Click **OK**.

20 Press Ctrl+A to select and Ctrl+C to copy all objects.

21 Press Ctrl+C to paste all objects.

22 Enter `1e-4` in the **x** edit field for **Displacements** in the **Paste** dialog box.

23 Click **OK**.



24 Click **Zoom Extents**.

25 From the **Draw** menu, select **Specify Objects>Rectangle**.

26 Enter `3e-5` in the **Width**, `1e-5` in the **Height**, and `-7e-5` in the **x** edit fields, respectively.

27 Click **OK**.

28 Press Ctrl+C followed by Ctrl+V to copy and paste the selected rectangle.

29 Type `5e-5` in the **x** edit field for **Displacements**.

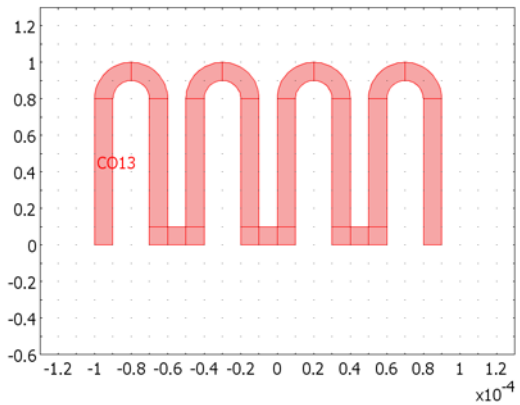
30 Click **OK**.

31 Press Ctrl+C followed by Ctrl+V to copy and paste the selected rectangle.

32 Type `5e-5` in the **x** edit field for **Displacements**.

33 Click **OK**.

34 Press Ctrl+A and click the **Union** button on the Draw toolbar to create one composite object.



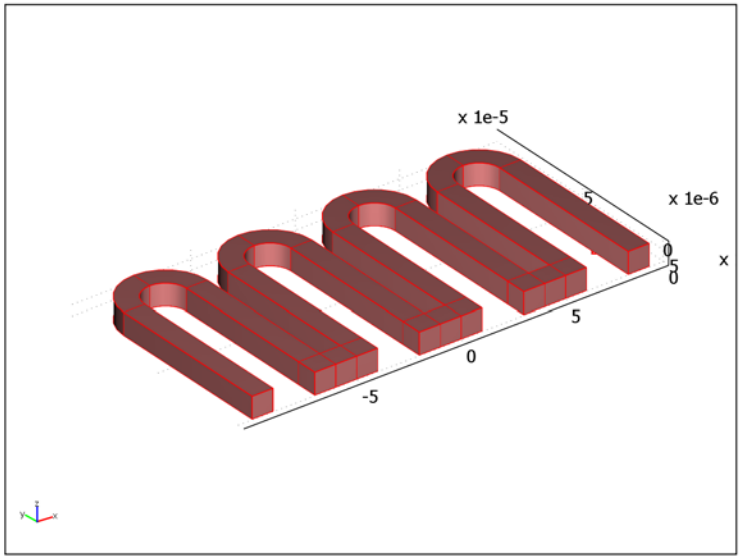
35 From the **Draw** menu, select **Extrude**.

36 Enter `1e-5` in the **Distance** edit field.

37 Click **OK**.

38 Click the **Headlight** button on the Camera toolbar.

The completed geometry in the drawing area should now look like that in the following figure.



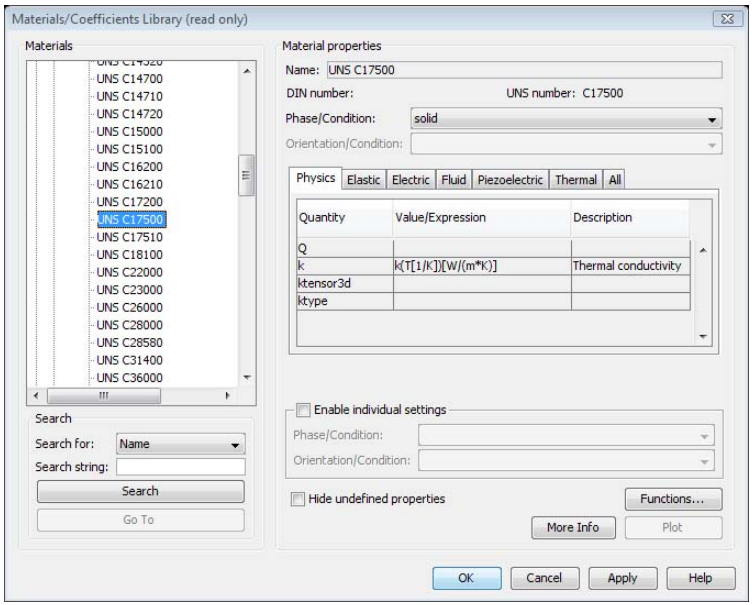
PHYSICS SETTINGS

Start by setting the properties and boundary conditions for the thermal analysis.

Subdomain Settings—Heat Transfer by Conduction

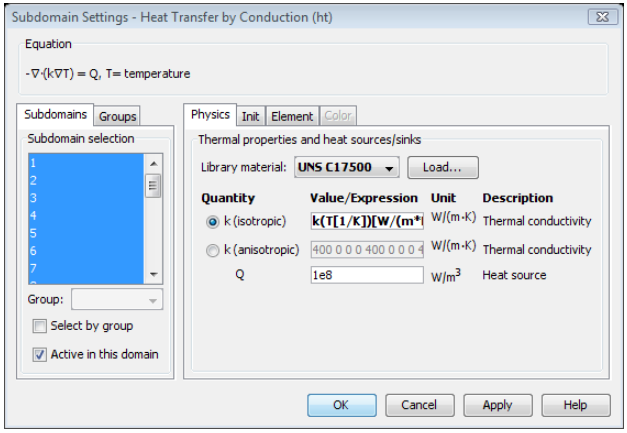
1. From the **Physics** menu, select **Subdomain Settings**.
2. Click the **Subdomain selection** list and press Ctrl+A to select all subdomains.
3. Click the **Load** button.
4. Click the **Material Library** node, which is second in the **Materials** list.
5. Click the **Al & Cu alloys** node.
6. Click the **Copper alloys** node.

7 Select the copper alloy **UNS C17500** from the list.



8 Click **OK**.

9 Enter `1e8` in the **Heat source** edit field.



10 Click **OK**.

Boundary Conditions—Heat Transfer by Conduction

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

2 Click the **Boundary selection** list.

3 Press Ctrl+A to select all boundaries.

4 In the **Boundary selection** list, press Ctrl and click Boundaries 2, 17, 26, 32, 52, 61, 67, 87, 96, 102, and 122 to clear them from the current selection. Note that you can also do this directly in the user interface by selecting all boundaries, clicking the right mouse button to keep the selection, and then selecting the boundaries corresponding to the attachment to the base one at the time. When you click on a boundary, it turns green. If this is the boundary you want to clear from the selection list, click the right mouse button. Repeat this procedure until all boundaries listed above are cleared from the selection.

5 Select **Heat Flux** from the **Boundary condition** list.

6 Enter 10 in the **Heat transfer coefficient** edit field and 298 in the **External temperature** edit field.

7 Click **OK**.

Subdomain Settings—Solid, Stress-Strain

1 From the **Multiphysics** menu, select the **Solid, Stress-Strain** application mode.

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

3 Select all the subdomains in the **Subdomain selection** list, if they are not already selected.

4 In the **Library material** list, select **UNS C17500**.

5 Click the **Load** tab. Note that the **Include thermal expansion** box is selected and that the variable for the temperature field, T, already appears in the **Strain temperature** edit field.

6 Type 293 in the **Strain ref. temperature** edit field. You can get the strain reference temperature from the Material Library. In this case, it is included in the notes for the thermal expansion coefficient function, alpha, in the Material Library.

7 Click **OK**.

Boundary Settings—Solid, Stress-Strain

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

2 Click the **Boundary selection** list and press Ctrl+D to clear the current selection.

3 Press Ctrl and click Boundaries 2, 17, 26, 32, 52, 61, 67, 87, 96, 102, and 122 to select the surfaces attached to the solid frame.

4 Select **Fixed** from the **Constraint condition** list.

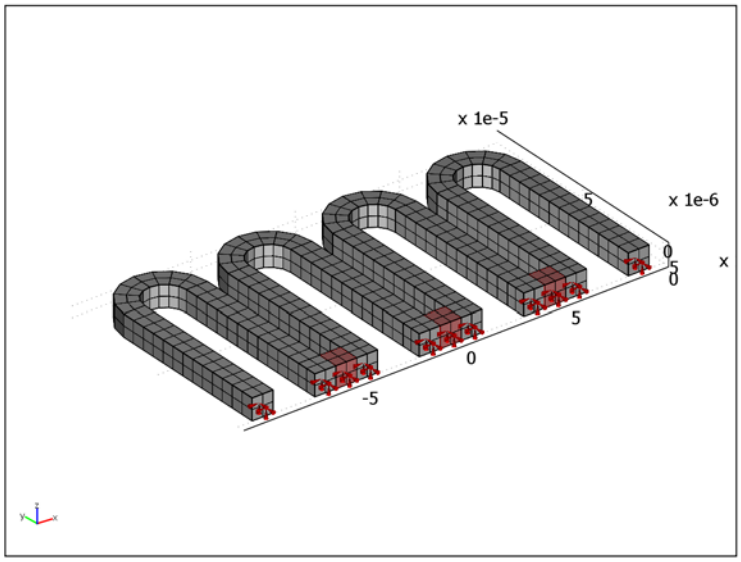
5 Click **OK**.

MESH GENERATION

1. Click the **Interactive Mesh** button.
2. Select Boundary 2, which is the left-most boundary attached to the solid frame.
3. Click the **Decrease Mesh Size** button to decrease the mesh size from normal to fine.
4. Click the **Decrease Mesh Size** button a second and a third time to decrease the mesh size to extra fine.
5. Click the **Mesh Selected (Mapped)** mesh button.
6. Click the **Subdomain Mode** button.
7. Select Subdomains 1–5, which are the five first domains from left to right. Note that you can do this by clicking the mouse until you get the desired subdomain highlighted, then you can right-click to save the selection. Then continue to the next subdomain, highlight it by clicking on it, and right-click to save the selection and so on until you have selected all five subdomains.
8. Click the **Mesh Selected (Swept)** button.

   The reason for not sweeping the mesh throughout all subdomains is that the meshing of the cube sections, which unite the U-shaped sections of the geometry, requires that you change the sweep direction in order to create only hexagonal mesh elements. If you instead mesh all U-shaped sections first, COMSOL Multiphysics detects the sweep dimension automatically by the fact that two opposite faces of the cubes are meshed. You can therefore first create a swept mesh for all U-shaped sections and then mesh the cubes to create a hexagonal mesh for the whole geometry.
9. Click the **Boundary Mode** button.
10. Select Boundaries 32, 67, and 102 by clicking on them in the user interface. Note that you can use the same strategy as outlined above—that is, to click on the desired boundary until it gets highlighted—then right-click to save the selection, and so on for multiple selections.
11. Click the **Mesh Selected (Mapped)** button.
12. Click the **Subdomain Mode** button.
13. Press Ctrl+D to clear the current selection.
14. Select Subdomains 7–12, 14–19, and 21–25 by using the strategy outlined in Point 7 above.
15. Click the **Mesh Selected (Swept)** button.
16. Select Subdomains 6, 13, and 20.

17 Click the **Mesh Selected (Swept)** button.



COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar. Note that the solution is fully coupled, which is not required in this case. You can solve the thermal balance first because it does not depend on the structural analysis. The structural analysis does require the temperature field in order to calculate the loads due to thermal expansion. If you are familiar with the use of the Solver Manager, you can use it to solve the problem sequentially.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 3-22, visualizing the surface temperature and the structural deformation of the device, follow these instructions:

1 Click the **Plot Parameters** button.

2 Click the **General** tab.

3 Clear the **Slice** box.

4 Select the **Boundary** box.

5 Select the **Deformed shape** box.

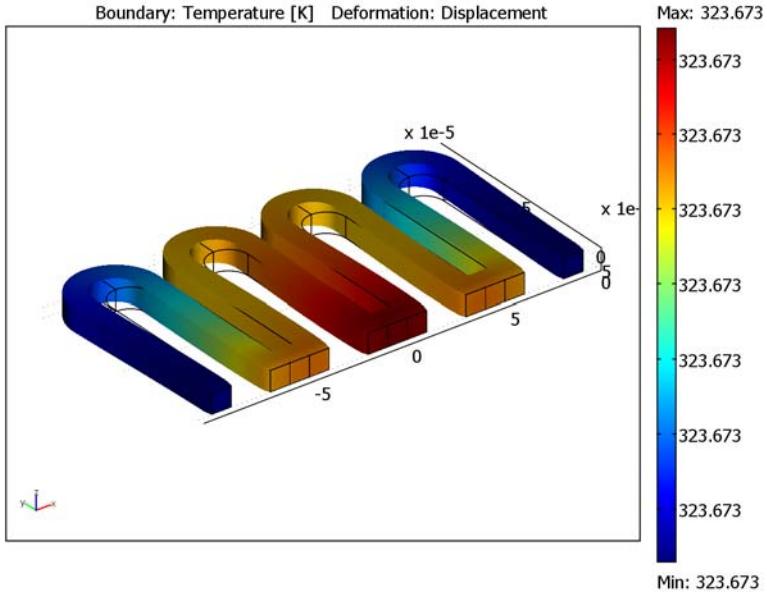
6 Click the **Boundary** tab.

7 In the **Expression** edit field type T.

8 Click the **Deform** tab.

9 On the **Subdomain Data** page, select **Solid, Stress-Strain (smsld)>Displacement** in the **Predefined quantities** list (the default option).

10 Click **OK**.



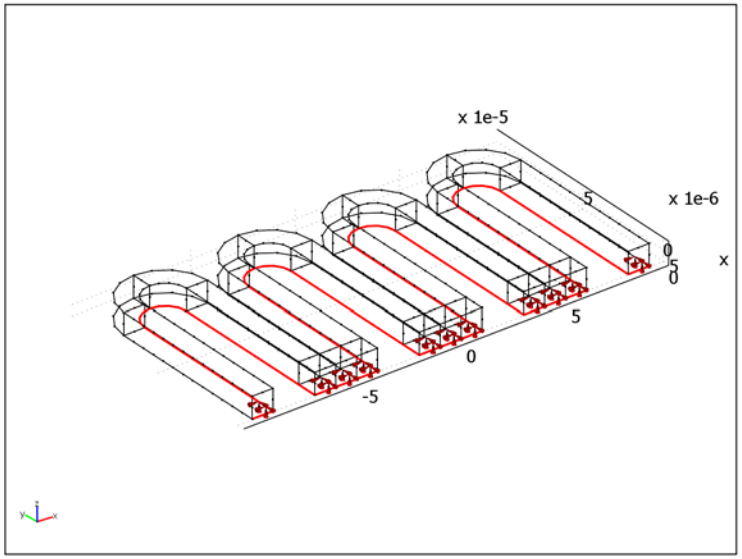
Create the deformation plot in Figure 3-23 as follows:

1 Choose **Postprocessing>Cross-Section Plot Parameters**.

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

3 Select the inner boundary segments marked in the following figure. To add a segment that you have highlighted in red by clicking with the mouse to the selection

use right-click. The segment should then turn blue in the drawing area. Repeat this procedure until you have selected all inner boundary segments.



4 In the **Predefined quantities** list select **Solid, Stress-Strain (smsld)>Total displacement**.

5 On the **General** page, click the **Title/Axis** button.

6 Click the option button next to the **Title** edit field. Leave the edit field empty to obtain a plot without title.

7 Click the option button next to the **First axis label** edit field, then enter the label `Position along the edge [m]`.

8 Click the option button next to the **Second axis label** edit field, then enter the label `Displacement [m]`.

9 Click **OK** to close the **Title/Axis Settings** dialog box.

10 Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the plot.

4

Microfluidics Models

This chapter presents several microfluidics models including those that describe AC electrokinetically adjusted fluid flow in a microchannel, pressure-driven flow and electrophoresis in a microchannel system, fluid-structure interaction, fluid flow in a star-shaped microchannel, capillary filling, and electroosmotic flow and lamella micromixer models.

AC Electrokinetically Enhanced Surface Reactions

Introduction

This model studies the use of AC electrokinetic forces to enhance the rate of transport of reactants to a reaction surface on the wall of a microchannel. It was developed for the MEMS Module by Gaurav Soni, Marin Sigurdson, and Carl Meinhart of the Department of Mechanical and Environmental Engineering, University of California, Santa Barbara.

The modeled system mixes a small concentration of a biological analyte with the fluid in a microchannel where a reaction surface is located on the channel walls. The flow velocity perpendicular to the surface is so small that the analyte, which is supposed to bind to an antibody ligand on this surface, is transported mainly by diffusion. The rate of the binding reaction on the surface is usually large enough to bind practically all analyte molecules appearing there. Thus, the process is said to be transport limited and, in order to increase the reaction rate, the system must increase the transport of molecules to the reaction surface.

AC electrokinetic forces can generate swirling patterns in the fluid and thereby enhance the transport of the analyte to the reaction surface (Ref. 1). Biological immunoassays, which detect an analyte through their binding response to an antibody ligand, can use these flow patterns to great advantage.

The AC electrokinetic forces arise when the fluid absorbs energy from an applied nonuniform AC electric field by means of Joule heating. The temperature increase changes the fluid's conductivity and permittivity. Consequently the fluid experiences an effective or time-averaged volume force, which depends on the conductivity and permittivity gradients and on the field intensity. By changing the shape of the electric field it is possible to alter the fluid-flow pattern so that required amounts of analyte molecules reach the reaction surface.

Model Definition

Figure 4-1 shows the model geometry, which consists of a section of the channel 40 μm high and 250 μm long. Two electrodes, each 60 μm wide, are located on the

lower boundary at distances of 50 µm and 130 µm from the inlet. The reaction surface, 20 µm wide, is located on the top wall, 90 µm from the inlet.

The fluid flows from left to right. The incoming flow profile is characteristic for fully developed laminar flow, that is, it is parabolic with zero velocity at the channel walls. An applied electrothermal force creates swirling patterns in the flow at the channel's center.

The two electrodes produce an AC electric field that heats the fluid and creates the electrothermal force. The model assumes that the electrodes are perfect heat conductors and remain at a constant ambient temperature. At the inlet and the outlet, the temperature gradually approaches the ambient. At all other boundaries the model assumes that the channel is thermally and electrically insulated.

The incoming flow has a small concentration of a biological analyte, which the reaction surface on the upper boundary transports and adsorbs. Any remaining concentration exits the channel with the fluid at the right boundary.

Having solved for the steady-state flow for a given electric field and the resulting electrothermal force, this example reviews a transient simulation of the material balance of the analyte, assuming that the initial concentration in the channel is zero and that a given concentration of the analyte is injected at the inlet at time zero.

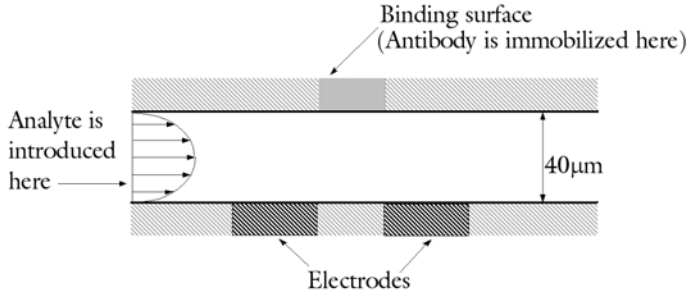


Figure 4-1: Model geometry for the microchannel with electrodes and a reaction surface.

FLUID FLOW

Fluid flow in the channel follows the Navier-Stokes equations

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \eta\nabla^2\mathbf{u} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{F}$$

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

where $\mathbf{u}$ denotes the velocity, ρ is the density, η is the dynamic viscosity, and p refers to the pressure. At steady state, the first time-dependent term disappears. The volume force $\mathbf{F}$ appearing in the equation is the electrothermal force $\mathbf{f}_E$ given by

$$\mathbf{F} = \mathbf{f}_E$$
$$\mathbf{f}_E = -0.5\left[\left(\frac{\nabla\sigma}{\sigma} + \frac{\nabla\varepsilon}{\varepsilon}\right)\cdot\mathbf{E}\frac{\varepsilon\mathbf{E}}{1+(\omega\tau)^2} + 0.5|\mathbf{E}|^2\nabla\varepsilon\right] \quad (4\text{-}1)$$

where σ is the conductivity, $\varepsilon = \varepsilon_r\varepsilon_0$ equals the fluid's permittivity, ω represents the electric field's angular frequency, and $\tau = \varepsilon/\sigma$ gives the fluid's charge-relaxation time. The field vector $\mathbf{E}$ contains the amplitude and orientation of the AC electric field but not its instantaneous value.

The following table gives the input data for the model:

NAME	VALUE	DESCRIPTION
ρ	1000 kg/m^3	Density of water
η	1.08·10^{-3} kg/(m·s)	Dynamic viscosity of water
σ	5.75·10^{-2} S/m	Conductivity of water
ε_r	80.2	Relative permittivity of water
ω	2π·15·10^3 rad/s	Angular frequency of the AC electric field

As a result of Joule heating, ε and σ are temperature dependent. You can rewrite the gradients of theses entities using chain differentiation, which yields

$$\nabla\varepsilon = (\partial\varepsilon/\partial T)\nabla T$$

and

$$\nabla\sigma = (\partial\sigma/\partial T)\nabla T$$

where T is the fluid's temperature. For water,

$$(1/\varepsilon)(\partial\varepsilon/\partial T) = -0.004\ \mathrm{K}^{-1}$$

and

$$(1/\sigma)(\partial\sigma/\partial T) = 0.02\ \mathrm{K}^{-1}$$

Thus you can rewrite the electrothermal force (Equation 4-1) as

$$\mathbf{f}_E = -0.5\varepsilon\left((0.016\ \mathrm{K}^{-1})\nabla T \cdot \mathbf{E}\frac{\mathbf{E}}{1+(\omega\tau)^2} + 0.5|\mathbf{E}|^2(-0.004\ \mathrm{K}^{-1})\nabla T\right)$$

The following table contains the boundary conditions for the incompressible Navier-Stokes equations:

BOUNDARY	CONDITION
Left	Parabolic inflow with average velocity 0.1 mm/s and zero velocity at the upper and lower boundaries
Upper	No slip condition
Lower	No slip condition
Right	Outflow with pressure p = 0

ELECTROSTATICS

Because the electrothermal force is a time-averaged entity, it is sufficient to solve the static electric field that corresponds to the root mean square (rms) value of the AC field. The rms value of the AC voltage is $V_{\mathrm{rms}} = 10$ V.

To solve the electrostatics problem, turn to Laplace's equation

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

with

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

and the constitutive equation

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$$

The boundary conditions for the electrostatic problem are as follows:

BOUNDARY	CONDITION
Left electrode	Electric potential, V = V_{rms}/2 = 5V
Right electrode	Electric potential, V = -V_{rms}/2 = -5V
Other boundaries	Electric insulation

HEAT TRANSFER

The power that a unit volume of fluid absorbs through Joule heating is

$$Q = \sigma|\mathbf{E}|^2$$

where $\mathbf{E}$ is the rms value of the electric field and σ is the fluid's conductivity. The heat source, Q, appears in the stationary heat balance equation

$$\nabla \cdot (-k\nabla T) = Q - \rho C_p \mathbf{u} \cdot \nabla T$$

where C_p denotes the heat capacity and k is the fluid's thermal conductivity. This is the nonconservative formulation of the heat balance, which is consistent with the assumption of a divergence-free flow field.

The following table gives the relevant input data for the heat-transfer problem:

NAME	VALUE	DESCRIPTION
ρ	1000 kg/m^3	Density of water
C_p	4.184·10^3 J/(kg·K)	Heat capacity of water
k	0.598 W/(m·K)	Thermal conductivity of water

In general, the Navier-Stokes equations along with the convection and conduction equation form a coupled system that you should solve simultaneously.

This example assumes an ambient temperature $T = 0$ °C, and the electrodes are held steady at this temperature. The flow rate is small, and you can therefore assume that the temperature decreases symmetrically at the inlet and the outlet. The magnitude of the temperature gradient at both boundaries is such that the fluid reaches the ambient temperature at a distance of 1 mm from the boundary. At all other boundaries the model assumes that the channel is insulated.

CONVECTION AND DIFFUSION OF THE ANALYTE

The material balance of the analyte comes from the equation

$$\delta_{ts}\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - \mathbf{u} \cdot \nabla c \,.$$

This equation gives the material balance in a nonconservative form because the flow field is divergence free. In this equation D denotes the diffusion coefficient and R represents the reaction rate. Here R equals zero because no reactions take place in the bulk of the fluid, only on the reaction surface.

The boundary conditions are as follows:

BOUNDARY	CONDITION
Left	The incoming flow has constant analyte concentration
Right	Remaining concentration leaves the system through convection

BOUNDARY	CONDITION
Reaction surface	Concentration consumed in the binding reaction as defined by Equation 4-2 (see next chapter)
Other boundaries	Boundaries are insulated and the concentration gradients normal to these boundaries equal zero

The following table gives the input data for the material balance:

NAME	VALUE	DESCRIPTION
δ_{ts}	1	Time-scaling coefficient
D	$1 \cdot 10^{-11}$ m^2/s	Diffusivity of the analyte in the fluid
R	0 M/s	No reaction takes place within the fluid
c_0	1 nM = 1 μmol/m^3	Inlet analyte concentration

BINDING REACTION

The reaction surface contains a total concentration R_t of antibody ligands. The portion of the bonded molecules is the concentration B. The binding rate depends on the analyte concentration on the surface, c, on the concentration of free antibodies, and on the association rate constant, k_{on}. Similarly, bonded antibodies dissociate with a rate that depends on the concentration of the bonded ligands and on the dissociation rate constant, k_{off}. Therefore, the equation that describes the material balance of adsorbed species (see Ref. 2) is:

$$\frac{\partial B}{\partial t} = k_{on} c (R_t - B) - k_{off} B \tag{4-2}$$

The reaction rate of the analyte on the surface equals the negative of the binding rate on the surface.

The table below gives the input data for the material balance of the adsorbed species:

NAME	VALUE	DESCRIPTION
k_{on}	10^8 (M·s)$^{-1}$ = 10^5 m^3/(mol·s)	Association rate constant
k_{off}	0.02 s^{-1}	Dissociation rate constant
R_t	$1.67 \cdot 10^{-11}$ M·m = $1.67 \cdot 10^{-8}$ mol/m^2	Total surface concentration of the antibody ligand

The model assumes that the antibodies do not diffuse on the surface and that there is no leakage of the molecules at the edges of the surface.

To study the effect of the applied electric field, you first run the model with $V_{rms} = 0$ V and then repeat the simulation for $V_{rms} = 10$ V.

STEP-RESPONSE ANALYSIS

Another interesting aspect to analyze is the system's behavior when injecting a fixed amount of analyte over a limited time with a sudden cutoff in the analyte supply. To simulate such an experiment, use the analyte inlet concentration expression

$$c(t) = \begin{cases} c_0 & t < t_1 \\ 0 & t > t_1 \end{cases} \quad (4\text{-}3)$$

with $t_1 = 1000$ s and $c_0 = 75$ nM = 75 μmol/m^3 (1 M ≡ 1 mol/l = 10^3 mol/m^3). For this analysis, modify the material balance input data according to the following table to obtain a reaction-rate limited process.

NAME	VALUE	DESCRIPTION
k_{on}	100 m^3/(mol·s)	Association rate constant
k_{off}	$5 \cdot 10^{-3}$ s^{-1}	Dissociation rate constant
R_t	$1.67 \cdot 10^{-11}$ mol/m^2	Total surface concentration of the antibody ligand

Results and Discussion

Figure 4-2 shows the flow profile and concentration distribution without any applied electric field. In this case, the flow is laminar and has a parabolic profile. The effect of the reaction surface on the analyte concentration is visible only in the narrow region near the surface. Compare it to the flow and concentration with an applied electric field (Figure 4-3). Now the flow profile is far from parabolic: it has two distinct swirls and a narrow region with high flow velocity between the electrodes. Both of these figures represent the situation 5 s after the system introduces analyte at the left boundary.

Figure 4-4 depicts the flow and concentration just 1 s after introducing the analyte. It shows more clearly how the swirling patterns in the flow focus the analyte on a narrower path near the reaction surface. This flow results in a difference in the adsorption rate of the molecules with and without the electric field, (Figure 4-5). The average number of adsorbed molecules—the ratio between the total amount and the surface width—on the surface increases more rapidly with the electric field (the curve with squares) than without the electric field (the curve with triangles).

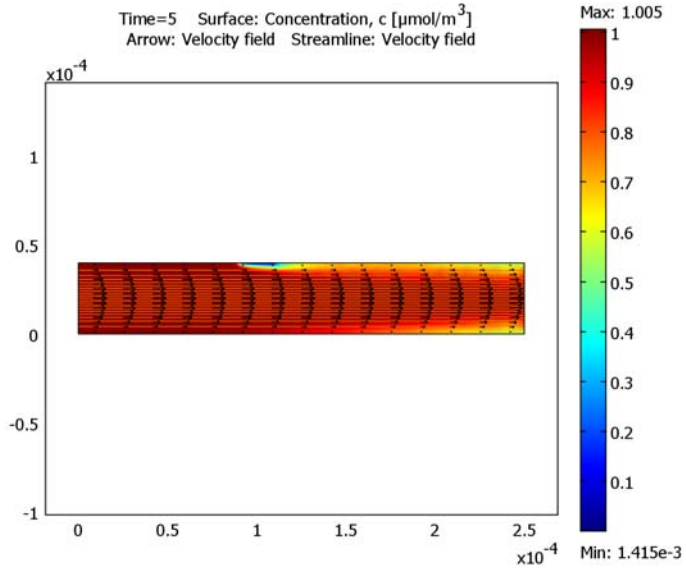


Figure 4-2: Microchannel flow and concentration at 5 s without any applied electric field.

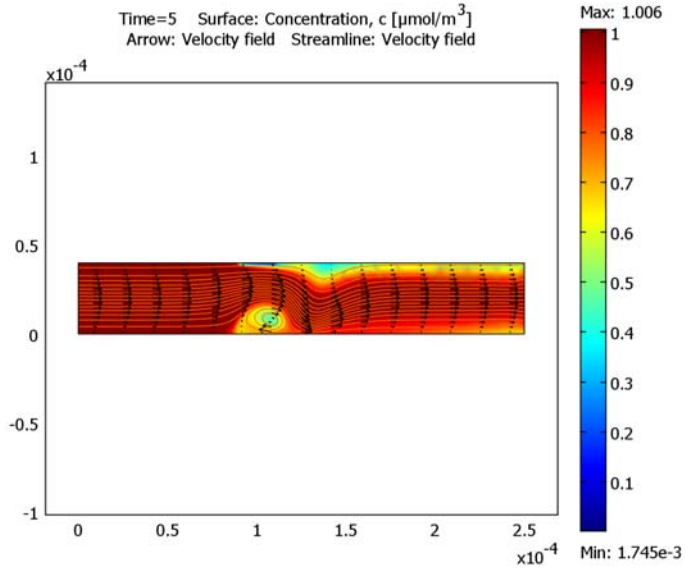


Figure 4-3: Microchannel flow and concentration at 5 s with an applied electric field.

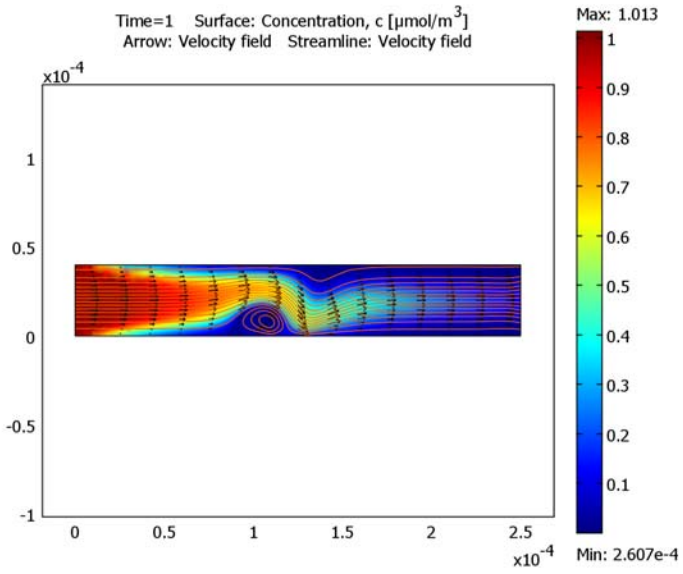


Figure 4-4: Microchannel flow and concentration at 1 s with an applied electric field.

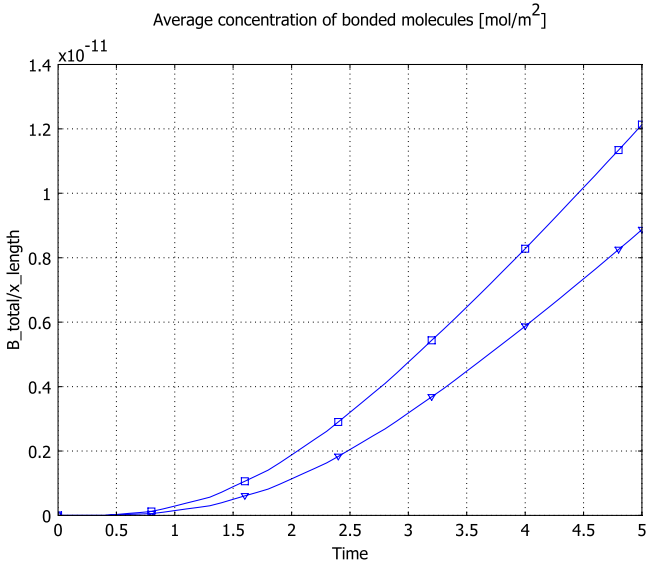


Figure 4-5: Binding of molecules on the reaction surface in the microchannel with (squares) and without (triangles) an applied electric field.

Figure 4-6 shows the result for the average concentration of bonded molecules of the third and final simulation, in which you cut off the analyte supply at $t = 1000$ s. During the phase when the analyte supply is kept constant, the concentration of molecules on the binding surface approaches a constant maximum value near 10^{-11} mol/m^2. When the supply at the inlet then stops, the concentration starts to decay. By varying the antibody ligand concentration and the association and dissociation rate constants, you can study the effects on the maximum concentration and the decay rate. Simulations of this kind can thus be useful for fitting a model to experimental data.

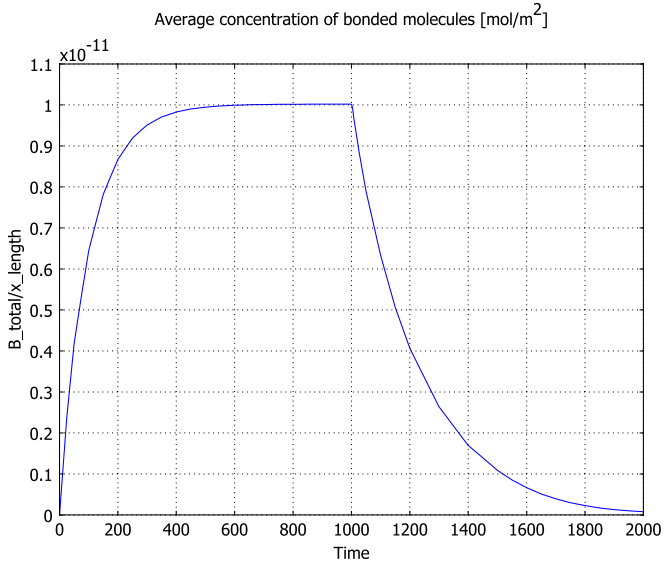


Figure 4-6: System response when the analyte supply at the inlet is cut off at t = 1000 s.

Modeling in COMSOL Multiphysics

This model solves the problem with two geometries and five application modes. Table 4-1 lists the geometries and their application modes.

The first geometry, named *channel*, is in 2D and represents the channel. Within this geometry the model uses four application modes: Electrostatics, Convection and Conduction, Incompressible Navier-Stokes, and Convection and Diffusion. The second geometry, named *surface*, is in 1D and simulates the reaction surface with the Diffusion application mode. The overall model couples this solution with the reaction

surface boundary condition of the Convection and Diffusion application mode on the first geometry. For this purpose you must define two extrusion-coupling variables.

You solve the model in three steps with different solvers in a progression using results from the previous step:

- First, solve the Electrostatics application mode with a stationary linear solver.
- Next, solve the Convection and Conduction and the Incompressible Navier-Stokes application modes together using a stationary nonlinear solver, because they form a coupled system through their subdomain settings.
- In the third step you use the time-dependent solver to solve the transport of the analyte. At this point the software solves two application modes simultaneously: Convection and Diffusion, and Diffusion.

COMSOL Multiphysics' solver scripting capabilities allow you to record these solving stages, a feature which greatly facilitates repeated simulations.

TABLE 4-1: GEOMETRY AND APPLICATION MODE DESCRIPTION

GEOMETRY	APPLICATION MODE	VARIABLES	DESCRIPTION
channel	Electrostatics	V	Solves the static electric potential in the channel
channel	Convection and Conduction	T	Solves the temperature distribution in the channel
channel	Incompressible Navier-Stokes	u, v, p	Solves the velocities in the x and y directions and the pressure distribution in the channel
channel	Convection and Diffusion	c	Solves the concentration of the analyte in the channel
surface	Diffusion	B	Solves the concentration of the binded antibodies on the reaction surface

References

1. A. Ramos, H. Morgan, N.G. Green, and A. Castellanos, "AC electrokinetics: A review of forces in microelectrode structures," *J. Phys. D: Appl. Phys.*, vol. 31, pp. 2338–2353, 1998.

2. D.G. Myszka, "Survey of the 1998 optical biosensor literature," *J. Mol. Recognit.*, vol. 12, pp. 390–408, 1999.

Model Library path:
`MEMS_Module/Microfluidics_Models/ac_electrokinetic_2d`

Modeling Using the Graphical User Interface

MODEL LIBRARY

1 In the **Model Navigator**, click the **New** tab, then click the **Multiphysics** button.

2 Click the **Add Geometry** button.

3 Enter these settings in the dialog box:

FIELD	VALUE
Geometry name	`channel`
Space dimension	2D
Independent variables	`x y z`

4 Click **OK**.

5 Click the **Add Geometry** button once again and enter these settings:

FIELD	VALUE
Geometry name	`surface`
Space dimension	1D
Independent variables	`x y z`
Unit system	None

Because the available unit systems give the wrong reference dimension for the 1D geometry, use the last setting to disable units for this geometry.

6 Click **OK**.

7 In the **Multiphysics** area, select the geometry **channel (2D)**.

8 In the list of application modes, select **MEMS Module>Electrostatics>Electrostatics**, then click the **Add** button in the **Multiphysics** area.

9 Select the application mode **COMSOL Multiphysics>Heat Transfer>Convection and Conduction**, then click the **Add** button.

10 Select **MEMS Module>Microfluidics>Incompressible Navier-Stokes**, then click **Add**.

11 Select **MEMS Module>Microfluidics>Convection and Diffusion>Transient analysis**, then click **Add**.

12 In the **Multiphysics** area, select the geometry **surface (1D)**.

13 Select **COMSOL Multiphysics>Convection and Diffusion>Diffusion>Transient analysis**. In the **Dependent variables** edit field type `B`, then click **Add**.

14 Click **OK**.

OPTIONS AND SETTINGS

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

2 Define the following names, expressions, and (optionally) descriptions; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
epsilon0	8.854188e-12[F/m]	Permittivity of free space
epsilonr_f	80.2	Relative permittivity, fluid
epsilon_f	epsilonr_f*epsilon0	Permittivity, fluid
k_f	0.598[W/(m*K)]	Thermal conductivity, fluid
rho_f	1000[kg/m^3]	Density, fluid
Cp_f	4.184[kJ/(kg*K)]	Heat capacity, fluid
eta_f	1.08e-3[Pa*s]	Dynamic viscosity, fluid
sigma_f	5.75e-2[S/m]	Electric conductivity, fluid
tau	epsilon_f/sigma_f	Charge relaxation time, fluid
D_a	1e-11[m^2/s]	Diffusion coefficient, analyte
omega	2*pi[rad]*15[kHz]	Angular frequency, AC electric field
V_rms	0[V]	Electric potential, RMS value
T_amb	0[degC]	Ambient temperature
u_av	0.1[mm/s]	Average flow velocity at the inlet
c0	1[umol/m^3]	Analyte concentration at the inlet
k_on	1e5[m^3/(mol*s)]	Association rate constant
k_off	0.02[1/s]	Dissociation constant
R_t	1.67e-8[mol/m^2]	Total surface concentration, antibody ligand

Later, you change the value of the electric potential to 10 V and re-solve the model.

GEOMETRY MODELING

First create the 2D geometry for the channel.

1 Click the **channel** tab in the drawing area.

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

3 In the dialog box, click the **Axis** tab, select the **Axes equal** check box, and enter these settings:

SETTING	VALUE
x min	-5e-5
x max	30e-5
y min	-5e-5
y max	10e-5

4 Click the **Grid** tab.

5 Clear the **Auto** check box and make these settings:

SETTING	VALUE
x spacing	1e-5
y spacing	1e-5

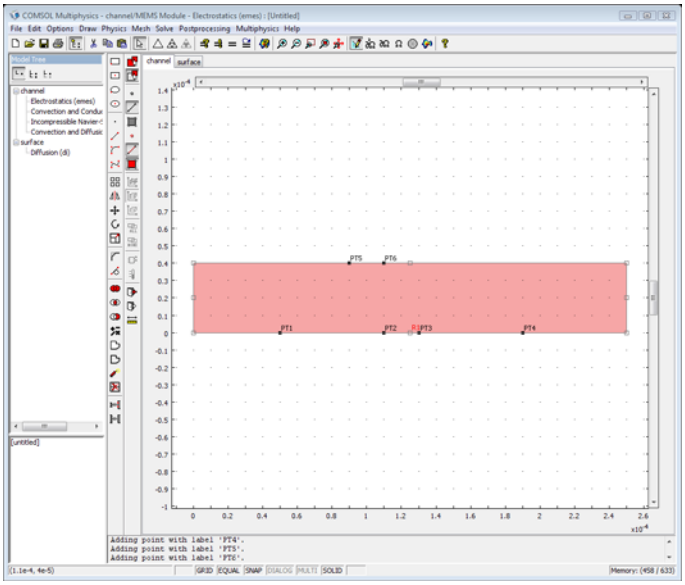
6 Click **OK**.

7 Click the **Rectangle/Square** button on the Draw toolbar and draw a rectangle with diagonally opposite corners at (0, 0) and ($2.5 \cdot 10^{-4}$, $4 \cdot 10^{-5}$).

8 Draw the following points by successively using the **Point** tool in the Draw toolbar.

NAME	x	y
PT1	0.5e-4	0
PT2	1.1e-4	0
PT3	1.3e-4	0
PT4	1.9e-4	0
PT5	0.9e-4	0.4e-4
PT6	1.1e-4	0.4e-4

The completed 2D geometry should look like that in the following picture:



The completed 2D geometry for a microchannel detector.

Next create the 1D geometry for the reaction surface.

1 Click the **surface** tab.

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

3 In the dialog box, click the **Axis** tab, then enter these settings:

SETTING	VALUE
x min	-5e-5
x max	30e-5

4 Click the **Grid** tab. Clear the **Auto** check box. In the **x spacing** edit field type `1e-5`, then click **OK**.

5 On the Draw toolbar select the **Line** tool and draw a line from $0.9 \cdot 10^{-4}$ to $1.1 \cdot 10^{-4}$.

The geometry is now complete.

Expressions and Coupling Variables

Follow these steps to create the expressions for computing the electrothermal force, to define the expressions and coupling variables needed to solve the binding reaction, and provide the integration-coupling variables needed for postprocessing.

Note: You create expressions separately for the two geometries.

Start by defining scalar expressions for the electrothermal force components.

1 Click the **channel** tab to select that geometry.

2 From the **Options** menu, choose **Expressions>Scalar Expressions**.

3 In the dialog box, enter the expressions in the following table for the x- and y-components of the electrothermal force. Note that this example uses the expressions `tmp1` and `tmp2` only to simplify the writing of `Fx_et` and `Fy_et`.

NAME	EXPRESSION
tmp1	(Tx*Ex_emes+Ty*Ey_emes)/(1+(omega*tau)^2)
tmp2	normE_emes^2
Fx_et	-0.5*epsilon_f*(0.016[1/K]*tmp1*Ex_emes-0.5*0.004[1/K]*tmp2*Tx)
Fy_et	-0.5*epsilon_f*(0.016[1/K]*tmp1*Ey_emes-0.5*0.004[1/K]*tmp2*Ty)

4 Click **OK**.

Next set the expressions and extrusion-coupling variables you need to solve the surface reaction.

1 From the **Options** menu, choose **Expressions>Boundary Expressions**.

2 In the **Boundary selection** list, select Boundary 5.

3 Create the following boundary expression (`c_surf` is an extrusion coupling variable that you define later):

NAME	EXPRESSION
react_bulk	k_off*c_surf-k_on*c*(R_t-c_surf)

COMSOL Multiphysics marks the unit of `react_bulk` as inconsistent because of the coupling variable. You can disregard this warning.

4 Click **OK**.

5 Click the **surface** tab to select that geometry.

6 From the **Options** menu, choose **Expressions>Subdomain Expressions**.

7 In the **Subdomain selection** list, select Subdomain 1.

8 Define the following subdomain expression (the term `c_bulk` is an extrusion-coupling variable that you define next); when done, click **OK**.

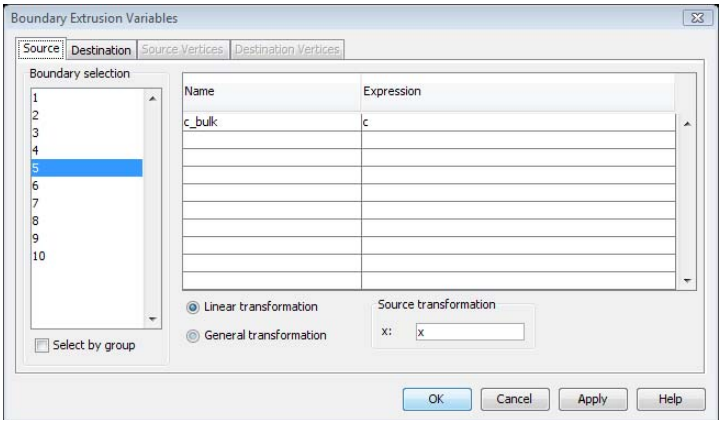
NAME	EXPRESSION
`react_surf`	`k_on*c_bulk*(R_t-B)-k_off*B`

9 Click the **channel** tab to select that geometry.

10 From the **Options** menu, choose **Extrusion Coupling Variables>Boundary Variables**.

11 Select Boundary 5. In the first row of the **Name** column type `c_bulk`, then type `c` in the corresponding **Expression** column.

12 Click the **General transformation** option button.

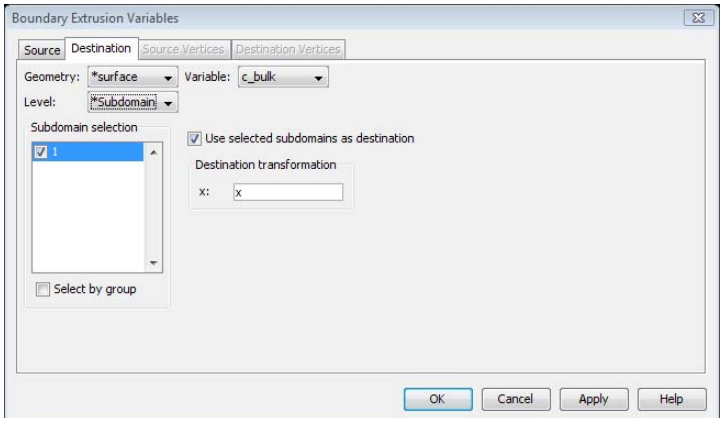


Configuring the source of the extrusion coupling variable for the channel geometry.

13 Click the **Destination** tab.

14 From the **Geometry** list select **surface**, and from the **Level** list select **Subdomain**.

15 In the **Subdomain selection** list, click the check box to select Subdomain 1. Make sure the **Use selected subdomains as destination** check box is selected.



Configuring the destination of the extrusion coupling variable for the channel geometry.

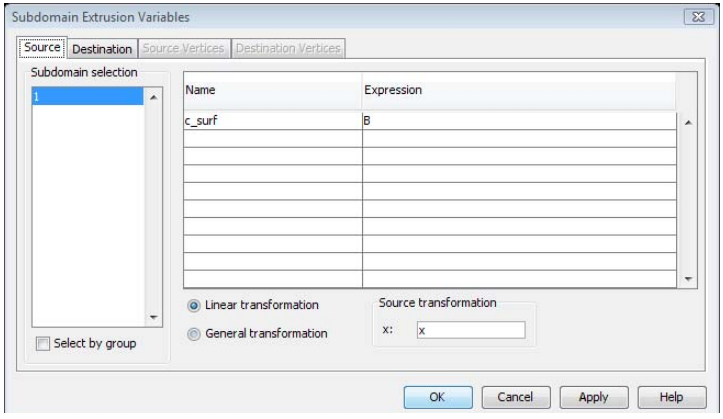
16 Click **OK**.

17 Verify that you still have the **surface** tab selected; if it is not selected, click it.

18 From the **Options** menu, choose **Extrusion Coupling Variables>Subdomain Variables**.

19 From the **Subdomain selection** list select **1**, go to the first row in the **Name** column and enter `c_surf`, then type `B` in the corresponding **Expression** column.

20 Click the **General transformation** option button.

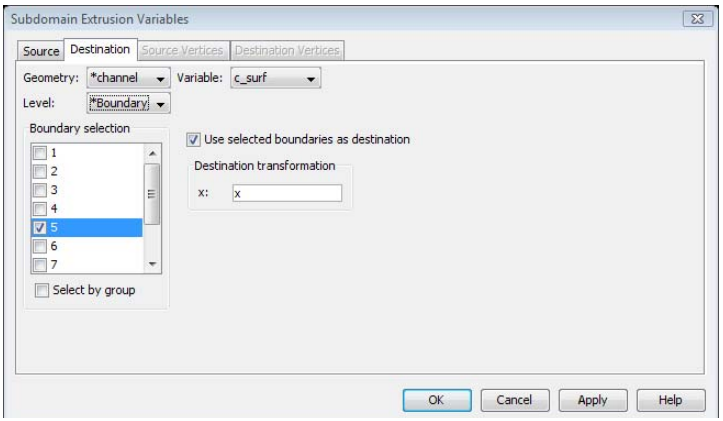


Configuring the source of the extrusion coupling variable for the surface geometry.

21 Click the **Destination** tab.

22 From the **Geometry** list select **channel**, and from the **Level** list select **Boundary**.

23 In the **Boundary selection** list, click the check box to select Boundary 5. Make sure the **Use selected boundaries as destination** check box is selected.



Configuring the destination of the extrusion coupling variable for the surface geometry.

24 Click **OK**.

Finally set the integration-coupling variables needed for postprocessing. They represent the total amount of bonded molecules on the reaction surface and its length, respectively. Their ratio thus gives the average concentration of bonded molecules at the surface.

1 Select the **surface** geometry.

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

3 Select Subdomain 1 and enter these settings:

NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
B_total	B	4	Selected
x_length	1	4	Selected

4 Click **OK**.

Subdomain Settings

1 From the **Multiphysics** menu, select **1 channel: Electrostatics (emes)**.

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

3 Select Subdomain 1.

4 Under the options for the **Constitutive relation** click the option button corresponding to $\mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}$.

5 In the **Relative permittivity** edit field type `epsilonr_f`, then click **OK**.

6 From the **Multiphysics** menu, select **2 channel: Convection and Conduction (cc)**.

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

8 Select Subdomain 1, then enter settings as in this table; when finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
k (isotropic)	`k_f`	Thermal conductivity
ρ	`rho_f`	Density
C_p	`Cp_f`	Heat capacity at constant pressure
Q	`sigma_f*normE_emes^2`	Heat source
u	`u`	x-velocity
v	`v`	y-velocity

9 From the **Multiphysics** menu, select **3 channel: Incompressible Navier-Stokes (mmglf)**.

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

11 In the dialog box select Subdomain 1, then enter these settings:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ	`rho_f`	Density
η	`eta_f`	Dynamic viscosity
F_x	`Fx_et`	Volume force, x dir.
F_y	`Fy_et`	Volume force, x dir.

12 Click the **Init** tab. In the **x-velocity** edit field, type `u_av`. Click **OK**.

13 From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.

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

15 Select Subdomain 1, then enter settings as in the following table; for the **Time-scaling coefficient** and the **Reaction rate**, leave the default settings. When finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
D (isotropic)	`D_a`	Diffusion coefficient
u	`u`	x-velocity
v	`v`	y-velocity

I6 From the **Multiphysics** menu, choose **5 surface: Diffusion (di)**.

I7 From the **Physics** menu, select **Subdomain Settings**.

I8 Select Subdomain 1, then enter these settings; when finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
D	0	Diffusion coefficient
R	`react_surf`	Reaction rate

Boundary Conditions

1 From the **Multiphysics** menu, choose **1 channel: Electrostatics (emes)**.

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

3 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 4	BOUNDARY 8	BOUNDARIES 1–3, 5–7, 9, 10
Boundary condition	Electric potential	Electric potential	Zero charge/ Symmetry
V_0	`V_rms/2`	`-V_rms/2`	

4 From the **Multiphysics** menu, choose **2 channel: Convection and Conduction (cc)**.

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

6 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARIES 1, 10	BOUNDARIES 4, 8
Boundary condition	Heat flux	Temperature
q_0	`-k_f*(T-T_amb)/1[mm]-nx*u*rho_f*Cp_f*T`	
T_0		`T_amb`

The default boundary condition (thermal insulation) applies to the boundaries not listed in the table.

7 From the **Multiphysics** menu, select **3 channel: Incompressible Navier-Stokes (mmglf)**.

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

9 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 10	BOUNDARIES 2–9
Boundary type	Inlet	Outlet	Wall
Boundary condition	Laminar inflow	Pressure, no viscous stress	No slip

SETTINGS	BOUNDARY 1	BOUNDARY 10	BOUNDARIES 2–9
U_0	u_av		
L_{entr}	1e-4		
Constrain end points to zero	Yes		
P_0		0	

10 From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.

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

12 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 10	BOUNDARIES 2–4, 6–9
Boundary condition	Concentration	Flux	Convective flux	Insulation/ Symmetry
c_0	c0			
N_0		react_bulk		

13 From the **Multiphysics** menu, select **5 surface: Diffusion (di)**.

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

15 Verify that the **Boundary condition** is set to **Insulation/Symmetry** on both boundaries.

16 Click **OK**.

MESH GENERATION

1 Select the **channel** geometry.

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

3 Click the **Boundary** tab.

4 Select Boundaries 4, 5, and 8.

5 In the **Maximum element size** edit field type `0.2e-6`.

6 Click the **Remesh** button to initialize the mesh for the **channel** geometry. Click **OK**.

7 Select the **surface** geometry.

8 Click the **Initialize Mesh** button on the Main toolbar to initialize the mesh for the **surface** geometry.

COMPUTING THE SOLUTION

You solve the model in three steps using three different solvers.

1 Click the **Solver Manager** button on the Main toolbar to launch the **Solver Manager**.

2 On the **Script** page, select the **Automatically add commands when solving** check box. With this setting, COMSOL Multiphysics records the subsequent solver commands so that you can reuse them when you later solve the model for $V_{\text{rms}} = 10$ V.

3 On the **Solve For** page, select **channel (2D)>Electrostatics (emes)**.

4 Click **Solve**.

5 Click the **Initial Value** tab. In the **Values of variables not solved for and linearization point** area, select the **Current solution** option button.

6 Return to the **Solve For** page. Select the application modes **channel (2D)>Convection and Conduction (cc)** and **channel (2D)>Incompressible Navier-Stokes (mmglf)**.

7 Click **Solve**.

8 Click the **Solver Parameters** button on the Main toolbar to launch the **Solver Parameters** dialog box.

9 From the **Solver** list, select **Time dependent**.

10 On the **General** page, type `0:0.1:5` in the **Times** edit field in the **Time stepping** area.

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

12 Return to the **Solver Manager**.

13 On the **Solve For** page, select the application modes **channel (2D)>Convection and Diffusion (chcd)** and **surface (1D)>Diffusion (di)**.

14 Click **OK** to close the **Solver Manager** dialog box.

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

POSTPROCESSING AND VISUALIZATION

Begin by visualizing the fluid flow and the analyte concentration in the flow channel after 5 s.

1 In the drawing area, select the **channel** geometry.

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

3 On the **General** page of the **Plot Parameters** dialog box, select the check boxes for **Surface**, **Arrow**, **Streamline**, and **Geometry edges**. Make sure the **Solution at time** list is initialized to **5**.

4 Click the **Surface** tab. From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**. In the **Unit** edit field, type `umol/m^3`.

5 Click the **Arrow** tab. In the **Plot arrows on** list select **Subdomains**.

6 Click the **Subdomain Data** tab. From the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

7 In the **Arrow parameters** area, find the **Arrow length** list and select **Proportional**.

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

9 Go to the **Streamline** page. Click the **Streamline Data** tab, then in the **Predefined quantities** list select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

10 From the **Streamline plot type** list, select **Magnitude controlled**.

11 Click the **Line Color** tab. Select the **Uniform color** option button. Click the **Color** button, then select the orange color corresponding to the RGB values (255, 102, 0). To do so, click the **RGB** tab and enter the values directly. Click **OK** to close the **Streamline Color** dialog box.

12 Return to the **General** page. From the **Plot in** list, select **New figure**.

13 Click **OK** to generate the plot in Figure 4-2 on page 249.

Next, generate the first graph in Figure 4-5 on page 250 with the following steps:

1 Select the **surface** geometry.

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

3 On the **General** page, verify that all solutions in the **Solutions to use** list are selected. From the **Plot in** list, select **New figure**.

4 Click the **Point** tab. In the **y-axis data** area, type `B_total/x_length` in the **Expression** edit field. In the **Coordinates** area, type `1e-4` in the **x** edit field.

5 Click the **Line Settings** button. From the **Line marker** list select **Triangle**, then click **OK** to close the **Line Settings** dialog box.

6 Click **OK**.

Leave the figure windows open to enable comparison with the solutions for the case where an electric field has been applied.

Re-Solve the Model with an Applied Electric Field

In this second part of the modeling session, you apply an external electric field.

OPTIONS AND SETTINGS

Choose **Options>Constants**. Change the **Expression** for `V_rms` to `10[V]`, then click **OK**.

COMPUTING THE SOLUTION

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

2 On the **Script** page, select **Solve using a script** check box. The following solver script appears in the script area (the orders between the entries in the `solcomp` and `outcomp` lists can vary):

3 Click **OK** to close the **Solver Manager**.

4 Click the **Solve** button on the Main toolbar. The software automatically repeats all the solving stages you recorded in the first part of this model to compute the solution for $V_{rms} = 10$ V.

POSTPROCESSING AND VISUALIZATION

1 In the drawing area, select the **channel** geometry.

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

3 On the **General** page, select **New figure** from the **Plot in** list. Click **Apply**.

The plot displayed in Figure 4-3 on page 249—visualizing the fluid flow and the analyte concentration in the flow channel after 5 s in the presence of an electric field —should now appear in the Figure 3 window. To plot the same quantities at $t = 1$ s, proceed with the following steps:

4 Still on the **General** page, from the **Solution at time** list select **1**.

5 From the **Plot in** list select **New figure**, then click **OK**.

The new figure window now contains a plot resembling that in Figure 4-4. This is the plot you see in the Model Navigator if you open the model from the Model Library.

Finally, finish reproducing Figure 4-5, which illustrates the binding rate of the analyte, by executing the following instructions:

1. Select the **surface** geometry.
2. From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
3. On the **Point** page, click the **Line Settings** button. From the **Line marker** list select **Square**, then click **OK** to close the **Line Settings** dialog box.
4. Click the **General** tab.
5. Select the **Keep current plot** check box.
6. Click the **Title/Axis** button.
7. Activate the **Title** edit field, then enter the title `Average concentration of bonded molecules [mol/m<sup>2</sup>]`.

   The HTML tags produce a superscript figure "2" for the exponent.
8. Click **OK** to close the **Title/Axis Settings** dialog box.
9. Click **OK** to generate the plot.

The two graphs in the Figure 2 window should now look like those in Figure 4-5.

To study an animation of the solution, click the **Animate** button on the Plot toolbar.

Step-Response Simulation

OPTIONS AND SETTINGS

From the **Physics** menu, select **Constants**. Edit the expressions for the four last constants according to the following table; when done, click **OK**.

NAME	EXPRESSION
c0	75[umol/m^3]
k_on	100[m^3/(mol*s)]
k_off	5e-3[1/s]
R_t	1.67e-11[mol/m^2]

PHYSICS SETTINGS

1. From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.
2. From the **Physics** menu, select **Boundary Settings**. Select Boundary 1.

3 Change the entry in the c_0 edit field to `c0*(t<1000[s])`, then click **OK**.

The logical expression implements the step function in Equation 4-3.

COMPUTING THE SOLUTION

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

2 Change the entry in the **Times** edit field to `0:25:950 975:1025 1050:50:2000`.

3 Set the **Relative tolerance** to `1e-4` and the **Absolute tolerance** to `1e-3`.

4 Click the **Time Stepping** tab.

5 From the **Time steps taken by solver** list, select **Intermediate**.

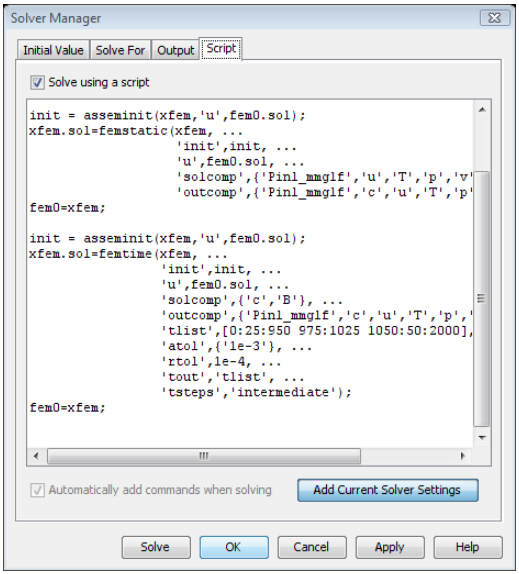
6 Click **OK** to close the **Solver Parameters** dialog box.

7 Click the **Solver Manager** button on the Main toolbar.

8 On the **Script** page, click the **Add Current Solver Settings** button.

A `femtime` command with the current solver settings appears in the script area.

9 Because this command should replace the previous one, cut out the complete *upper* `femtime` command together with the `asseminit` command line immediately before it as well as the `fem0=xfem;` line immediately after it. When you are done, the contents of the script area should be as in the following figure (again, the entries in the `solcomp` and `outcomp` lists can be ordered differently).



10 Click **OK** to close the **Solver Manager**.

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

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 4-6, follow these steps:

1 Select the **surface** geometry.

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

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

4 On the **Point** page, click the **Line Settings** button. From the **Line marker** list select **None**, then click **OK** to close the **Line Settings** dialog box.

5 Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the plot.

Transport in an Electrokinetic Valve

Introduction

This model presents an example of pressure-driven flow and electrophoresis in a microchannel system.

Researchers often use a device similar to the one in this model as an electrokinetic sample injector in biochips to obtain well-defined sample volumes of dissociated acids and salts and to transport these volumes. The model presents a study of a pinched injection cross valve during the focusing, injection, and separation stages. Inspiration for the model comes from a study by Ermakov and others (Ref. 1). Focusing is obtained through pressure-driven flow of the sample and buffer solution, which confines the sample in the focusing channel. When the system reaches steady state, the pressure-driven flow is turned off and an electric field is applied along the channels. This field drives the dissociated sample ions in the focusing zone at right angles to the focusing channel and through the injection channel. A clean separation of the sample ions is important, so the model examines the effect on ion separation of different configurations of the electric field.

This specific case does not account for electroosmosis because the channel surfaces are subjected to a treatment that minimizes the extension of the electric double layer.

Model Definition

Figure 4-7 shows a 2D cross section of the geometry in the *xz*-plane and points out the different channels and boundaries. The horizontal channel serves as the focusing channel, while the vertical channel is the injection channel. The actual model is in 3D with rectangular pipes whose corners are rounded. For geometry dimensions refer to Table 4-3 on page 279.

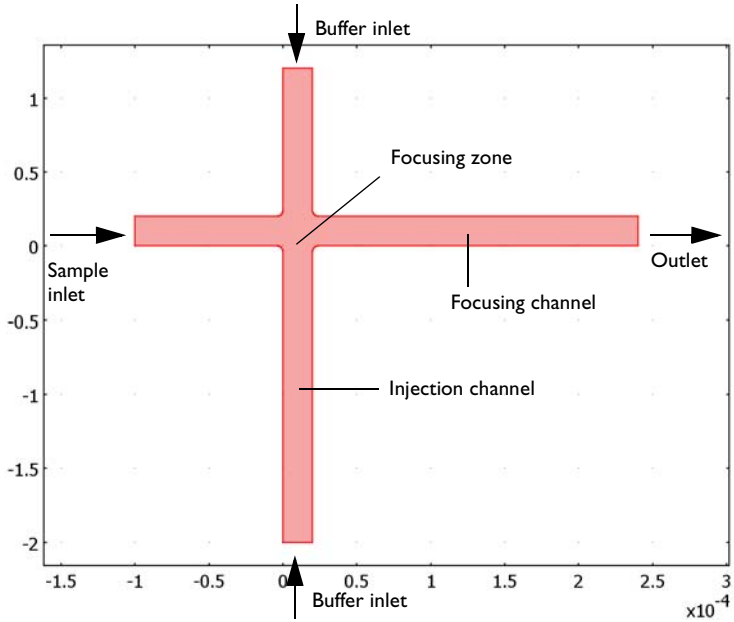


Figure 4-7: The focusing stage involves pressure-driven flow of both the sample and the buffering solution. The device applies an electric field over the focusing channel.

The device operation and hence the modeling procedure takes place in two stages: focusing and injection.

In the focusing stage, the device injects a buffering solution through pressure-driven convection into the vertical channels from the top and bottom. At the same time, it forces the sample solution through the horizontal focusing channel (see Figure 4-7). The buffering solution neutralizes the acids contained in the sample except for a very thin region confined to the crossing between the horizontal and vertical channels. This means that the dissociated ions are only in a needle-shaped region in the focusing zone.

Next, in the injection stage the device turns off the convective flow and then applies a vertical field to migrate the sample from the focusing channel to the injection point at the lower end of the vertical channel. The sample ions are negatively charged and migrate in opposite direction to the electric field. This model studies two different configurations (See Table 4-2) for the applied electric field. In the first configuration (Injection stage, Mode A) electric field is only applied in the vertical direction. In the second configuration (Injection stage, Mode B) the electric field is applied in both the

horizontal and vertical directions (Figure 4-8).The horizontal field focuses the sample during the initial part of the injection stage in order to obtain a well-separated sample.

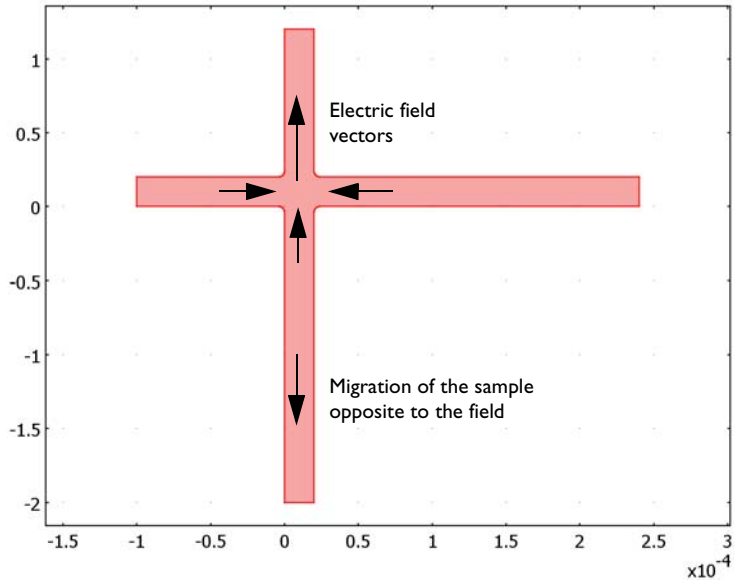


Figure 4-8: During the injection stage, the device turns off convective flow and applies an electric field. The horizontal field avoids the broadening of the sample, while the vertical field injects the sample into the vertical channel in the direction opposite to the electric field.

TABLE 4-2: APPLIED ELECTRIC FIELD CONFIGURATION

INLET	MODE A	MODE B
Sample inlet	Electric insulation	Electric potential, V = -1V
Outlet	Electric insulation	Electric potential, V = 0V
Upper buffer inlet	Electric potential, V = -3.2V	Electric potential, V = -3.2V
Lower buffer inlet	Electric potential, V = 0V	Electric potential, V = 0V

The model assumes that the charged sample concentration is very low compared to other ions dissolved in the solution. This implies that the sample concentration does not influence the solution's conductivity and that you can neglect the concentration gradients of the charge-carrying species, which are present in a much higher concentration than the sample ions. Such an electrolyte is known as a supporting electrolyte.

Several equations describe the model: the Stokes flow equations, the equation for current balance, and a mass balance using the Nernst-Planck equation. This model uses the steady-state solution for the focusing stage as the initial condition for the injection stages.

Now consider the formulation of the model equations.

THE FOCUSING STAGE

The Stokes flow equations give the global mass a momentum balance in the focusing stage:

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

In these equations, η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ is the velocity (m/s), p is the pressure (Pa).

The total balance of charges for a supporting electrolyte comes from the divergence of the current-density vector, which in a supporting electrolyte is given by Ohm's law:

$$\mathbf{i} = -\kappa \nabla V$$

Here κ is the electrolyte's conductivity (S/m) and V is the potential (V). The balance of current at steady state then becomes

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

which gives

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

The flux vector for the sample ions comes from the Nernst-Planck equation

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_{\mathrm{m}i} F c_i \nabla V + c_i \mathbf{u}$$

which leads to the following mass balance equation at steady state for species i:

$$\nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m}i} F c_i \nabla V + c_i \mathbf{u}) = 0$$

Here c_i is the concentration (mol/m^3), D_i represents the diffusivity (m^2/s), z_i equals the charge number (which equals 1 for this model), $u_{\mathrm{m}i}$ is the mobility (s·mol/kg), and F is Faraday's constant (C/mol).

For the pressure-driven flow, assume that the flow has fully developed laminar form in all inlets, that all sides have no-slip conditions, and that the fluid flows freely out from the end of the focusing channel.

The boundary conditions for the charge balance determine the potential at the respective inlet and outlet boundary

$$V = V_{0,i}$$

where i denotes the index for each boundary. This model also assumes that all wall boundaries are insulating:

$$\nabla V \cdot \mathbf{n} = 0$$

The boundary conditions for the mass balance of the sample during the focusing stage appear below. The equation

$$c = c_{\text{in}}$$

gives the concentration at the inlet of the sample, while the equation

$$c = c_{\text{buffer}}$$

gives the concentration of the buffer at the inlet of the two vertical channels, and the buffer inlets are at both boundaries in the vertical channel. At the outlet boundary, convection and migration are the dominating transport mechanisms (that is, diffusion is negligible), so that

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_{\text{m}i} F c_i \nabla V + c_i \mathbf{u}) \cdot \mathbf{n}$$

THE INJECTION STAGE

In the injection and separation stages, the device turns the flow off and changes the configuration of the electric field. You again solve the charge-balance equations but with new boundary conditions:

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

The mass balance for the dilute species comes from a time-dependent mass balance:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\text{m}i} F c_i \nabla V) = 0$$

The model assumes that the convective contribution is zero.

The boundary conditions for the current-balance equation imply that the potential is locked at all boundaries except for the walls,

$$V = V_{0,i}$$

Further assume the walls are electrically insulated, which yields

$$\nabla V \cdot \mathbf{n} = 0$$

As opposed to the focusing state, the boundary conditions for the mass balance are changed. In the injection stage, set the concentration at the inlet boundary:

$$c = c_{\text{in}}$$

For all other boundaries, assume that migration is the dominating transport mechanism, so that

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_{\text{m}i} F c_i \nabla V) \cdot \mathbf{n} \tag{4-4}$$

The time-dependent solution requires an initial condition for the mass balance, which you obtain from the steady-state solution of the focusing stage:

$$c(t = 0) = c_{\text{focus}}$$

Results and Discussion

This example analyzes the focusing stage and two configurations for the injection stages. Recall that the first injection-stage configuration (Mode A) applies the electric field only over the injection channel while the inlet and outlet boundaries of the focusing channel are insulated; the second injection-stage configuration (Mode B) applies the electric field over both channels.

Figure 4-9 shows the steady-state concentration distribution during the focusing stage along with the distribution at the beginning of the injection stage. Note that the vertical flows from the upper and lower injection channels focus the concentration on

a very narrow region near the crossing area of the channels. Further away from the crossing area, however, the concentration spreads again more equally over the channel.

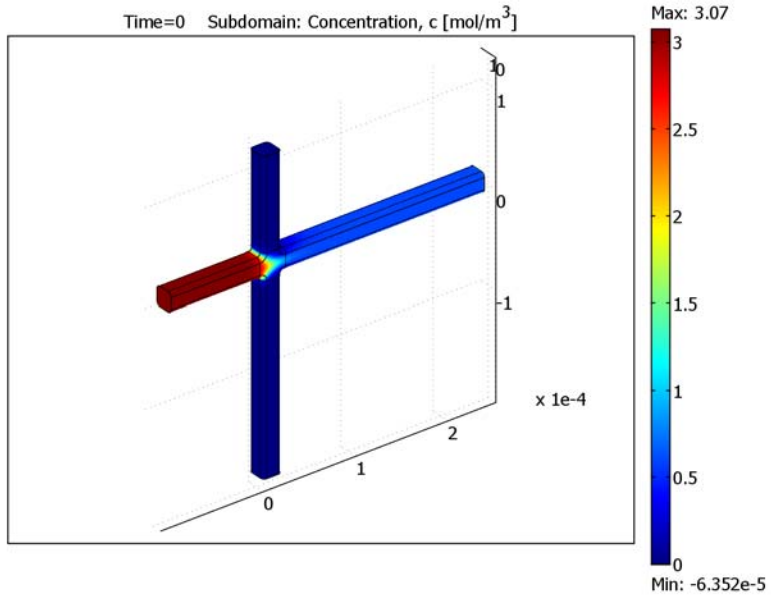


Figure 4-9: The steady-state concentration distribution during the focusing stage and prior to the injection stage.

Figure 4-10 and Figure 4-11 compare the concentration distribution for the two configurations at two times, specifically 0.06 s and 0.12 s after the beginning of the injection stage. The figures on the left show that for Mode A the concentration boundary is practically stationary in the horizontal direction. Consequently, the vertical electric field can continuously draw ions from the focusing channel, which results in poor separation and a poorly defined sample volume of the substance. For Mode B the situation is very different. The horizontal electric field draws the concentration boundary to the left, and the channels separate rapidly. Consequently,

this scheme draws a well-defined sample volume of the substance into the injection channel.

Figure 4-10: The concentration distribution at a time 0.06 s after starting the injection stage for the Mode A configuration (left) and Mode B configuration (right).

Figure 4-11: The concentration distribution at a time 0.12 s after starting the injection stage for the Mode A configuration (left) and Mode B configuration (right).

It is also possible to observe the difference between the two configurations if you look at the concentration along a line through the middle of the injection channel, examining it at several times after the start of the injection stage (Figure 4-12). The maximum concentration moves down the injection channel with time. The peaks are higher in the upper axis corresponding to Mode A, but they are much wider than for Mode B. A considerable amount of concentration appears at the left of the peak, and the sample remains attached to the focusing area—resulting in an unwanted distortion of the sample package. The narrow peaks of Mode B, on the other hand, form nice bell

curves throughout the downward transport in the injection channel, resulting in a well-defined sample package.

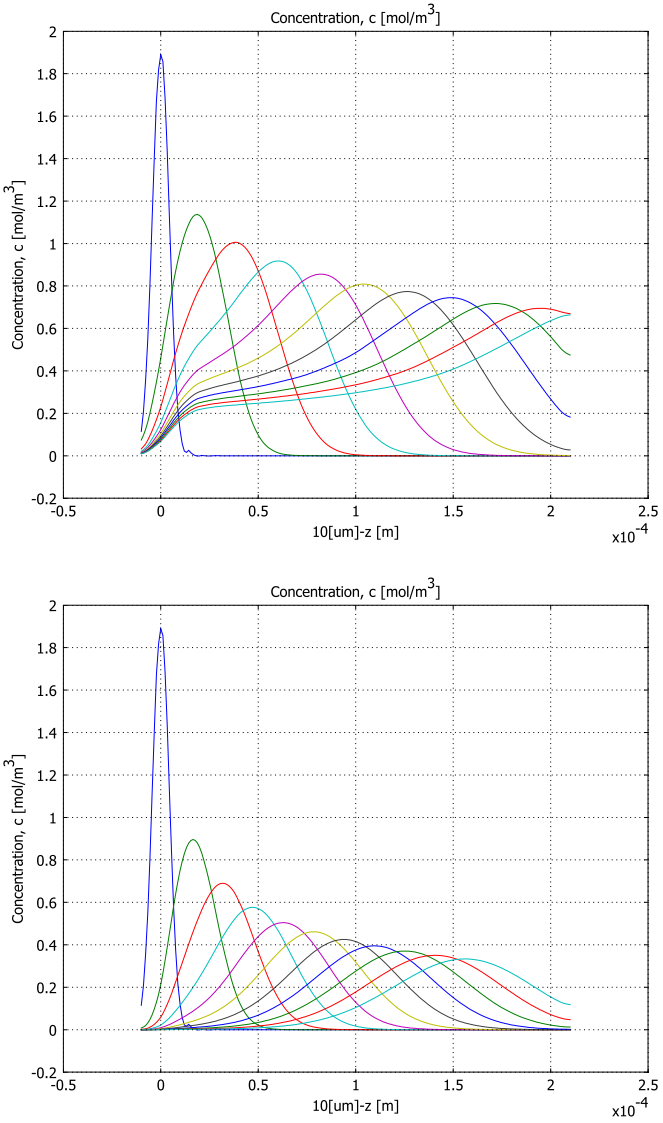


Figure 4-12: Concentration profile for Mode A (top) and Mode B (bottom) along the injection channel at various time steps: 0 s, 0.06 s, 0.12 s, 0.18 s, 0.24 s, 0.30 s, 0.36 s, 0.42 s, 0.48 s, 0.54 s, and 0.6 s after initialization of the injection stage. The origin of the x-axis marks the centerline of the focusing channel.

This study illustrates that modeling is extremely valuable in the investigation of electrophoretic transport. You can vary the configuration of the potential to obtain even better focusing and injection stages for the valve under study.

Modeling in COMSOL Multiphysics

APPLICATION MODES

In COMSOL Multiphysics you define the model with three application modes:

- The Stokes Flow application mode solves the fluid flow in the channels with Stokes equations.
- The Conductive Media DC application mode solves the equation for current balance.
- The Electrokinetic Flow application mode solves the Nernst-Planck equation.

GEOMETRY MODELING

Table 4-3 gives the dimensions of the model geometry. To draw it, proceed in four steps:

1. Initialize the geometry with simple blocks that represent the crossing of the channels.
2. Create a 2D work plane geometry in which you draw the cross section of the channel and a few assisting objects.
3. To finalize to channel crossing, apply the revolve operator to the 2D objects and subtract the resulting 3D objects from the original 3D blocks.
4. Finally apply the extrude operator to the 2D channel cross section to create the channels.

TABLE 4-3: MODEL DIMENSIONS

	HORIZONTAL CHANNEL	VERTICAL CHANNEL	CROSSING AREA
Dimensions (μm)			
- x	340	20	28
- y	20	20	20
- z	20	340	28
Position (μm)			
- x	-100	0	-4
- y	0	0	0

TABLE 4-3: MODEL DIMENSIONS

	HORIZONTAL CHANNEL	VERTICAL CHANNEL	CROSSING AREA
- z	0	-200	-4
Rounding (μm)			
- radius	4	4	4
- direction	in	in	out

COMPUTING THE SOLUTION

The operation of the actual device proceeds in two stages, the focusing stage and the injection stage. This model simulates two settings of the injection stage so in total it works in three phases.

The first phase defines the subdomain settings and boundary conditions for the focusing phase. Then the model solves the application modes sequentially with a nonlinear solver in the following sequence:

1. Stokes Flow application mode
2. Conductive Media DC application mode
3. Electrokinetic Flow application mode

Each step uses the solution from the previous one. The model stores the last solution for use as the initial value for the consequent modeling.

In the second phase you change the subdomain settings and boundary conditions to handle the injection stage Mode A. In a real device you would turn off the convective flow; in the model you simulate this by setting the velocity parameters of the Electrokinetic Flow application mode to zero. Thus it uses no information from the Stokes Flow application mode.

Solving the second phase starts from the stored solution of the first phase, and the model solves the Conductive Media DC application mode with a nonlinear solver. Then you select a time-dependent solver and solve the Electrokinetic Flow application mode. This solution is the result for the injection stage Mode A.

In the third phase you again change subdomain settings and boundary conditions but this time for the injection stage Mode B; you then solve for the final solution the same way as in the second phase.

Reference

1. S.V. Ermakov, S.C. Jacobson, and J.M. Ramsey, *Technical Proc 1999 Int'l Conf. on Modeling and Simulation of Microsystems*, Computational Publications, 1999.

Model Library path:
`MEMS_Module/Microfluidics_Models/electrokinetic_valve_3d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, select the **New** page, and from the **Space dimension** list select **3D**.

2 Click the **Multiphysics** button.

3 In the **Application Modes** tree, select **MEMS Module>Microfluidics>Stokes Flow**. Click **Add**.

4 In the **Application Modes** tree, select **MEMS Module>Electrostatics>Conductive Media DC**. Click **Add**.

5 In the **Application Modes** tree, select **MEMS Module>Microfluidics>Electrokinetic Flow>Transient analysis**. Click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

Next define some constants for the model.

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

2 In the dialog box that opens, specify names, expressions, and (optionally) descriptions for the following constants; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
u_a	0.2[mm/s]	Average velocity, sample inlet
w_a	0.67[mm/s]	Average velocity, buffer inlets
rho	1e3[kg/m^3]	Fluid density
eta	1e-3[Pa*s]	Fluid viscosity
D	1e-9[m^2/s]	Sample ion diffusivity

NAME	EXPRESSION	DESCRIPTION
Rg	8.314[J/(mol*K)]	Gas constant
T	298[K]	Fluid temperature
nu	D/(Rg*T)	Sample ion mobility
sigma	1[S/m]	Electric conductivity, electrolyte
c_in	0.05*3.5[g/l]/(22+35)[g/mol]	Sample ion concentration, inlet

GEOMETRY MODELING

3D Geometry—Step 1

Start the geometry by creating a simple set of rectangular blocks.

1. Click the **Block** tool on the 3D Draw toolbar and create two rectangular blocks using the settings from the following table; keep all other settings at their default values.

BLOCK	AXIS BASE POINT			LENGTH		
	X	Y	Z	X	Y	Z
BLK1	-4e-6	0	-4e-6	28e-6	20e-6	28e-6
BLK2	-20e-6	0	-20e-6	60e-6	20e-6	60e-6

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

Work Plane Geometry

Next create a 2D geometry on a work plane. After you extrude and revolve the objects, they shape the 3D geometry.

1. From the **Draw** menu, choose **Work Plane Settings**.
2. On the **Quick** page, click the **y-z** option button. Type `-4e-6` in the associated **x** edit field. Click **OK**.
3. Click the **Geom2** tab to activate the 2D work plane geometry.
4. Shift-click the **Rectangle/Square** button on the Draw toolbar.
5. Create a rectangle as in the following table; when done, click **OK**.

SIZE		POSITION		
WIDTH	HEIGHT	BASE	X	Y
20e-6	20e-6	Corner	0	0

6. Click the **Zoom Extents** button on the Main toolbar.
7. Click the **Fillet/Chamfer** button on the Draw toolbar.

8 In the dialog box go to the **Vertex selection** area, open the menu tree under **R1**, then select the four corners. Click the **Fillet** option button, and in the **Radius** edit field type `4e-6`. Click **OK**.

9 Shift-click the **Rectangle/Square** button on the Draw toolbar. Create a rectangle as in the following table; when done, click **OK**.

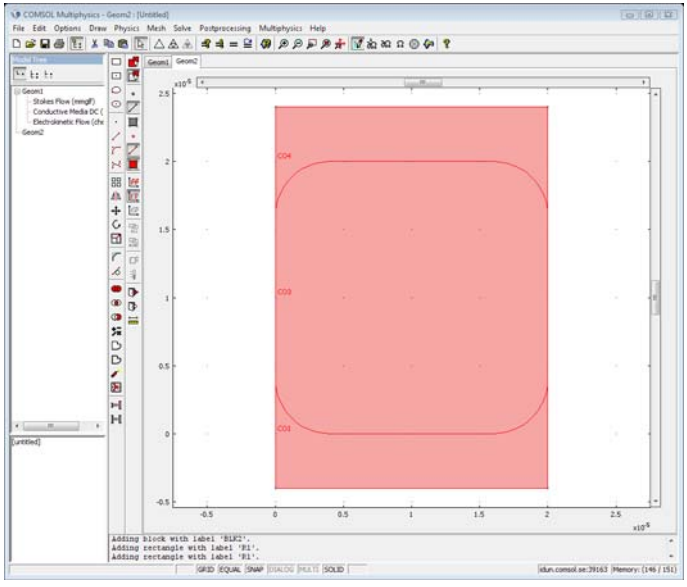
OBJECT	SIZE		POSITION		
	WIDTH	HEIGHT	BASE	X	Y
R1	20e-6	28e-6	Corner	0	-4e-6

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

11 Verify that the **Keep interior boundaries** check box is selected.

12 In the **Set formula** edit field, type `CO1+R1`. Click **OK**.

13 Click the **Split Object** button on the Draw toolbar.



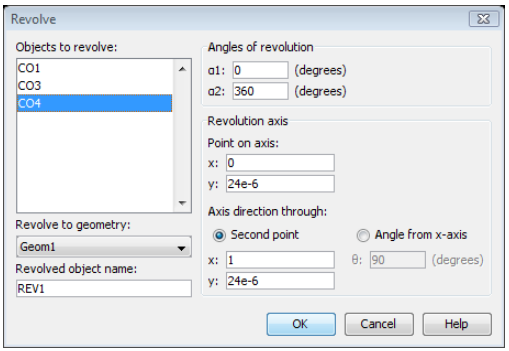
Zoom-in view of the completed 2D geometry.

3D Geometry—Step 2

After creating the work plane geometry, keep **Geom2** activated and use it to shape the 3D geometry.

1 From the **Draw** menu, choose **Revolve**.

2 In the resulting dialog box, enter settings as in the following figure.



Settings for the Revolve operation.

3 Click **OK**. The revolved object automatically becomes activated in **Geom1**.

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

5 In the dialog box that appears, specify the following settings, then click **OK**.

DISPLACEMENT			ARRAY SIZE		
X	Y	Z	X	Y	Z
28e-6	0	-28e-6	2	1	2

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

7 In the **Set formula** edit field, type `BLK2-REV1-REV2-REV3-REV4`. Click **Apply**.

8 In the **Set formula** edit field, type `BLK1*CO1`. Click **OK**.

9 Click the **Geom2** tab.

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

11 From the **Objects to extrude** list, select **CO3**. In the **Distance** edit field, type `-96e-6`. Click **OK**.

12 Click the **Geom2** tab.

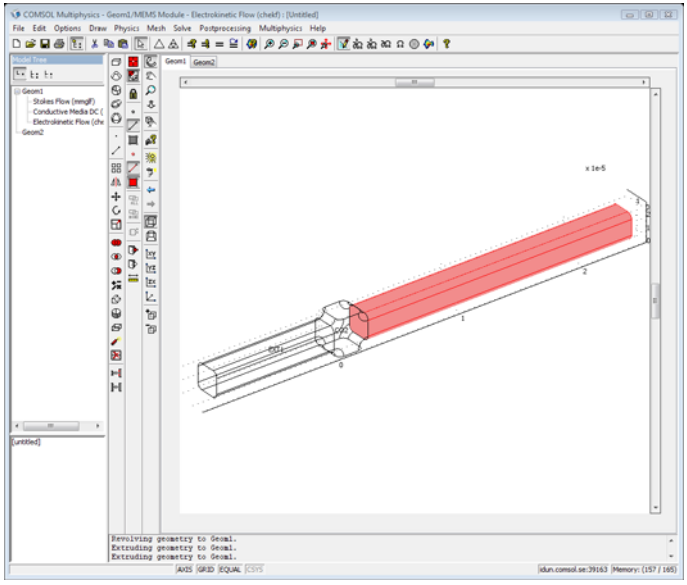
13 From the **Draw** menu, choose **Work Plane Settings**.

14 On the **Quick** page, click the **y-z** button, and in the corresponding **x** edit field type `24e-6`. Click **OK**.

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

16 In the dialog box that appears, set the **Distance** to `216e-6`. Click **OK**.

The following figure shows the 3D geometry when you have executed this step.



3D geometry after an extrusion operation on one of the arms.

17 Click the **Geom2** tab.

18 From the **Draw** menu, choose **Work Plane Settings**.

19 On the **Quick** page, click the **x-y** button. In the associated **z** edit field, type `-4e-6`. Click **OK**.

20 From the **Draw** menu choose **Extrude**. Set the **Distance** to `-196e-6`, then click **OK**.

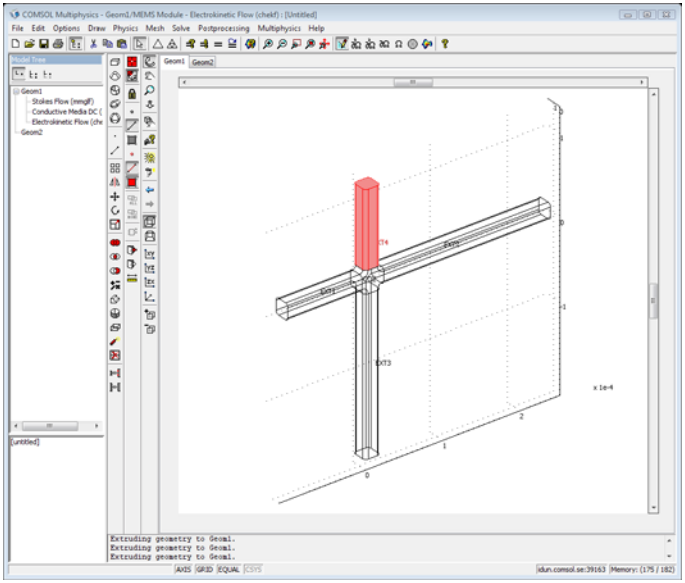
21 Click the **Geom2** tab.

22 From the **Draw** menu, choose **Work Plane Settings**.

23 On the **Quick** page, click the **x-y** button. In the associated **z** edit field type `24e-6`. Click **OK**.

24 From the **Draw** menu, choose **Extrude**. Set the **Distance** to `96e-6`, then click **OK**.

The completed geometry should look like that in the following figure.



The completed 3D geometry after extrusion of all four arms.

PHYSICS SETTINGS—THE FOCUSING STAGE

Subdomain Settings

1 From the **Multiphysics** menu, choose **1 Geom1: Stokes (mmglf)**.

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

3 In the **Subdomain selection** list, select all the subdomains.

4 Enter the settings from the following table. When done, click **OK**.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

5 From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (emdc)**.

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

7 For all subdomains, set σ to `sigma`. Click **OK**.

8 From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.

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

10 With all subdomains still selected, enter the settings in the following table; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	D
R	0
u_m	nu
z	-1
u	u
v	v
w	w
V	V

Boundary Conditions

1 From the **Multiphysics** menu, choose **1 Geom1:Stokes (mmglf)**.

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

3 Specify the following boundary conditions (for boundaries not listed in the table, the default No slip condition applies); when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 26	BOUNDARY 54
Boundary type	Inlet	Inlet	Outlet
Boundary condition	Laminar inflow	Laminar inflow	Pressure, no viscous stress
U_0	u_a	w_a	
L_{entr}	1e-4	1e-4	
Constrain outer edges to zero	Yes	Yes	
P_0			0

4 From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (emdc)**.

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

6 Click in the **Boundary selection** list and press Ctrl+A to select all boundaries. From the **Boundary condition** list, select **Electric insulation**.

7 Edit the boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 54
Boundary condition	Electric potential	Ground
V_0	-1	-

8 From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.

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

10 Specify boundary settings as in the following table (for boundaries not listed, the default Insulation/Symmetry condition applies); when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 26	BOUNDARY 54
Boundary condition	Concentration	Concentration	Convective flux
c_0	c_in	0	-

MESH GENERATION

1 Click **Geom1** to activate the 3D geometry.

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

COMPUTING THE SOLUTION—THE FOCUSING STAGE

First, compute the solution for the velocity field, and then use that solution when solving the mass-transport problem.

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

2 Click the **Solve For** tab.

3 From the **Solve for variables** tree, select **Geom1 (3D)>Stokes (mmglf)**.

4 Click the **Solve** button.

5 When the solver has finished, click the **Initial Value** tab.

6 Click the **Current solution** option button in the **Initial value** area, then return to the **Solve For** page.

7 From the **Solve for variables** tree, select **Geom1 (3D)>Conductive Media DC (emdc)**.

8 Click **Solve**

9 From the **Solve for variables** tree, select **Geom1 (3D)>Electrokinetic Flow (chekf)**.

10 Click **Solve**.

11 On the **Initial Value** page, click the **Store Solution** button.

12 Click **OK** to close the **Solver Manager**.

PHYSICS SETTINGS—INJECTION STAGE, MODE A

Subdomain Settings

1 From the **Multiphysics** menu, choose **3 Geom1: Electrokinetic Flow (chekf)**.

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

3 In the **Subdomain selection** list, select all the subdomains, then change the settings for velocity parameters as in the following table; when done, click **OK**.

PROPERTY	VALUE
u	0
v	0
w	0

Boundary Conditions

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

2 Select Boundaries 1, 21, 26, and 54 (the inlets and outlets).

3 From the **Boundary condition** list, select **Flux**.

4 In the $\mathbf{N}_0$ edit field, type `-nmflux_c_chekf`.

The predefined boundary variable `nmflux_c_chekf` gives the outward normal electrophoretic flux, $\mathbf{N}_i \cdot \mathbf{n}$.

5 Click **OK**.

6 From the **Multiphysics** menu, choose **2 Geom1: Conductive Media DC (emdc)**.

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

8 Change the boundary settings as in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 54	BOUNDARY 21	BOUNDARY 26
Boundary condition	Electric insulation	Electric potential	Electric potential
V_0	-	0	-3.2

COMPUTING THE SOLUTION—INJECTION STAGE, MODE A

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

2 Click the **Script** tab. Select the **Automatically add commands when solving** check box.

This setting instructs the software to record the subsequent solver settings and commands, which you can then reuse when solving Mode B.

3 Click the **Initial Value** tab. In the **Initial value** area, click the **Stored solution** option button. This makes the steady-state solution from the focusing stage the initial solution.

4 Click the **Solve For** tab.

5 In the **Solve for variables** tree, select **Geom1 (3D)>Conductive Media DC (emdc)**.

6 Click **Solve**.

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

8 From the **Analysis** list, select **Transient**.

9 In the **Time stepping** area go to the **Times** edit field and enter `0:0.03:0.6`.

10 Click **OK**.

11 Activate the **Solver Manager** window.

12 Click the **Initial Value** tab.

13 In the **Initial value** area, click the **Current solution** option button.

14 Click the **Solve For** tab.

15 In the **Solve for variables** tree, select **Geom1 (3D)>Electrokinetic Flow (chekf)**.

16 Click **Solve**.

17 Click **OK**.

POSTPROCESSING AND VISUALIZATION—INJECTION STAGE, MODE A

Reproduce the plot in Figure 4-9 on page 276 with the following steps:

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

2 On the **General** page, select the **Subdomain** and **Geometry edges** check boxes in the **Plot type** area and clear all the others.

3 From the **Solution at time** list, select **0**.

4 Click the **Subdomain** tab. From the **Predefined quantities** list on the **Color Data** page, select **Electrokinetic Flow (chekf)>Concentration, c**. Click **Apply**.

5 Click the **Go to Default 3D View** button on the Camera toolbar, then click the **Zoom Extents** button on the Main toolbar.

To visualize the solution at two later times, as in the left panels of Figure 4-10 and Figure 4-11 on page 277, do as follows:

6 Return to the **Subdomain** page of the **Plot Parameters** dialog box.

7 Clear the **Color scale** check box in the **Element color** area.

8 Click the **General** tab. From the **Solution at time** list, select **0.06**. Click **Apply** to generate the plot in the left panel.

9 From the **Solution at time** list, select **0.12**. Click **OK** to generate the plot in the left panel.

To make an animation of the solution, click the **Animate** button on the Plot toolbar. On the **Animate** page of the **Plot Parameters** dialog box, you can customize the movie settings.

Generate the upper plot of Figure 4-12, by executing the following instructions:

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

2 On the **General** page, select **Interpolated times** from the **Select via** list.

3 In the **Times** edit field, type `0:0.06:0.6`.

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

5 In the **Predefined quantities** list, select **Electrokinetic Flow (chekf)>Concentration, c**.

6 In the **x-axis data** area, click the option button next to the **Expression** button and then click **Expression**.

7 In the **Expression** edit field, type `10[um]-z`. Click **OK**.

8 In the **Cross-section line data** area, enter the settings listed in the following table; when done, click **OK**.

CROSS-SECTION LINE DATA			
x0	1e-5	x1	1e-5
y0	1e-5	y1	1e-5
z0	2e-5	z1	-2e-4
Line resolution			200

PHYSICS SETTINGS—INJECTION STAGE, MODE B

Boundary Conditions

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

2 Change the boundary settings for the Conductive Media DC application mode to those in the following table:

SETTINGS	BOUNDARY 1	BOUNDARIES 21, 54	BOUNDARY 26
Boundary condition	Electric potential	Electric potential	Electric potential
V_0	-1	0	-3.2

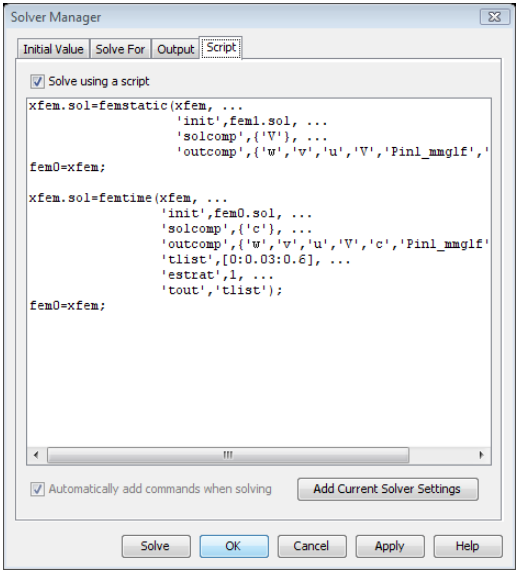
3 Click **OK**.

COMPUTING THE SOLUTION—INJECTION STAGE, MODE B

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

2 On the **Script** page, select the **Solve using a script** check box.

3 Click **Solve** to execute the script you see in the edit window.



4 Click **OK** to close the **Solver Manager**.

POSTPROCESSING AND VISUALIZATION—INJECTION STAGE, MODE B

Generate the plots in the right panels of Figure 4-10 and Figure 4-11 on page 277 as follows:

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

2 On the **General** page, select **0.06** from the **Solution at time** list. Click **Apply**.

This generates the right plot in Figure 4-10.

3 Repeat Step 2 but select **0.12** from the **Solution at time** list to generate the right plot in Figure 4-11.

4 From the **Solution** at time list, select **0**.

5 Click **OK** to close the dialog box and generate the plot you see when you open the model from the Model Library.

Finally, generate the lower plot in Figure 4-12 with the following steps:

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

2 Accept the settings from Mode A by clicking **OK**.

ALE Fluid-Structure Interaction

Introduction

The following example demonstrates techniques for modeling fluid-structure interactions in COMSOL Multiphysics. It illustrates how fluid flow can deform surrounding structures and how to solve for the flow in a continuously deforming geometry using the arbitrary Lagrangian-Eulerian (ALE) technique.

The model geometry consists of a horizontal flow channel in the middle of which is an obstacle, a narrow vertical structure (Figure 4-13). The fluid flows from left to right, except the obstacle forces it into a narrower path in the upper part of the channel, and it imposes a force on the structure's walls resulting from the viscous drag and fluid pressure. The structure, being made of a deformable material, bends under the applied load. Consequently, the fluid flow also follows a new path, so solving the flow in the original geometry would generate incorrect results.

The ALE method handles the dynamics of the deforming geometry and the moving boundaries with a moving grid. COMSOL Multiphysics computes new mesh coordinates on the channel area based on the movement of the structure's boundaries and on so called mesh smoothing. The Navier-Stokes equations that solve the flow are formulated for these moving coordinates.

The structural mechanics portion of the model does not require the ALE method, and COMSOL Multiphysics solves it in a fixed coordinate system as usual. However, the strains the model computes in this way are the only source for computing the deformed coordinates with ALE.

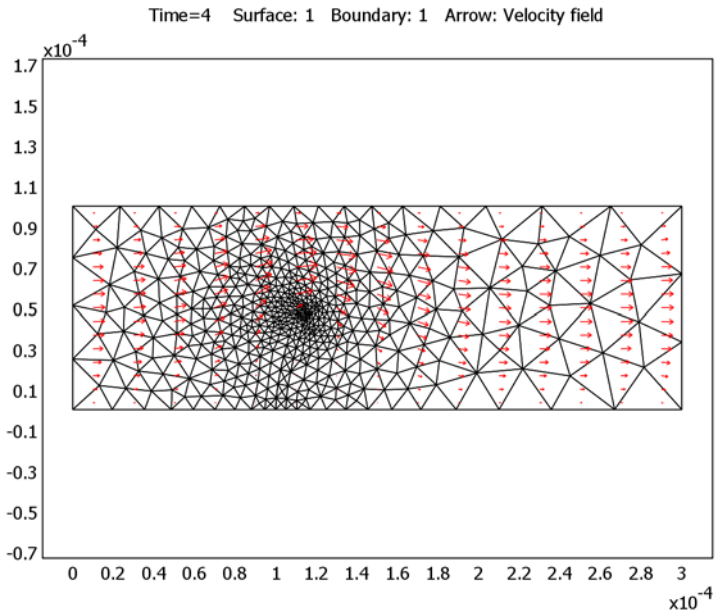


Figure 4-13: Fluid flows into this horizontal flow channel from the left, and it enters with a parabolic velocity profile. A narrow vertical structure in the channel (the straight vertical structure) forces the flow into a narrower path. Due to fluid pressure and viscous drag, the originally vertical structure bends (the vertical structure shifted to the right). This simulation models the fluid flow in a deformed, moving mesh that follows the movement of the bending structure.

Model Definition

In this example the flow channel is 100 µm high and 300 µm long. The vertical structure—5 µm wide, 50 µm high, and with a semicircular top—sits 100 µm away from the channel's left boundary. Assume that the structure is long in the direction perpendicular to the image.

The fluid is a water-like substance with a density $\rho = 1000$ kg/m^3 and dynamic viscosity $\eta = 0.001$ Pa·s. To demonstrate the desired techniques, assume the structure consists of a flexible material with a density $\rho = 7850$ kg/m^3 and Young's modulus $E = 200$ kPa.

The model consists of a fluid part, solved with the Navier-Stokes equations in the flow channel, and a structural mechanics part, which you solve in the obstacle. A Moving

Mesh (ALE) application mode makes sure the flow domain is deformed along with the obstacle.

Transient effects are taken into account in both the fluid and the structure. The structural deformations are modeled using large deformations in the Plane Strain application mode. The displacements and displacement velocities are denoted u, v, u_t, and v_t, respectively. Fluid flow is described by the Navier-Stokes equations, where the velocity components and pressure are denoted u_2, v_2, and p_2, respectively.

FLUID FLOW

The fluid flow in the channel is described by the Navier-Stokes equations for the velocity field, $\mathbf{u} = (u, v)$, and the pressure, p, in the spatial (deformed) moving coordinate system:

$$\begin{aligned} \rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot [-p\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho((\mathbf{u} - \mathbf{u}_m) \cdot \nabla)\mathbf{u} &= \mathbf{F} \\ -\nabla \cdot \mathbf{u} &= 0 \end{aligned} \tag{4-5}$$

In these equations, $\mathbf{I}$ denotes the unit diagonal matrix and $\mathbf{F}$ is the volume force affecting the fluid. Assume that no gravitation or other volume forces affect the fluid, so that $\mathbf{F} = 0$. The coordinate system velocity is $\mathbf{u}_m = (u_m, v_m)$.

At the channel entrance on the left, the flow has fully developed laminar characteristics with a parabolic velocity profile but its amplitude changes with time. At first flow increases rapidly, reaching its peak value at 0.215 s; thereafter it gradually decreases to a steady-state value of 5 cm/s. The centerline velocity in the x direction, u_{in} (see Figure 4-16 on page 300), with the steady-state amplitude U comes from the equation

$$u_{\text{in}} = \frac{U \cdot t^2}{\sqrt{(0.04 - t^2)^2 + (0.1t)^2}} \tag{4-6}$$

where t must be expressed in seconds.

At the outflow (right-hand boundary), the condition is $p = 0$. On the solid (non deforming) walls, no-slip conditions are imposed, $u = 0, v = 0$, while on the deforming interface the velocities equal the deformation rate, $u_0 = u_t$ and $v_0 = v_t$.

STRUCTURAL MECHANICS

The structural deformations are solved for using an elastic formulation and a nonlinear geometry formulation to allow large deformations.

For boundary conditions, the obstacle is fixed to the bottom of the fluid channel. All other object boundaries experience a load from the fluid, given by

$$\mathbf{F}_T = -\mathbf{n} \cdot (-p\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \quad (4\text{-}7)$$

where $\mathbf{n}$ is the normal vector to the boundary. This load represents a sum of pressure and viscous forces.

MOVING MESH

The motion of the deformed mesh is modeled using Winslow smoothing. For more information on this formulation, please refer to "The Moving Mesh Application Mode" on page 401 in the COMSOL Multiphysics Modeling Guide. This is the default smoothing when using the predefined Fluid-Structure Interaction coupled application modes. The boundary conditions control the displacement of the moving mesh with respect to the initial geometry. At the boundaries of the obstacle, this displacement is the same as the structural deformation. At the exterior boundaries of the flow domain, the deformation is set to zero in all directions.

Results and Discussion

Figure 4-14 shows the geometry deformation and flow at t = 4 s when the system is close to its steady state. Due to the channel's small dimensions, the Reynolds number of the flow is small (R << 100), and the flow stays laminar in most of the area. The swirls are restricted to a small area behind the structure. The amount of deformation

as well as the size and location of the swirls depend on the magnitude of the inflow velocity.

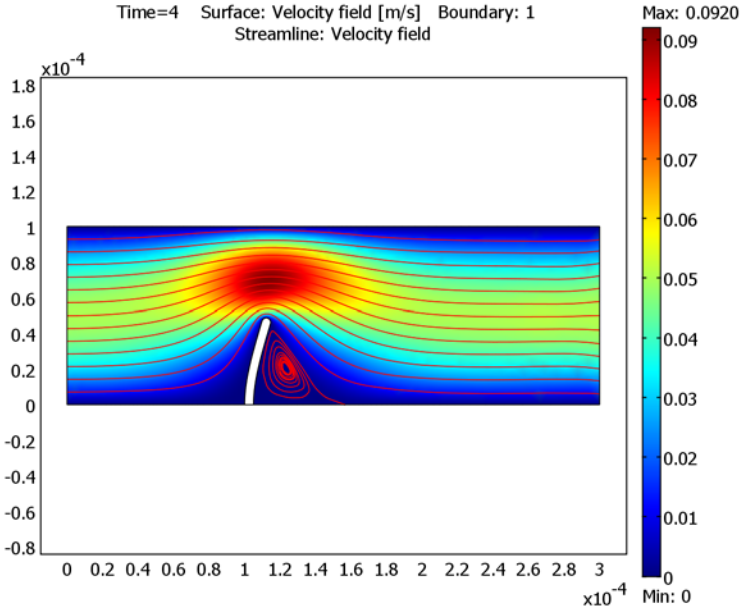


Figure 4-14: Flow velocity and geometry deformation at t = 4 s. The streamlines indicate the flow direction and the color scale indicates flow-velocity magnitude. Here the geometry deformation is scaled by unity.

Figure 4-15 shows the mesh velocity at $t = 0.15$ s. The boundaries of the narrow structure are the only moving boundaries of the flow channel. Therefore the mesh velocity also has its largest values near the structure. Depending on the current state of the deformation—whether it is increasing, decreasing or stationary—the mesh velocity can have a very different distribution. Figure 4-16 further illustrates this point; it compares the average inflow velocity to the horizontal mesh velocity and the horizontal mesh displacement just beside the top of the structure at the physical point $(1.05 \cdot 10^{-4}, 0.5 \cdot 10^{-4})$. Most of the time the deformation follows the inflow velocity quite closely. Whenever the inflow velocity starts to decrease, the deformation also decreases, which you can observe as the negative values on the horizontal mesh

velocity. Toward the end of the simulation, when inflow and structure deformation approach their steady-state values, the mesh velocity also decreases to zero.

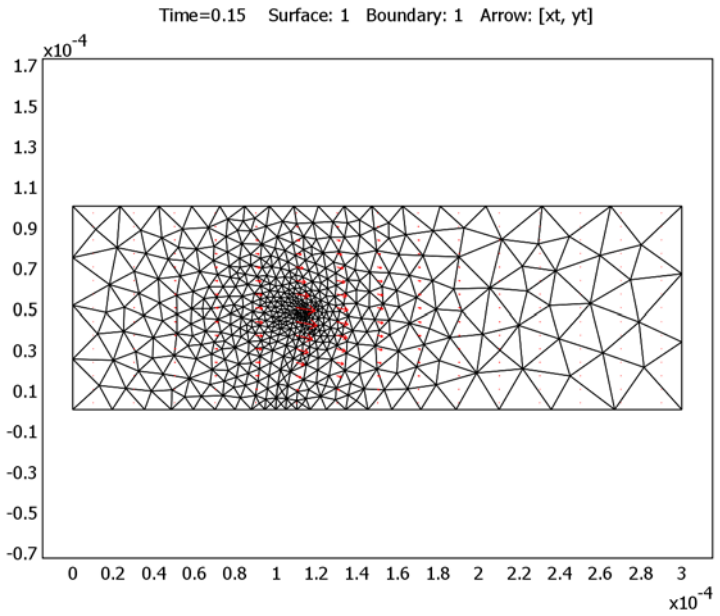


Figure 4-15: Mesh velocity (arrows) and mesh and geometry deformation at t = 0.15 s.

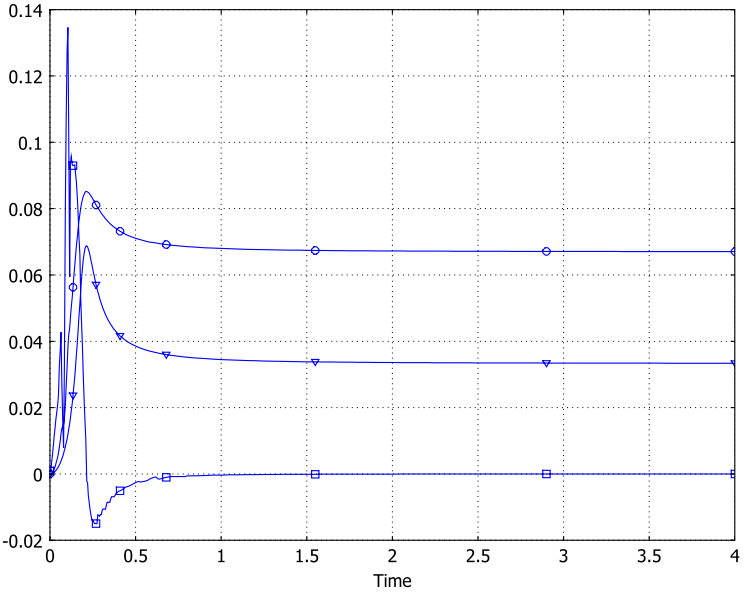


Figure 4-16: Inflow velocity, horizontal mesh velocity, and mesh deformation. The curve with triangles shows the average x direction velocity at the inflow boundary (m/s); the curve with circles shows 10^4×mesh displacement in the x direction (dx_ale; m) at the geometry point ($1.05 \cdot 10^{-4}$, $0.5 \cdot 10^{-4}$); and the curve with squares shows 10^3×mesh velocity in the x direction (xt; m/s), also at the point ($1.05 \cdot 10^{-4}$, $0.5 \cdot 10^{-4}$).

Figure 4-17 and Figure 4-18 compare the meshes at different times. The first image shows the initial mesh, which you generate prior to solving the model. This mesh is equally distributed around the top of the structure. The second image shows the mesh in its deformed form. Because the structure deforms more in the horizontal direction,

the mesh also changes more in this direction: On the left, the mesh elements are stretched; on the right, they are compressed in the x direction.

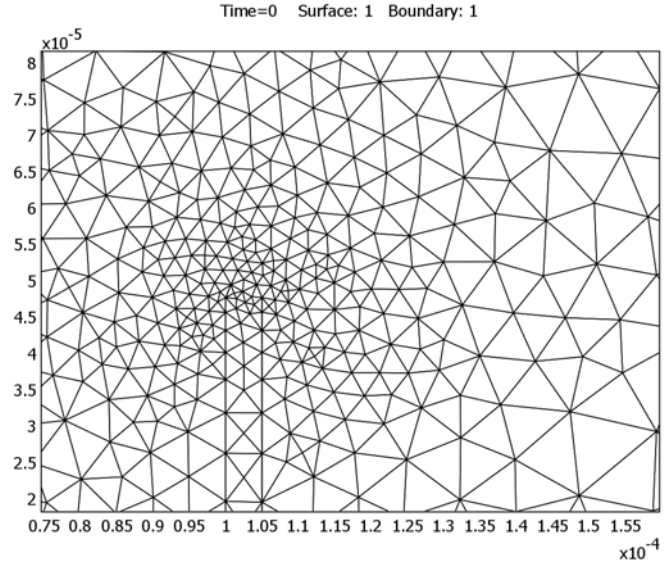


Figure 4-17: Initial (undeformed) geometry and mesh near the top of the structure.

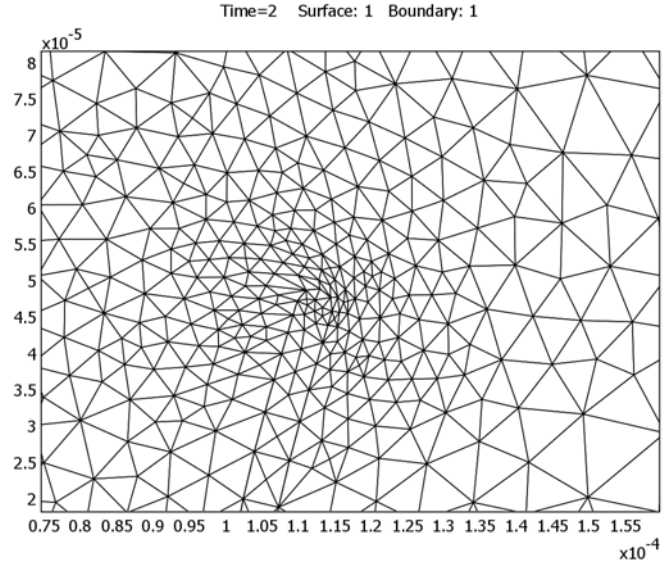


Figure 4-18: Deformed geometry and deformed mesh near the top of the structure at $t = 2$ s.

Modeling in COMSOL Multiphysics

This example implements the model using three application modes, which the predefined Fluid-Structure Interaction multiphysics entry sets up automatically. First, the Incompressible Navier-Stokes application mode computes the fluid dynamics. It is active only in the area of the flow channel.

Second, the Plane Strain application mode solves the model's structural mechanics portion. You activate it only in the area of the narrow structure. To get a more accurate computation of the large strains, the large deformation analysis type is the default setting. The deformation velocity solved with this application mode acts as the boundary condition for the Incompressible Navier-Stokes and the Moving Mesh (ALE) application modes.

Third, the Moving Mesh (ALE) application mode solves for the deformed mesh

Model Library path: `MEMS_Module/Microfluidics_Models/fluid_structure_interaction`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the **Model Navigator**, select **2D** from the **Space dimension** list.
2. From the **Application Modes** list, select **MEMS Module>Fluid-Structure Interaction> Plane Strain with Fluid Interaction>Transient analysis**.
3. Click **OK** to close the **Model Navigator**.

GEOMETRY MODELING

1. Shift-click the **Rectangle/Square** button on the Draw toolbar.
2. In the **Width** edit field type `3e-4`, and in the **Height** edit field type `1e-4`. Click **OK**.
3. Click the **Zoom Extents** button on the Main toolbar.
4. From the **Options** menu, choose **Axes/Grid Settings**.
5. On the **Grid** page, clear the **Auto** check box, then go to the **X spacing** and **Y spacing** edit fields and in each one type `2.5e-6`. Click **OK**.

6 Click the **Zoom Window** button on the Main toolbar, then left-click and drag the mouse approximately from the point $(0.9 \cdot 10^{-4}, -0.1 \cdot 10^{-4})$ to $(1.2 \cdot 10^{-4}, 0.7 \cdot 10^{-4})$.

7 Click the **2nd Degree Bézier Curve** button on the Draw toolbar, then left-click nine points as in the following table; when done, right-click to complete the curve.

POINT	X	Y
1	1e-4	0
2	1e-4	4.00e-5
3	1e-4	4.75e-5
4	1e-4	5.00e-5
5	1.025e-4	5.00e-5
6	1.05-4	5.00e-5
7	1.05-4	4.75e-5
8	1.05-4	4.00e-5
9	1.05-4	0

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

PHYSICS SETTINGS

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

2 In the **Constants** dialog box, define the following constants with names, expressions, and (optionally) descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
eta	1e-3[Pa*s]	Fluid viscosity
rho	1000[kg/m^3]	Fluid density
U	3.33[cm/s]	Inlet mean velocity at steady state
E	200[kPa]	Young's modulus

3 From the **Options** menu, choose **Scalar Expressions**.

4 Define the following expression (the description is optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
u_in	U*t^2/ sqrt(t^4-0.07[s^2]*t^2+0.0016[s^4])	Inlet mean velocity

Subdomain Settings

1 In the **Multiphysics** menu, make sure **Incompressible Navier-Stokes (mmglf)** is selected.

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

3 Select Subdomain 1. From the **Group** list, select **Fluid domain**, then apply the following settings:

PROPERTY	VALUE
ρ	rho
η	eta

4 Select Subdomain 2, then select **Solid domain** from the **Group** list. This deactivates the incompressible Navier-Stokes equations in Subdomain 2 (the solid).

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

6 From the **Multiphysics** menu, select **Plane Strain (smpn)**.

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

8 Select Subdomain 1, then select **Fluid domain** from the **Group** list to deactivate the structural mechanics equations in the fluid.

9 Select Subdomain 2, then select **Solid domain** from the **Group** list. In the **E** edit field for the Young's modulus, type `E`.

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

11 From the **Multiphysics** menu, select **Moving Mesh (ALE)**.

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

13 Apply the following settings by selecting from the **Group** list.

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
Group	Fluid domain	Solid domain

For the fluid domain, this means that the displacements are free. In the solid domain, the deformation of the solid determines the mesh displacement.

Boundary Conditions

1 From the **Multiphysics** menu, select **Incompressible Navier-Stokes (mmglf)**.

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

3 Select Boundaries 7–10, then select **Structural velocity** from the **Group** list.

4 For the remaining active boundaries, apply the following settings:

SETTINGS	BOUNDARY 1	BOUNDARY 6	ALL OTHERS
Boundary type	Inlet	Outlet	Wall
Boundary condition	Laminar inflow	Pressure, no viscous stress	No slip
U_0	`u_in`		
P_0		0	

5 Click **OK**.

6 From the **Multiphysics** menu, select **Plane Strain (smpn)**.

7 In the **Boundary Settings** dialog box, select Boundary 4. Then select **Fixed** from the **Constraint condition** list.

8 Select Boundaries 7–10, then select **Fluid load** from the **Group** list. This sets up the edge loads using the Lagrange multipliers and specifies them to be defined as force/area.

9 Click **OK**.

10 From the **Multiphysics** menu, select **Moving Mesh (ALE)**.

11 In the **Boundary Settings** dialog box, select the following groups from the **Group** list to apply the appropriate mesh displacements:

SETTINGS	BOUNDARIES 7–10	ALL OTHERS
Group	Structural displacement	Fixed

MESH GENERATION

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

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

3 Click the **Custom mesh size** button, then set the **Element growth rate** to `1.2`.

4 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

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

2 In the **Times** edit field type `0:0.005:0.4 0.41:0.01:0.8 0.85:0.05:4`.

3 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 4-14 (this is also the plot that appears in the **Model Navigator** and when you open the prepared model file), follow these steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, find the **Plot type** area. Select the **Surface**, **Boundary**, and **Streamline** check boxes; clear all the other check boxes.
3. Click the **Surface** tab. From the **Predefined quantities** list on the **Surface Data** page, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.
4. Click the **Boundary** tab. Type 1 in the **Expression** edit field on the **Boundary Data** page.
5. Click the **Uniform color** option button, then click the **Color** button. Set the color to black, then click **OK** to close the **Boundary Color** dialog box.
6. Click the **Streamline** tab. From the **Predefined quantities** list on the **Streamline Data** page, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.
7. Click the **Specify start point coordinates** option button. In the **X** and **Y** edit fields enter these expressions:

X	`linspace(0,0,15) linspace(1.2e-4,1.2e-4,3)`
Y	`linspace(0,1e-4,15) linspace(0,0.35e-4,3)`

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

Lamella Mixer

Introduction

At the macroscopic level, systems usually mix fluids using mechanical actuators or turbulent 3D flow. At the microscale level, however, neither of these approaches is practical or even possible. This model demonstrates the mixing of fluids using laminar-layered flow in a MEMS mixer.

To characterize the fluid flow's turbulent behavior scientists generally use the Reynolds number

$$\mathrm{Re} = \frac{\rho u L}{\eta}$$

where ρ is the fluid density, u is flow velocity, L is a characteristic length, and η is the fluid's dynamic viscosity. Turbulent flow takes place when the Reynolds number is high, typically when $\mathrm{Re} > 2000$. At MEMS scales, the width of a channel is in the range of $100\ \mu\mathrm{m}$ and the velocity is approximately $1\ \mathrm{cm/s}$. In this case, for water-like substances Re is close to unity. The fluid flow is thus clearly laminar, so effective mixing of fluids in MEMS devices requires other means.

Figure 4-19 shows a section of a component that uses layered flow to improve mixing. The mixer has several lamellae of microchannels, and the two fluids being mixed are alternated for every second layer. Pressure forces the fluid to travels in the channels from back to front. The fluid enters a larger space, the mixing chamber (visible at the front of the image). The figure does not include this chamber, but it covers the area beyond where the grid of the microchannel ends. Near the ends of the microchannels the mixing chamber has distinct lamellae of the two fluids, but this separation vanishes towards the end of the chamber.

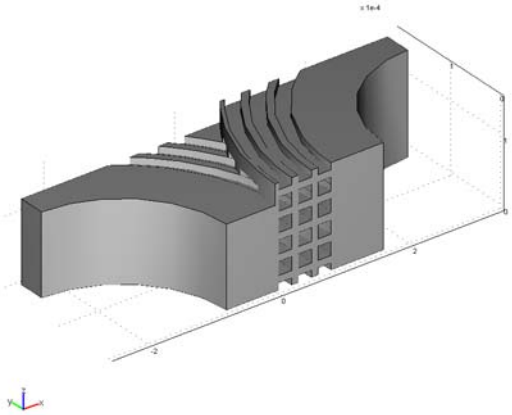


Figure 4-19: Geometry of a lamella mixer (mixing chamber not visible).

Model Definition

This model analyzes the steady-state condition of the fluid flow as well as the convection and diffusion of a dissolved substance in a lamella mixer. The geometry in Figure 4-20 corresponds to Figure 4-19 except it includes only a small vertical section of the mixer with a height of 30 µm. The model starts from a plane in the middle of the channel bending to the left and ends at a plane in the middle of the channel bending to the right.

Each microchannel in the mixer has a quadratic cross section with a side of 20 µm. Because of the chosen geometry, microchannel height in the model is only 10 µm. To create the curved channel shape, the model uses concentric circles with inner radii of 240 µm, 270 µm, and 300 µm. Except for the direction of the curvature, the geometry and dimensions of the channel layers are the same.

The fluid exiting the microchannels enters a mixing chamber of length is 200 µm and width 80 µm.

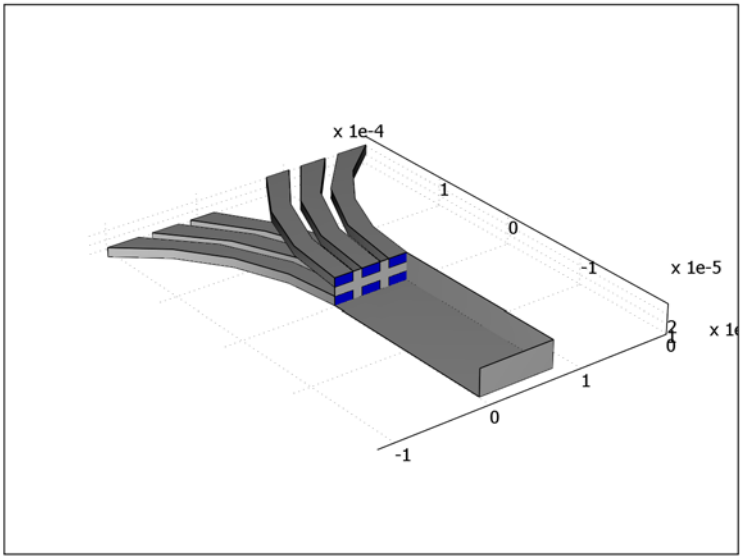


Figure 4-20: The model geometry for a lamella mixer takes advantage of symmetry so it is not necessary to model the entire height of the device.

You solve the fluid flow in the channels and in the chamber with the incompressible Navier-Stokes equations

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot [(-p)\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \mathbf{F}$$
$$-\nabla \cdot \mathbf{u} = 0 \qquad (4\text{-}8)$$

where ρ is fluid density, $\mathbf{u} = (u, v, w)$ is the flow-velocity field, p is fluid pressure, $\mathbf{I}$ is the unit diagonal matrix, η is the fluid's dynamic viscosity, and $\mathbf{F} = (f_x, f_y, f_y)$ is a volume force affecting the fluid. In this model, the fluid is water with $\rho = 1000$ kg/m^3, $\eta = 0.001$ Pa·s, and $\mathbf{F} = \mathbf{0}$ because there are no volume forces.

The system applies a pressure of 10 Pa on all six microchannel inputs to drive the flow through the mixing chamber to where there is zero pressure. At the chamber exit the flow velocity has components only in the normal direction of the boundary.

On the microchannel and mixing-chamber walls, the no-slip boundary condition applies. However, in the vertical direction, due to the geometry, you can use a symmetry boundary condition.

The following convection-diffusion equation describes the concentration of the dissolved substances in the fluid:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - \mathbf{u} \cdot \nabla c \tag{4-9}$$

where c is the concentration, D is the diffusion coefficient, and R is the reaction rate. In this model, $D = 10^{-10}$ m^2/s, and R = 0 because the concentration is not affected by any reactions.

There is a concentration of 50 mol/m^3 on the input boundaries of the channels curving to the left, but the channels curving to the left have zero concentration. At the output boundary of the mixing chamber the substance flows through the boundary by convection. The walls of the channels and the chamber are insulated for this dissolved substance, and on the top and bottom boundaries you use a symmetry boundary condition.

Results and Discussion

Figure 4-21 details fluid flow in the mixer. On a PC screen you can see a gradual change in the color of the slices, which indicates a laminar parabolic flow. The streamlines do not show swirls, and there are only small changes in the flow direction. The figure also shows that the maximum velocity of the microchannels is at the model's boundary because it is located in the middle of the channel. In the mixing chamber, the change of flow velocity is visible only in horizontal direction because the chamber is high and flow at the model boundaries is unchanged.

The peak velocity is roughly 1.4 mm/s in the microchannels and 0.5 mm/s in the mixing chamber. Given the corresponding lengths (20 µm and 80 µm), the Reynolds numbers are Re = 0.028 and Re = 0.04, so the flow is clearly laminar.

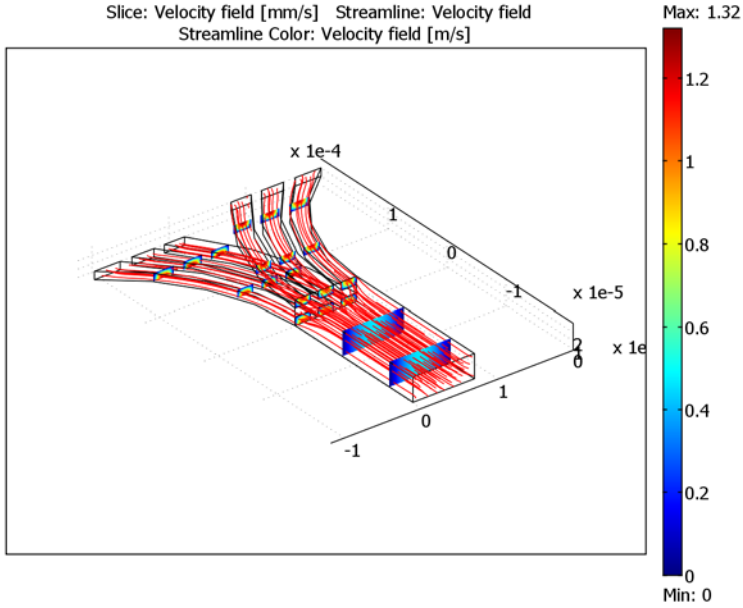


Figure 4-21: Fluid flow in the lamella mixer.

Figure 4-22 shows the concentration distribution on the model boundaries. The inflow channels see a constant concentration of 0 or 50 mol/m^3 depending on the channel. Mixing starts when the fluid enters the mixing chamber. At the entrance there is a clear separation of the concentration, but this diminishes toward the end of the chamber. On the sides of the mixing chamber where the flow velocity is smaller the mixing is better than at its center. The mixing, however, is not perfect, and a reduced flow velocity, a longer mixing chamber, or some other means to increase mixing is preferable.

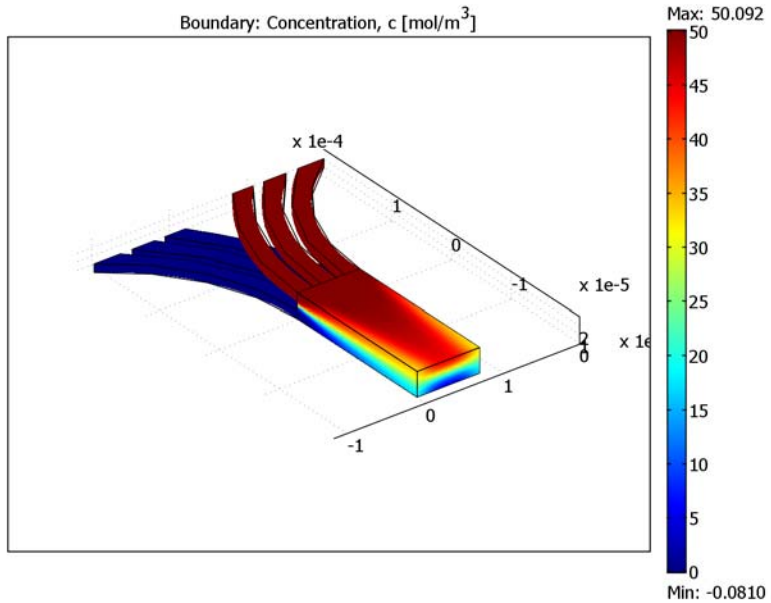


Figure 4-22: Concentration plot on the boundaries of the lamella mixer model.

To get another point of view, examine Figure 4-23, which shows the concentration profile at the chamber's centerline. Near the channels the transition is very rapid, but closer to the chamber's end the profile has a flatter sigmoid shape. On the chamber's sides the concentration profile has the same shape, but its amplitude is between approximately 17 mol/m^3 and 33 mol/m^3.

If you generalize the concentration profile to cover the entire component (Figure 4-19 on page 308), the profile would be a wave-like curve where concentration would alternate between its minimum and maximum values with a spatial frequency related to the layer thickness.

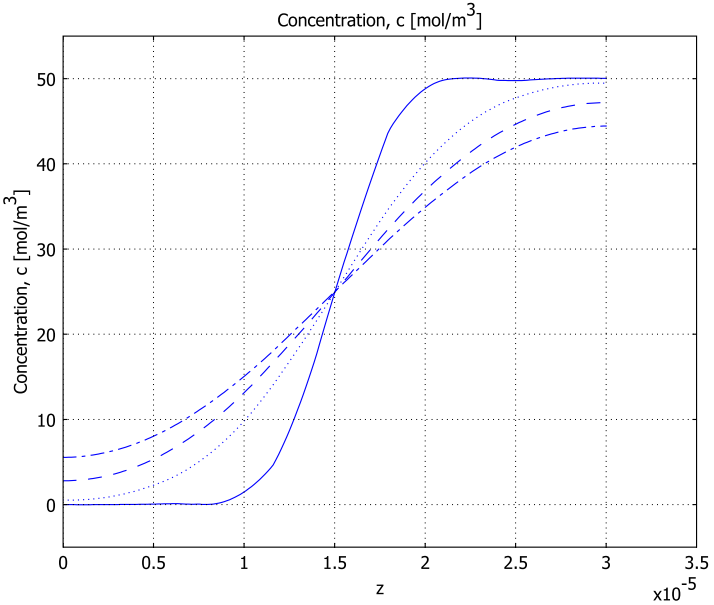


Figure 4-23: Concentration profile along a line in the z direction in the middle of the mixing chamber at various distances from the microchannels: 20 µm (solid), 80 µm (dotted), 140 µm (dashed), and 200 µm (dash-dotted).

Modeling in COMSOL Multiphysics

In COMSOL Multiphysics you build the model with two application modes: The Incompressible Navier-Stokes application mode solves the fluid flow, and the Convection and Diffusion application mode solves the transport of the concentration within the fluid. For both modes use the default values for the equation forms: For the Incompressible Navier-Stokes application mode the default value is the full stress tensor formulation in Equation 4-8; for the Convection and Diffusion application mode the default value is the non-conservative equation form in Equation 4-9. The selection for the Convection and Diffusion application mode ensures that no artificial accumulation of concentration arises when solving the model.

Because the concentration does not affect the fluid flow it is not necessary to solve the application modes simultaneously. By solving them sequentially, first using the Navier-Stokes equations, you improve the solution's convergence and reduce the solution time. Using this technique it takes only a few minutes to solve this model.

It is good practice to save the solution steps in a solver script using the Solver Manager. You can then use this script when trying different values for pressure, concentration, and diffusion coefficients.

To create the 3D geometry (in this example named Geom1), start with three 2D geometries named Geom2, Geom3, and Temp and extrude the 2D drawings. The geometry Temp is a temporary drawing area for creating initial objects that you copy to Geom2 and Geom3, which are work planes in the *xy*-plane located at $z = 0$ and $z = 0.2 \cdot 10^{-4}$ m, respectively. They show the geometry viewed from the top so that the upper channels curve to the right and the lower channels curve to the left.

Model Library path: `MEMS_Module/Microfluidics_Models/lamella_mixer`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Open the **Model Navigator**, and on the **New** page click the **Multiphysics** button.
2. Click **Add Geometry**. From the **Space dimension** list, select **3D**. Click **OK**.
3. From the list of application modes, select **MEMS Module>Microfluidics>Incompressible Navier-Stokes>Steady-state analysis**. Click **Add**.
4. From the list of application modes, select **MEMS Module>Microfluidics>Convection and Diffusion**. Click **Add**.
5. Click **Add Geometry**. From the **Space dimension** list, select **2D**. Click **OK**. This action creates the geometry **Geom2 (2D)**.
6. Click **Add Geometry**, then click **OK**. This creates the geometry **Geom3 (2D)**.
7. Click **Add Geometry**. In the **Geometry Name** edit field, type `Temp`. Click **OK**.
8. Click **OK** to close the **Model Navigator**.

COMSOL Multiphysics opens in the Draw mode with the geometry **Temp** activated.

GEOMETRY MODELING

Initial Drawings

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

2 On the **Axis** page, enter **x-y limits** settings as given in this table; when done, click **OK**.

NAME	VALUE
x min	-25e-5
x max	25e-5
y min	-25e-5
y max	25e-5

You are now ready to draw the initial geometries.

1 Draw six concentric circles centered at the point (–2.4e-4, 0) with radii 2.4e-4, 2.6e-4, 2.7e-4, 2.9e-4, 3.0e-4, and 3.2e-4, respectively. To do so, shift-click on the **Ellipse/Circle (Centered)** button on the Draw toolbar and enter the data in the dialog box.

2 Shift-click on the **Rectangle/Square** button on the Draw toolbar, then enter the following **Size** and **Position** settings:

NAME	VALUE
Width	3.2e-4
Height	2e-4
Base	Corner
x	-2.4e-4
y	0

3 Click **OK**.

4 From the **Edit** menu, choose **Select All**.

5 Click the **Union** button on the Draw toolbar.

6 Click the **Split Object** button on the Draw toolbar.

2D Geometries

1 In the **Temp** geometry, select the objects CO5, CO9, and CO13 (first select CO5 and then Ctrl-click on the other two objects).

2 From the **Edit** menu, choose **Copy**.

3 Click the **Geom2** tab.

4 From the **Edit** menu, choose **Paste**. In the dialog box that appears, leave the displacement values at zero. Click **OK**.

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

6 Select the new objects CO1, CO2, and CO3.

7 Click the **Mirror** button on the Draw toolbar. In the dialog box that appears, click **OK**.

8 From the **Edit** menu, choose **Cut**.

9 Click the **Geom3** tab.

10 From the **Edit** menu, choose **Paste**.

11 In the dialog box that appears, type `0.8e-4` in the **x** edit field; leave the **y** edit field at zero. Click **OK**.

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

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

14 On the **Quick** page, type `0.2e-4` in the **z** edit field. Click **OK**.

15 Click the **Geom2** tab.

16 Shift-click the **Rectangle/Square** button, then enter the following **Size** and **Position** settings:

NAME	VALUE
Width	`0.8e-4`
Height	`2e-4`
Base	Corner
x	0
y	`-2e-4`

17 Click **OK**.

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

3D Geometry

1 Click the **Geom2** tab.

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

3 From the **Objects to extrude** list, select **CO1**, **CO2**, and **CO3**.

4 In the **Distance** edit field, type `1e-5`. Click **OK**.

5 Click the **Geom2** tab.

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

7 From the **Objects to extrude** list, select **R1**.

8 In the **Distance** edit field, type `3e-5`. Click **OK**.

9 Click the **Geom3** tab.

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

11 In the **Objects to extrude** list, select all of them.

12 In the **Distance** edit field, type `1e-5`. Click **OK**.

13 When the software activates **Geom1**, click the **Zoom Extents** button on the Main toolbar.

OPTIONS AND SETTINGS

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

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

NAME	EXPRESSION	DESCRIPTION
p0	10[Pa]	Driving pressure
rho	1e3[kg/m^3]	Density of water
eta	1e-3[Pa*s]	Dynamic viscosity of water
c0	50[mol/m^3]	Input concentration
D_i	1e-10[m^2/s]	Isotropic diffusion coefficient of the substance in water

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Geom1: Incompressible Navier-Stokes (mmglf)**.

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

3 From the **Subdomain selection** list, select all the subdomains.

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

5 In the **Dynamic viscosity** edit field, type `eta`.

6 Click **OK**.

7 From the **Multiphysics** menu, select **2 Geom1: Convection and Diffusion (chcd)**.

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

9 In the **D (isotropic)** edit field, type `D_i`.

10 In the **u** edit field type `u`, in the **v** edit field type `v`, and in the **w** edit field type `w`.

11 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Geom1: Incompressible Navier-Stokes (mmglf)**.

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

3 Enter boundary settings from the following table. When done, click **OK**. For the exterior boundaries that are not explicitly mentioned, the default no-slip boundary condition applies.

SETTINGS	BOUNDARIES 1, 6, 11, 38, 41, 42	BOUNDARIES 3, 8, 13, 17, 18, 24, 31, 37	BOUNDARY 16
Boundary type	Inlet	Wall	Outlet
Boundary condition	Pressure, no viscous stress	Slip	Pressure, no viscous stress
p_0	p0		0

4 From the **Multiphysics** menu, select **2 Geom4: Convection and Diffusion (chcd)**.

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

6 Enter boundary settings from the following table. The **Insulation/Symmetry** condition is the default and need not be set. Do not specify any conditions for the interior boundaries (number 19, 21, 27, 28, 33, and 34). When done, click **OK**.

SETTINGS	BOUNDARIES 1, 6, 11	BOUNDARIES 38, 41, 42	BOUNDARY 16	ALL OTHERS
Boundary condition	Concentration	Concentration	Convective flux	Insulation/ Symmetry
c_0	0	c0		

MESH GENERATION

1 Activate **Geom1**.

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

3 From the **Predefined mesh sizes** list on the **Global** page, select **Extremely fine**.

4 Click **OK** to close the **Free Mesh Parameters** dialog box.

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

COMPUTING THE SOLUTION

Solve the model with the default solver. You can review the default settings in the **Solver Parameters** dialog box.

The first time you solve the model, it is a good idea to record the solution steps and use them later when solving the model with different values. To automate this process, use solver scripting.

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

2 Click the **Script** tab.

3 Select the **Automatically add commands when solving** check box.

4 Click the **Solve For** tab.

5 In the **Solve for variables** list, select **Geom1 (3D)>Incompressible Navier-Stokes (mmglf)**.

6 Click **Solve**.

7 Click the **Initial Value** tab.

8 In the **Values of variables not solved for and linearization point** area, click the **Current solution** button.

9 Click the **Solve For** tab.

10 In the **Solve for variables** list, select **Geom1 (3D)>Convection and Diffusion (chcd)**.

11 Click **Solve**.

12 Click the **Script** tab.

13 Clear the **Automatically add commands when solving** check box.

14 Click **OK**.

If you want to solve the model with other parameter values, follow the steps below. Alternatively, you can go through the steps already listed. In the latter case, remember to skip the tasks (Steps 2 and 3) that would add extra lines to the script.

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

2 Click the **Script** tab.

3 Select the **Solve using a script** check box.

4 Click **Solve**.

5 Clear the **Solve using a script** check box.

6 Click **OK**.

POSTPROCESSING AND VISUALIZATION

First inspect the fluid flow by reproducing the plot in Figure 4-21.

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

2 On the **General** page, go to the **Plot type** area and select the **Slice**, **Streamline**, and **Geometry edges** check boxes. Clear all the other check boxes.

3 Click the **Slice** tab.

4 From the **Predefined quantities** list in the **Slice data** area, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

5 From the **Unit** list, select **mm/s**.

6 In the **Slice positioning** area, set **x levels** to 0 and **y levels** to 5.

7 Click the **Streamline** tab.

8 From the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

9 From the **Streamline plot type** list, select **Magnitude controlled**.

10 On the **Density** page, set the **Min distance** to 0.01 and the **Max distance** to 0.025.

11 Click **OK**.

12 Click the **Go to Default 3D View** button on the Camera toolbar, then click the **Zoom Extents** button on the Main toolbar.

Next, reproduce the plot of the concentration field given in Figure 4-22.

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

2 On the **General** page, go to the **Plot type** area and select the **Boundary** and **Geometry edges** check boxes. Clear all the other check boxes.

3 On the **Boundary** page, go to the **Predefined quantities** list and select **Convection and Diffusion (chcd)>Concentration, c**. Click **OK**.

4 Click the **Go to Default 3D View** button on the Camera toolbar, then click the **Zoom Extents** button on the Main toolbar.

Finally draw the concentration profiles on the centerline of mixing chamber displayed in Figure 4-23.

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

2 On the **Line/Extrusion** page, select **Convection and Diffusion (chcd)>Concentration, c** from the **Predefined quantities** list.

3 From the **x-axis data** list, select **z**. Enter the following **Cross-section line data**:

SETTING	VALUE	SETTING	VALUE
x0	4e-5	x1	4e-5
y0	-2e-5	y1	-2e-5
z0	0	z1	3e-5
Line resolution			200

4 Click **Apply**.

5 Click the **General** tab.

6 Select the **Keep current plot** check box.

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

8 Change the values in the **y0** and **y1** edit fields to `-8e-5`.

9 Click the **Line Settings** button. Set **Line style** to **Dotted line**, then click **OK**.

10 Click **Apply**.

11 Change the values in the **y0** and **y1** edit fields to `-14e-5`.

12 Click the **Line Settings** button. Set **Line style** to **Dashed line**, then click **OK**.

13 Click **Apply**.

14 Change the values in the **y0** and **y1** edit fields to `-20e-5`.

15 Click the **Line Settings** button. Set **Line style** to **Dash-dot line**, then click **OK**.

16 Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the plot.

Electroosmotic Flow in a Biochip

This model was developed by Dr. Jordan MacInnes at the University of Sheffield, UK. The modeling work at his department has been combined with experimental studies.

Introduction

Miniature laboratories (Ref. 1) are required to efficiently analyze the information in human DNA, and they can facilitate tailor-made diagnosis and treatment of hereditary diseases for individuals. A problem that arises in these lab-on-chip devices concerns the transport of the liquid samples and other solutions in the chip, which are of very small dimensions. Moving parts of micrometer scale make the chips very expensive and fragile and are therefore to be avoided if at all possible. An alternative method for transporting fluid in the samples is through electrokinetic effects, where charged ions in the solutions are subjected to an electric field. These ions can drag the entire solution through the channels in the microchip from one analyzing point to the other.

Two mechanisms can drive the flow of a saline solution in an electric field. In the presence of solid surfaces, like the micromachined surfaces of the channels of a biochip, a charged solution is formed close to the wall surfaces. This layer is referred to as a *diffuse double layer*. Depending on the material used, it is formed by negatively or positively charged groups on the wall's surfaces. The electric field displaces the charged liquid in the charged double layer generating an *electroosmotic flow*. Figure 4-24 shows the velocity field shortly after the application of the electric field.

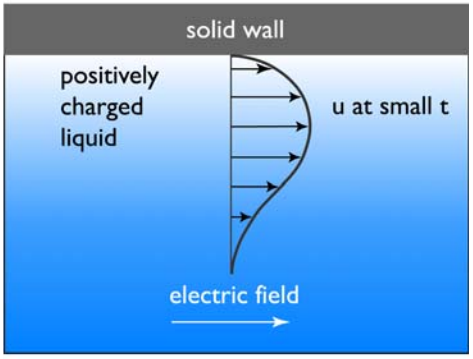


Figure 4-24: Velocity field near a solid wall. The fluid flows in the direction of the electric field.

A force is imposed on the positively charged solution close to the wall surface, and the fluid starts to flow in the direction of the electric field. The velocity gradients perpendicular to the wall give rise to viscous transport in this direction. In the absence of other forces, the velocity profile eventually becomes almost uniform in the cross section perpendicular to the wall. The time constant of the overall flow is roughly 1 ms, while the flow in the double layer responds to changes far more rapidly. The layer model of MacInnes (Ref. 1) replaces the double layer with the Helmholtz-Smoluchowski relationship between wall velocity and wall electric field (Ref. 2).

The second effect arises due to differences in mobility and charge of the ionic species. Negatively and positively charged ions migrate in different directions, and these ions drag water molecules, to different extents, through the channel system. Water is dragged by the sodium ions, which can coordinate more water molecules than the chloride ions in the solution. This type of flow is called electrophoretic flow; Figure 4-25 depicts its basic principle.

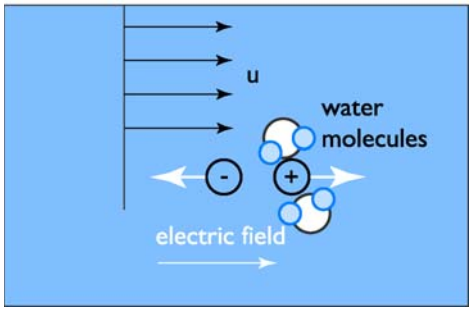


Figure 4-25: Electrophoretic flow.

This particular model does not include the mass balances of dissolved species in the sample (see Ref. 1), but you could easily add these through the Electrokinetic Flow application mode. As another possible model extension, you could use a time-dependent expression for the voltage at the inlet and outlet boundaries.

Model Definition

The flow in the chip is given by the electroosmotic effect just described. To simulate this type of flow, the model must couple the electric potential distribution in the ionic solution in the chip and the equations for fluid flow.

Figure 4-26 shows the chip's geometry. The potential difference imposed between its different parts produces a flow in the vertical or horizontal direction, depending on

the direction of the imposed field. Mode A generates a horizontal flow from right to left in the main channel; Mode B generates a flow that is vertical in the vertical channels and horizontal, from right to left, in the part of the main channel that unites the vertical branches.

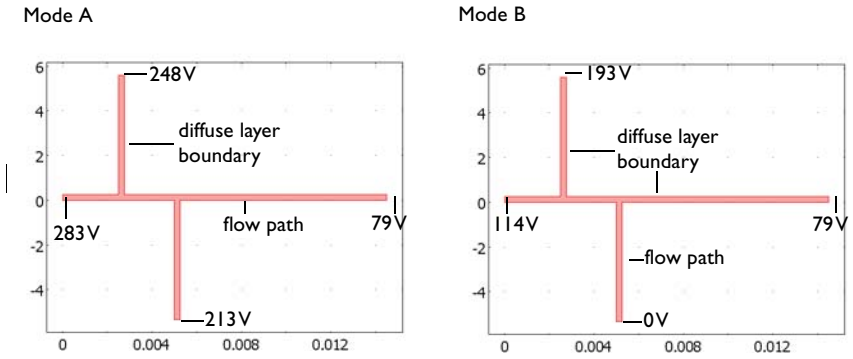


Figure 4-26: Geometry and electric field setup in the two modes: Mode A, where the flow is expected to flow in the horizontal branch, and Mode B, with flow in the vertical branch.

You set the potentials at the open boundaries, where the fluid is allowed to enter or leave the channel system. The wall boundaries are denoted diffuse layer boundaries. From the published work of Dr. MacInnes (Ref. 1), you can expect the flow to be laminar and of low Reynolds number. This implies that you can use the Stokes Flow application mode. The Stokes flow equations are almost the same as the Navier-Stokes equations with the exception that they assume that the inertial term $\rho\mathbf{u}\cdot\nabla\mathbf{u}$ is zero. Therefore they describe flow with a very low Reynolds number and very small inertial forces. Unlike the Navier-Stokes equations, the Stokes equations form a nearly linear system of equations.

The Stokes flow equations are

$$\rho\frac{\partial\mathbf{u}}{\partial t} - \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] = \mathbf{F} \qquad (10)$$

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

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

The boundary conditions, according to the notations just given, are

$$\mathbf{u} = \frac{\varepsilon_0 \varepsilon_r \zeta_0}{\eta} \nabla V \qquad \text{diffuse layer, wall}$$

$$[-p\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] \cdot \mathbf{n} = 0 \qquad \text{voltage boundary and inlet}$$

$$p = 0 \ , [\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] \cdot \mathbf{n} = 0 \qquad \text{outlet}$$

where ε_0 denotes the permittivity of free space (F/m), ε_r is the relative permittivity of water (dimensionless), ζ_0 refers to the *zeta potential* at the channel wall (V), and V denotes the potential (V). For a more detailed review of the diffuse layer wall boundary condition, see Ref. 1 and Ref. 3.

Assuming that there are no concentration gradients for the ions carrying the current, it is possible to express the current balance in the channel through Ohm's law and the balance equation for current density:

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

Here σ denotes the conductivity (S/m) and the expression within the brackets represents the current density (A/m^2).

The corresponding boundary conditions for the current balance are

$$-\sigma \nabla V \cdot \mathbf{n} = 0 \qquad \text{diffuse layer, wall}$$

$$V = V_0 \qquad \text{voltage boundary, inlet or outlet}$$

where V_0 corresponds to the voltage shown in the previous figure at the neutral boundaries. At these boundaries, the potential and current distribution in the chip determine if the fluid enters or exits the chip or stays at rest.

The relevant material properties for water are listed in the following table.

PROPERTY	VALUE	DESCRIPTION
ρ	10^3 kg/m^3	Fluid density
η	10^{-3} kg/(m·s)	Dynamic viscosity
σ	0.11845 S/m	Electric conductivity
ε_r	80.2	Relative permittivity
ζ_0	0.1 V	Zeta potential

Results

Figure 4-27 shows the potential distribution for Mode A in the chip. From this plot it is clear that the largest potential differences are in the horizontal direction. This also implies that the main flow is in the same direction.

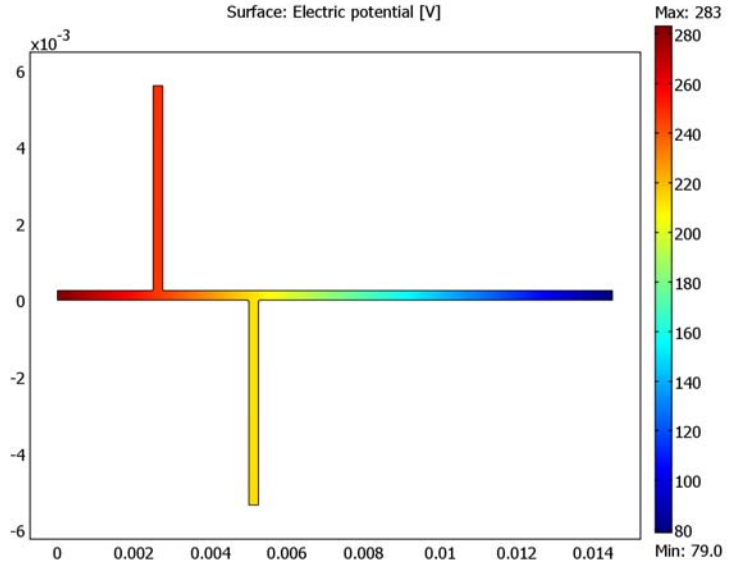


Figure 4-27: Potential distribution in the chip when electric field from mode A is applied.

The plot in Figure 4-28 shows that the average velocity in the channel is approximately 1 mm/s. The largest velocity is at the corner walls where the electric field is large. This clearly shows the effect of the driving force located at the walls. In normal pressure-driven flow, the velocity at the solid surfaces is zero. In fact, looking at the pressure field, you would find that it is constant in the channels.

Studying the velocity flow lines in the channel, Figure 4-29 shows that flow takes a small deviation at the T-junctions in the chip. This can also be detected in the color scale of the velocity, which decreases in the middle of the junction.

Regulating the potential can quickly and efficiently change the path of the flow in the channels. This makes it possible to mix different solutions in different branches of the chip. Figure 4-30 shows a different flow direction with the same magnitude as the potential configuration given in Mode A. In this plot you can also find the corner effects and the low-velocity regions in the T-junctions, as the channel width increases.

Figure 4-31 shows that the flow decreases in the outer parts of the turns while a maximum is seen in the inner parts. This maximum is larger in this case compared to the first case. This is because the electric field is much stronger around the corners compared to the straight path in the first simulation.

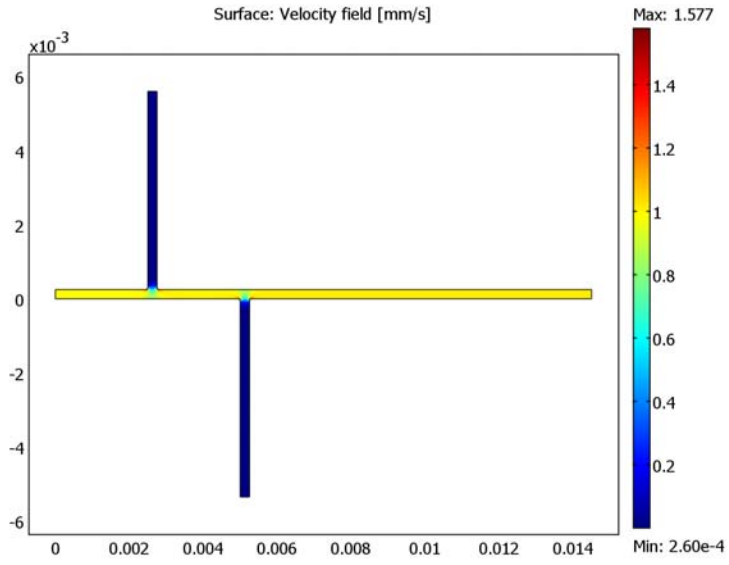


Figure 4-28: Velocity distribution in the chip with the electric field from Mode A applied.

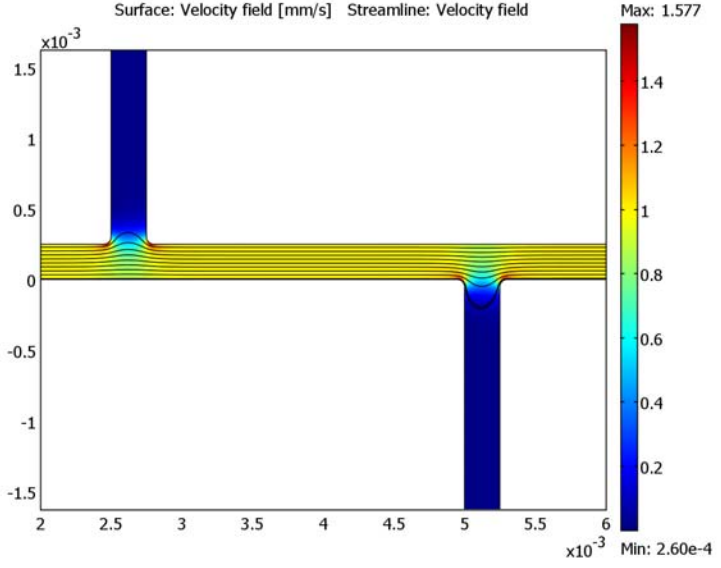


Figure 4-29: Close-up of the velocity field. The surface color is given by the modulus of the velocity vector and the flow lines by the velocity field.

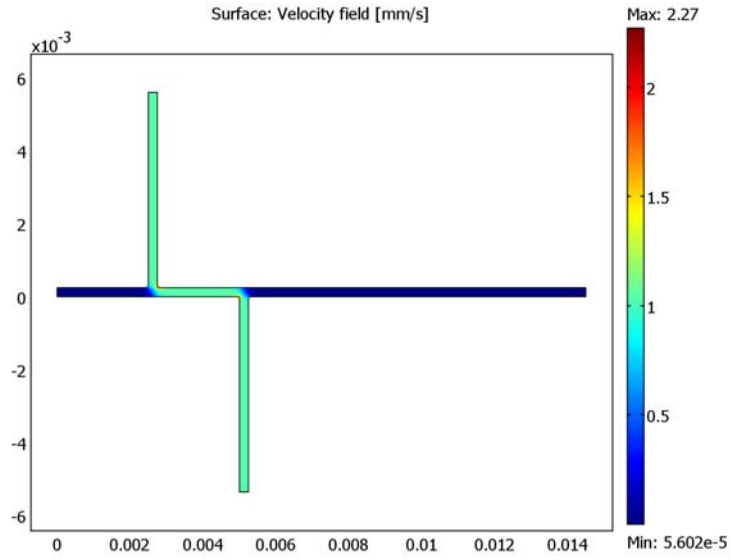


Figure 4-30: Flow distribution in the chip with the electric field from Mode B applied.

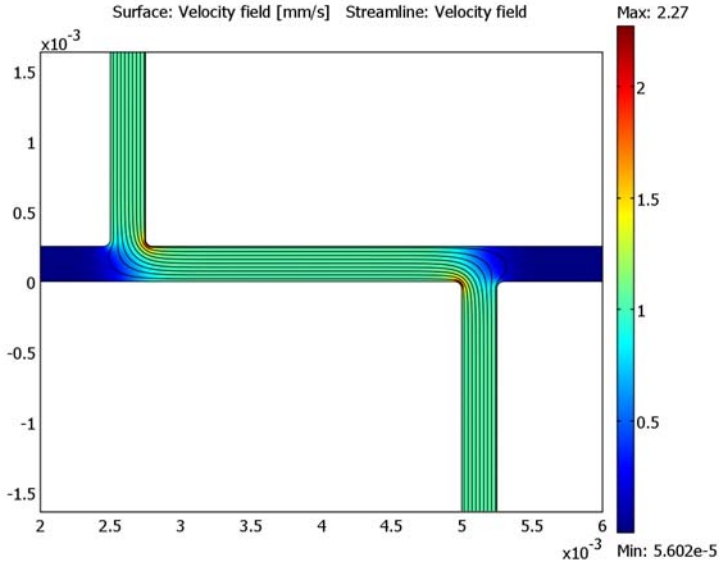


Figure 4-31: Close-up of the flow distribution near the T-junctions.

References

1. J.M. MacInnes, "Computation of Reacting Electrokinetic Flow in Microchannel Geometries," *J. Chem. Eng. Sci.*, vol. 57, no. 21, pp. 4539–4558, 2002.

2. R.F. Probstein, *Physicochemical Hydrodynamics*, Wiley-Interscience, 1994.

3. W. Menz, J. Mohr, and O. Paul, *Microsystems Technology*, Wiley-VCH Verlag GmbH, 2001.

Model Library path: `MEMS Module/Microfluidics_Models/electroosmotic_biochip`

Modeling Using the Graphical User Interface

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

2 From the **Application Modes** list, select **MEMS Module>Microfluidics>Electroosmotic Flow>Stokes Flow**.

3 Click **OK**.

OPTIONS AND SETTINGS

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

2 Define the following constants for water's material properties; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
eta	1e-3[Pa*s]	Dynamic viscosity
rho	1e3[kg/m^3]	Density
sigma	0.11845[S/m]	Conductivity
eps_r	80.2[F/m]	Relative permittivity
zeta0	0.1[V]	Zeta potential

GEOMETRY MODELING

You can easily create the geometry using the CAD tools in COMSOL Multiphysics.

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

2 In the **Size** area of the **Rectangle** dialog box, enter the **Width** `0.25e-3` and the **Height** `5.35e-3`. In the **Position** area, set **x** to `2.5e-3` and **y** to `2.5e-4`. Click **OK**.

3 Repeat this procedure to create two additional rectangles with the following properties:

SETTINGS	RECTANGLE 2	RECTANGLE 3
Width	0.25e-3	1.45e-2
Height	5.35e-3	2.5e-4
x	5e-3	0
y	-5.35e-3	0

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

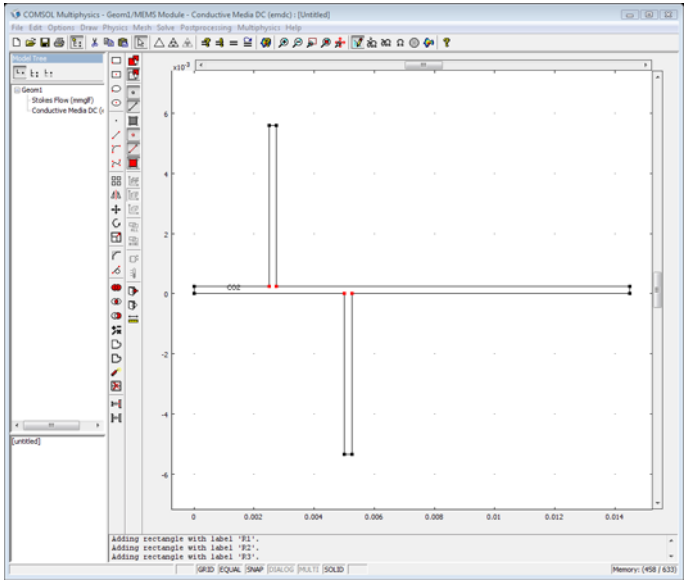
5 Press Ctrl+A to select all geometry objects.

6 Click the **Union** button on the Draw toolbar.

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

8 From the **Draw** menu, select **Fillet/Chamfer**.

9 In the drawing area, Ctrl-click to select the four vertices connecting the vertical channels with the horizontal one (Vertices 3, 5, 8, and 10).



10 In the **Fillet/Chamfer** dialog box, specify the fillet **Radius** 0.5e-4.

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

This completes the geometry modeling stage.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Stokes Flow (mmglf)**.

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

3 Select Subdomain 1.

4 In the ρ edit field, type `rho`, and in the η edit field, type `eta`. Click **OK**.

5 In the **Multiphysics** menu, switch to the **2 Conductive Media DC (emdc)** application mode.

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

7 In the σ edit field, type `sigma`. Click **OK**.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Stokes Flow (mmglf)**.

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

3 Specify boundary conditions according to the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2–4, 6–8, 10, 11, 13–16	BOUNDARIES 5, 9, 12
Boundary type	Outlet	Wall	Open boundary
Boundary condition	Pressure, no viscous stress	Electroosmotic velocity	Normal stress
p_0	0		
E_x		`Ex_emdc`	
E_y		`Ey_emdc`	
ζ		`zeta0`	
f_0			0

4 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

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

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

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 9	BOUNDARY 12	BOUNDARIES 2-4, 6-8, 10, 11, 13-16
Type	Electric potential	Electric potential	Electric potential	Electric potential	Electric insulation
V_0	283	248	213	79	

MESH GENERATION

1. From the **Mesh** menu, select **Free Mesh Parameters**.
2. Click the **Custom mesh size** button, then set the **Mesh curvature factor** to `0.6`.
3. Click the **Boundary** tab. From the **Boundary selection** list, select **1**, **5**, **9**, and **12**.
4. In **Maximum element size** edit field, type `1e-4`.
5. Click the **Remesh** button to generate the mesh.
6. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

Follow these instructions to generate the plot in Figure 4-27:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, make sure that only the **Surface** and **Geometry edges** plot types are selected.
3. On the **Surface** page, select **Conductive Media DC (emdc)>Electric potential** from the **Predefined quantities** list on the **Surface Data** page.
4. Click **Apply**.

Proceed to generate the plots in Figure 4-28 and Figure 4-29 with these steps:

1. On the **Surface** page, select **Stokes Flow (mmglf)>Velocity field** from the **Predefined quantities** list on the **Surface Data** page. From the **Unit** list, select **mm/s**.
2. Click **Apply** to obtain the plot in Figure 4-28.
3. On the **Streamline** page, select the **Streamline plot** check box.
4. From the **Predefined quantities** list on the **Streamline Data** page, select **Stokes Flow (mmglf)>Velocity field**.
5. From the **Streamline plot type** list, select **Magnitude controlled**. Set the **Density** to `9`.
6. On the **Line Color** page, click first the **Uniform color** option button and then the **Color** button. In the **Streamline Color** dialog box, select the black swatch, then click **OK**.
7. Click the **Advanced** button. Set the **Maximum number of integration steps** to `4000`.
8. Click **OK** to close the **Advanced Streamline Parameters** dialog box.
9. Click **OK** in the **Plot Parameters** dialog box.
10. From the **Options** menu, select **Axes/Grid Settings**.

11 On the **Axis** page, specify the following settings:

x min	2e-3
x max	6e-3
y min	-1e-3
y max	1e-3

12 Click **OK** to generate the plot in Figure 4-29.

PHYSICS SETTINGS—MODE B

Now switch the electric field to Mode B (see the right panel of Figure 4-26).

Boundary Conditions

1 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

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

3 Modify the boundary conditions according to the table below; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 9
Boundary condition	Electric potential	Electric potential	Electric potential
V_0	114	193	0

COMPUTING THE SOLUTION—MODE B

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

POSTPROCESSING AND VISUALIZATION—MODE B

The plot that appears in the drawing area when the solver has finished reproduces the one in Figure 4-31. To generate the plot in Figure 4-30, follow these steps:

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

2 On the **Streamline** page, clear the **Streamline plot** check box, then click **OK**.

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

Low-Voltage Electroosmotic Micropump

Micropumps, especially those based on electroosmotic flow (EOF), are essential components in microfluidic lab-on-a-chip devices, because they contain no moving parts and are relatively easy to integrate in microfluidic circuits during fabrication. One major drawback in the conventional design of electroosmotic micropumps is the use of a high driving voltage. Therefore, the development of a low-voltage cascade EOF pump is interesting, because it could draw power from batteries and be suitable for portable devices (Ref. 1).

This model, simulated in 2D, shows how to use the MEMS Module to study the electroosmotic flow described by the electroosmotically-induced boundary velocity.

The model uses the predefined Electroosmotic Flow multiphysics coupling, which builds on the Stokes Flow and the Conductive Media DC application modes.

Introduction

When a polar liquid (such as water) and a solid (such as glass) come into contact, the solid surface acquires an electric charge, which influences the charge distribution within the liquid and causes a 2-layer charge distribution called the electric double layer or EDL (Ref. 2). The charges close to the wall are strongly drawn toward the surface, but the application of an electric field can change the charge distribution deeper in the fluid (Figure 4-32).

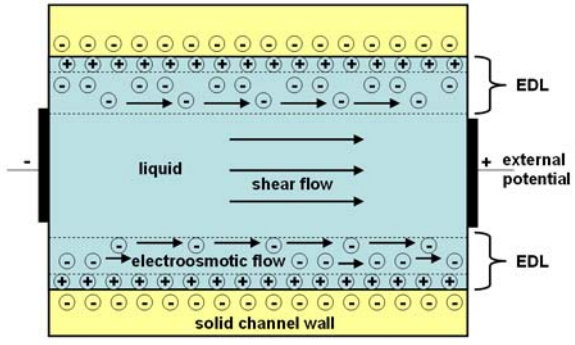


Figure 4-32: Diagram of an electric double layer and the principle of electroosmotic flow.

Because the thickness of the electric double layer is typically on the order of nanometers, you can model the electroosmotic flow velocity, u_{eof}, as a boundary velocity

$$u_{eof} = \mu_{eof}\boldsymbol{E} = \mu_{eof}\nabla V \tag{4-11}$$

where μ_{eof} is the fluid's empirically obtained electroosmotic mobility, and $\boldsymbol{E}$ is the strength of the electric field tangential to the surface. Due to the fluid's viscous force, all the fluid in the channel moves at once.

To study the electroosmotic pumping effect, this discussion works with results published by A. Brask and others (Ref. 1) as well as Y. Takamura and others (Ref. 3). The original pump was designed to work as an effective pressure source for low applied voltages. The main idea is to connect multiple pumps in series to build up pressure (Figure 4-33). Each elementary pump consists of ten narrow channels followed by a wide single channel. The EOF in the narrow channel section acts as a high-pressure pump with a forward electric field. In the wide channel section the electric field is reversed, but here the induced back pressure is small compared to the pressure produced by the narrow channel section. After flowing through one such pump section, the accumulated voltage is zero while the electroosmotically generated pressure maintains a net flow. This feature ensures a low operating voltage, which is an attractive feature that allows the pump to be operated by batteries.

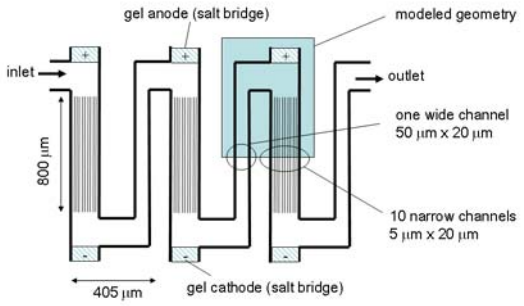


Figure 4-33: Top view of the low-voltage cascade EOF pump with three steps (adapted from Ref. 1 and Ref. 3).

Model Definition

The model geometry (Figure 4-34) contains only half of one pump section (Ref. 1). The flow pattern in the upper half of this section equals that in the lower half, thus reducing the geometry's complexity.

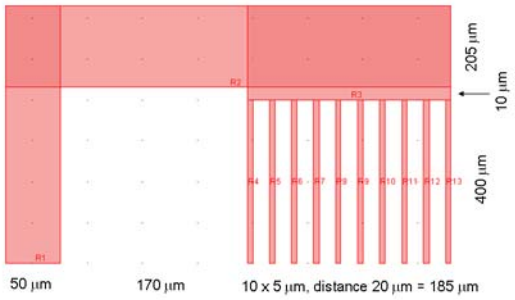


Figure 4-34: The 2D geometry. To more clearly show the dimensions, this diagram extends the aspect ratio in the y direction.

The governing equations for flow, defined by the Stokes flow are:

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

where $\mathbf{u}$ is the velocity, η is the viscosity, and p is the pressure inside the fluid.

The model uses the Pressure boundary condition for the inlet and the outlets. To analyze the free-flow condition, there are no pressure gradients in the flow. The Neutral boundary condition for the outlets would be more precise, but in practice it leads to numerical instabilities and less accurate results. In addition, a model can use the Velocity boundary condition in a parametric analysis to study the maximum back pressure against which the pump can operate. The electroosmotic velocity boundary condition is assigned on the other boundaries. This defines the boundary velocity according to Equation 4-11.

For a conductive material, you can calculate the electric potential from the equation

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

where σ is the electric conductivity of the fluid and V is the electric potential. The model employs the Electric potential boundary condition to set the potential equal to

$V_0 = 10$ V on the electrode and to $V_0/2$ on the channel ends. At all other boundaries, the model uses the Electric insulation boundary condition.

Further, the model assumes that the fluid in the pump is water with the following material properties: density, $\rho = 1000$ kg/m^3; dynamic viscosity, $\eta = 0.001$ Pa·s; electroosmotic mobility, $\mu_{eo} = 0.06$ mm^2/(V·s); relative permittivity, $\varepsilon_r = 78.5$; and isotropic electric conductivity, $\sigma = 0.01$ S/m.

You start the modeling by selecting a predefined Electroosmotic Flow multiphysics coupling from the Model Navigator, which adds the two application modes to the model. You can then build the model using the predefined index groups in the **Boundary Settings** dialog boxes. For example, you can assign boundaries to the Electrode, Outlet, or Electroosmosis groups, which automatically set up the actual boundary conditions discussed earlier in this section.

Results and Discussion

Figure 4-35 shows the flow field when there is no applied pressure. The flow streamlines show an interesting curved behavior close to the electrode caused by the stronger electric field. Even though the electroosmotic velocity always points downward, the larger number of small channels forces a net flow through the pump: the flow through the left channel is directed upward and that through the smaller channels downward.

Figure 4-36 further illustrates this effect. In the absence of an applied pressure, the smaller channels have flat flow-velocity profiles. In the wider channel, in contrast, the forced flow leads to a laminar flow profile. Note also that at the wider channel's boundaries, electroosmosis leads to a boundary flow in the opposite direction.

Figure 4-37 plots the flow through the pump against an applied back pressure. It gives an estimate of the strength of a single pump step. Increasing the back pressure decreases the flow, with the graph intersecting the zero line at 124 Pa. To obtain the pump's total strength, multiply this value by the number of steps. For the pump depicted in Figure 4-33, the result corresponds to a total maximum back pressure of roughly 372 Pa.

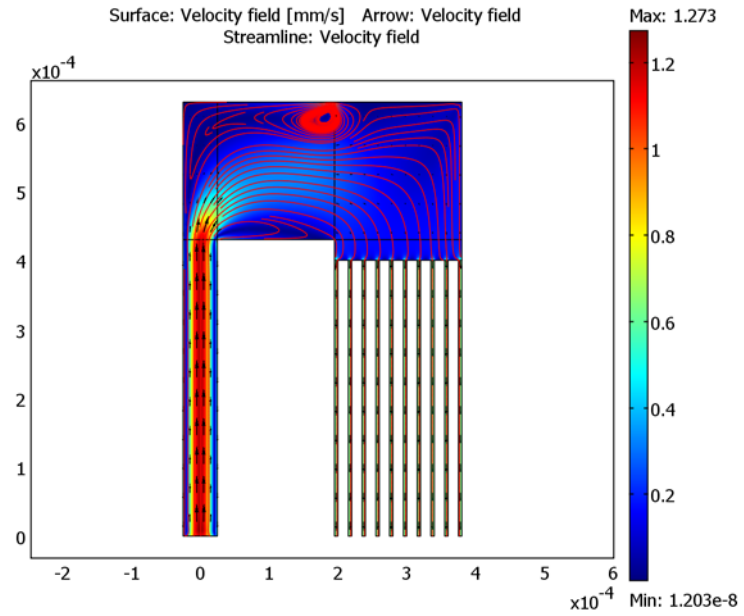


Figure 4-35: Flow streamlines.

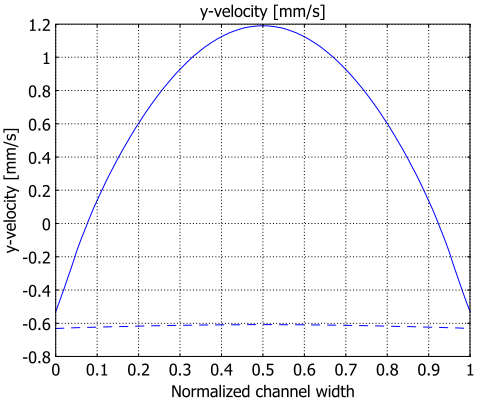


Figure 4-36: The inlet (solid) and outlet (dashed) velocity profiles.

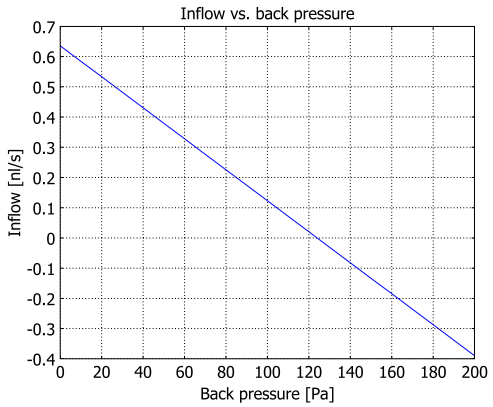


Figure 4-37: Influx versus back pressure.

Modeling in COMSOL Multiphysics

To solve this model using the MEMS Module in COMSOL Multiphysics, you need the Stokes Flow and Conductive Media DC application modes. However, to simplify the model set-up, use the predefined Electroosmotic Flow multiphysics coupling, which adds those two application modes and implements the required couplings between the fluid and the electric field.

Because the flow has no effect on the electric field, you can first solve for the electric potential and then use that solution when computing the flow and pressure fields.

The first solution for the total flux is rather inaccurate. Thus it is a good idea to refine the solution using weak constraints. The advantage of this option is that it computes the fluxes very accurately; for more information on this topic, see the section "Using Weak Constraints" on page 300 in the *COMSOL Multiphysics Modeling Guide*.

This example involves a parametric study to find the maximum back pressure against which the pump can operate. For this analysis you add an integration variable that calculates the flux through the inlet channel, which you plot as a function of the applied back pressure.

References

1. A. Brask, G. Goranovic, and H. Bruus, "Theoretical analysis of the low-voltage cascade electroosmotic pump," *Sens. Actuators B Chem.*, vol. 92, pp. 127–132, 2003.

2. N.-T. Nguyen and S.T. Wereley, *Fundamentals and Applications of Microfluidics*, Artech House, 2002.

3. Y. Takamura, H. Onoda, H. Inokuchi, S. Adachi, A. Oki, and Y. Horiike, "Low-voltage electroosmosis pump for stand-alone microfluidics devices," *Electrophoresis*, vol. 24, pp. 185–192, 2003.

Model Library path:
`MEMS Module/Microfluidics_Models/electroosmotic_micropump_2d`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

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

3 From the **Application Modes** list, select **MEMS Module>Microfluidics>Electroosmotic Flow>Stokes Flow**.

4 Click **OK**.

OPTIONS AND SETTINGS

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

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

NAME	EXPRESSION	DESCRIPTION
sigma	0.01[S/m]	Electric conductivity, water
V0	10[V]	Applied voltage
d	20[um]	Device thickness
eps_r	78.5	Relative permittivity, water
mu_eo	0.06[mm^2/(V*s)]	Electroosmotic mobility
p0	0[Pa]	Outlet pressure

GEOMETRY

You can import the geometry as a COMSOL Multiphysics binary file, `electroosmotic_micropump.mphbin`. Step-by-step instructions for how to manually create the geometry are available in an appendix on page 347.

1 From the **File** menu, select **Import>CAD Data From File**.

2 From the **Files of type** list, select **COMSOL Multiphysics file (*.mphtxt; *.mphbin; ...)**.

3 Browse to the directory where the file `electroosmotic_micropump_2d.mphbin` is stored (the same directory as the model file, that is, `models/MEMS_Module/Microfluidics_Models` under the COMSOL Multiphysics installation folder).

4 Click **Import**.

PHYSICS SETTINGS

Subdomain Settings—Conductive Media DC

1 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

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

3 From the **Subdomain selection** list, select all the subdomains (press Ctrl+A).

4 In the **d** edit field, type `d`.

5 In the σ edit field, type `sigma` to specify an isotropic conductivity.

6 Click **OK**.

Boundary Conditions—Conductive Media DC

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

2 Click in the **Boundary selection** list, then press Ctrl+A to select all boundaries.

3 From the **Group** list, select **Electroosmosis**.

4 Select Boundary 16.

5 From the **Group** list, select **Electrode**. In the $\mathbf{V_0}$ edit field, type `V0`.

6 Select the inlet and all outlet boundaries (Boundaries 2, 11, 20, 25, 30, 35, 40, 45, 50, 55, and 60). Note that you can easily do this by clicking and dragging in the drawing area to enclose the desired boundaries. From the **Group** list select **Electrode**, then type `V0/2` in the $\mathbf{V_0}$ edit field.

7 On the **Groups** page, type `Middle potential` in the **Name** edit field.

8 Click **OK**.

Subdomain Settings—Stokes Flow

1 From the **Multiphysics** menu, select **1 Stokes Flow (mmglf)**.

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

3 Select all the subdomains (press Ctrl+A).

4 On the **Physics** page, the default settings apply to water, so you need only set the **Channel thickness** to `d`.

5 On the **Microfluidic** page, set the **Relative permittivity** ε_r to `eps_r`.

6 Click **OK**.

Boundary Conditions—Stokes Flow

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

2 Specify boundary conditions as in the following table. The table lists only those **Boundary type** and **Boundary condition** settings that you explicitly need to change, having chosen the appropriate entry from the **Group** list.

SETTINGS	BOUNDARY 2	BOUNDARIES 11, 20, 25, 30, 35, 40, 45, 50, 55, 60	ALL OTHERS
Group	Inlet	Outlet	Electroosmosis
Boundary condition	Pressure	Pressure, no viscous stress	
p_0	0	p0	
μ_{eo}			`mu_eo`

Again, click and drag in the drawing area to quickly select all **Outlet** boundaries. To conveniently select the **Electroosmosis** boundaries, first select Boundary 1 and then select the **Select by group** check box.

3 Click **OK**.

MESH GENERATION

For this model, a mixed mesh is suitable: use mapped quad meshes for the elongated channels and a free mesh for the rest of the geometry.

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

2 Click the **Boundary** tab. For all of the boundaries in the following table, select the **Constrained edge element distribution** check box, then enter a value in the **Number of edge elements** edit field as indicated in the table. Note that the boundaries in the last row are all in the same line at the lower ends of the narrow channels; you can select all of them most easily by using the mouse to enclose them in the drawing area.

BOUNDARIES	NUMBER OF EDGE ELEMENTS
1	90
2	20
10, 19, 24, 29, 34, 39, 44, 49, 54, 59	80
11, 20, 25, 30, 35, 40, 45, 50, 55, 60	8

3 Click the **Subdomain** tab. Select Subdomains 1, 4, and 7–15 (the channels).

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

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

6 On the **Global** page, select **Extra fine** from the **Predefined mesh sizes** list.

7 Click the **Subdomain** tab. Select Subdomains 2, 3, 5, and 6.

8 In the **Subdomain mesh parameters** area, set the **Maximum element size** to `1e-5`.

9 Click the **Mesh Selected** button, then click **OK**.

As you can verify in the **Mesh Statistics** dialog box (that you open from the **Mesh** menu), the completed mesh consists of about 8200 quadrilateral and 6887 triangular elements.

COMPUTING THE SOLUTION

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

2 Click the **Solve For** tab.

3 From the **Solve for variables** list, select **Conductive Media DC (emdc)**.

4 Click **Solve**. Doing so should result in roughly 48,600 degrees of freedom, and the solution time should be a couple of seconds.

5 Click the **Initial Value** tab. In the **Value of variables not solved for and linearization point** area, click the **Current solution** button.

6 Click the **Solve For** tab. In the **Solve for variables** list select **Stokes Flow (mmglf)**.

7 Click **Solve**. The solution time for this solving stage should be roughly four times longer than for the electrostatics part (this time you solve for about 117,700 DOFs).

8 Click **OK**.

POSTPROCESSING AND VISUALIZATION

First study the velocity-field distribution inside the pump by reproducing the combined surface and streamline plot given in Figure 4-35.

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

2 On the **General** page, select the **Surface**, **Arrow**, **Streamline**, and **Geometry edges** check boxes in the **Plot type** area. Clear all the others.

3 Click the **Surface** tab. On the **Surface Data** page, verify that the selection in the **Predefined quantities** list is **Stokes Flow (mmglf)>Velocity field**. From the **Unit** list, select **mm/s**.

4 Click the **Arrow** tab. On the **Subdomain Data** page, verify that the selection in the **Predefined quantities** list again is **Stokes Flow (mmglf)>Velocity field**.

5 In the **Arrow positioning** area, click the **Vector with coordinates** option button for **x points**. In the associated edit field type `-2.5e-5:1e-5:2.5e-5 1.975e-4:2e-5:3.775e-4`.

6 In the **Arrow parameters** area, select **3D arrow** from the **Arrow type** list. Click the **Color** button. In the **Arrow Color** dialog box, click the black swatch, then click **OK**.

7 Click the **Streamline** tab. On the **Streamline Data** page, verify that the selection in the **Predefined quantities** list is **Stokes Flow (mmglf)>Velocity field**. From the **Streamline plot type** list, select **Uniform density**. Set the **Separating distance** to `0.02`.

8 Click **OK** to generate the plot.

Next use domain plots to analyze the inlet and outlet velocity profiles.

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

2 On the **General** page, click the **Title/Axis** button at the bottom of the dialog box. Go to the **Axis settings for line and point plots** area. Select the option button next to the edit field for the **First axis label**, then enter the text `Normalized channel width`. Click **OK**.

3 Select the **Keep current plot** check box.

4 Click **Line/Extrusion** tab.

5 In the **Plot type** area, click the **Line plot** button. Select Boundary 2.

6 In the **y-axis data** area, select **Stokes Flow (mmglf)>y-velocity** from the **Predefined quantities** list. From the **Unit** list, select **mm/s**.

7 In **x-axis data** area, click the **Expression** option button, then click the associated **Expression** button. In the **Expression** edit field, type `s` (this is a predefined variable for the normalized distance along the boundary). Click **OK**.

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

9 Select Boundary 11.

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

11 Click **OK** to reproduce the plot in Figure 4-36.

Next study the total fluxes through the inlet and outlets.

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

2 From the **Boundary selection** list, select **2**.

3 In the **Expression to integrate** area, type `(-nx*u-ny*v)*d` in the **Expression** edit field and `nl/s` in the **Unit** edit field to obtain the result expressed in nanoliters per second. The constant `d` gives the structure's thickness, while –`nx` and –`ny` are the x- and y-components of the inward-pointing normal vector.

4 Click **Apply**.

This setup should result in a value of 0.638 nl/s, a value that appears in the message log at the bottom of the user interface.

Next, compute the total flux through the outlets.

5 Using the mouse, select the outlet boundaries (Boundaries 11, 20, 25, 30, 35, 40, 45, 50, 55, and 60).

6 Click **OK**.

The resulting value of –0.618 nl/s differs slightly from the value for the inlet. You can evaluate all the other boundaries and observe that due to numerical inaccuracies the walls appear to leak slightly. Reducing this mass "leak" requires a finer mesh. For the purpose of the present analysis, assume the error to be small enough (roughly 3%) to continue the analysis.

FINDING THE MAXIMUM BACK PRESSURE

Finally make a parametric study where you vary the back pressure and identify the maximum back pressure from a plot of flux vs. pressure. Start by defining a global integration variable for the influx.

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

2 From the **Boundary selection** list, select **2**.

3 In the **Name** edit field type `Inflow`, and in the **Expression** edit field type `(-nx*u-ny*v)*d` (that is, the same expression you used for the flux studies).

4 Click **OK**.

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

6 From the **Solver** list, select **Parametric**. In the **Parameter name** edit field, type `p0` and in the **Parameter values** edit field, type `0:10:200`.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar. Solving this parametric study can take several minutes.

Next, plot the inflow as a function of the back pressure (see Figure 4-37).

1 From the **Postprocessing** menu, select **Global Variables Plot**.

2 In the **Expression** field, type `Inflow*1[m^3/nl]`, then click the **Add Entered Expression** button immediately to the right of the edit field. Multiplying the boundary integration variable `Inflow` (which has no unit, but by its definition is the inflow value measured in m^3/s) by the factor `1[m^3/nl]` gives the result in nanoliters/second.

3 Click the **Title/Axis** button. Enter the **Title** `Inflow vs. back pressure`, the **First axis label** `Back pressure [Pa]`, and the **Second axis label** `Inflow [nl/s]`.

4 Click **OK** to close the **Title/Axis Settings** dialog box.

5 Click **OK** to close the **Global Variables Plot** dialog box and generate the plot.

By zooming in on the plot you can see that the inflow changes sign (that is, turns into an net outflow) around 124 Pa.

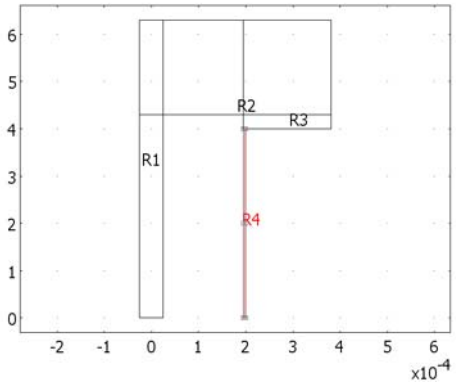
Appendix—Geometry Modeling

Follow these instructions to create the geometry by hand.

1 Shift-click the **Rectangle/Square** button on the Draw toolbar on the left side of the user interface and create the following rectangles:

PROPERTY	R1	R2	R3	R4
Width	50e-6	405e-6	185e-6	5e-6
Height	630e-6	200e-6	230e-6	400e-6
x	-25e-6	-25e-6	195e-6	195e-6
y	0	430e-6	400e-6	0

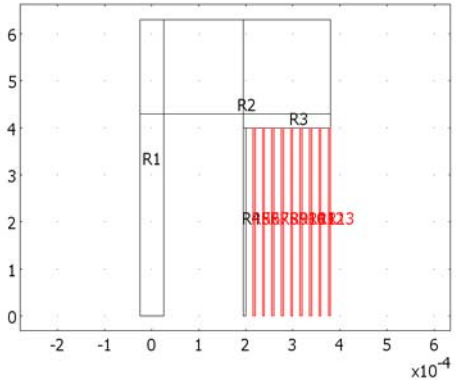
2 Click the **Zoom Extents** button on the Main toolbar.



The geometry before creating the array of narrow channels.

3 Select **R4**, then click the **Array** button on the Draw toolbar.

4 In the **Displacement** area, for **x** enter `20e-6` and for **y** enter `0`. In the **Array size** area, for **x** enter `10` and for **y** enter `1`. Click **OK**.



The geometry after creating the array of channels.

Electroosmotic Micromixer

This model was originally done in COMSOL Multiphysics by H. Chen, Y. T. Zhang, I. Mezic, C. D. Meinhart, and L. Petzold of the University of California, Santa Barbara (Ref. 1 and Ref. 2).

Microlaboratories for biochemical applications often require rapid mixing of different fluid streams. At the microscale, flow is usually highly ordered laminar flow, and the lack of turbulence makes diffusion the primary mechanism for mixing. While diffusional mixing of small molecules (and therefore of rapidly diffusing species) can occur in a matter of seconds over distances of tens of micrometers, mixing of larger molecules such as peptides, proteins, and high molecular-weight nucleic acids can require equilibration times from minutes to hours over comparable distances. Such delays are impractically long for many chemical analyses. These problems have led to an intense search for more efficient mixers for microfluidic systems.

Most microscale mixing devices are either passive mixers that use geometrical stirring, or active mixers that use moving parts or external forces, such as pressure or electric field.

In a passive mixer, one way of increasing the mixing is by "shredding" two or several fluids into very thin alternating layers, which decreases the average diffusion length for the molecules between the different fluids. However, these mixers often require very long mixing channels because the different fluids often run in parallel. Another way of improving mixing efficiency is to use active mixers with moving parts that stir the fluids. At the microscale level moving parts in an active mixer are very fragile. One alternative is to use electroosmotic effects to achieve a mixing effect that is perpendicular to the main direction of the flow.

This model takes advantage of electroosmosis to mix fluids. The system applies a time-dependent electric field, and the resulting electroosmosis perturbs the parallel streamlines in the otherwise highly ordered laminar flow.

Model Definition

This example of a rather simple micromixer geometry (Figure 4-38) combines two fluids entering from different inlets into a single 10 μm wide channel. The fluids then enter a ring-shaped mixing chamber that has four microelectrodes placed on the outer wall at angular positions of 45, 135, –45, and –135 degrees, respectively. Assume that

the aspect ratio (channel depth to width) is large enough that you can model the mixer using a 2D cross-sectional geometry. The material parameters relevant for the model are given in Table 4-4.

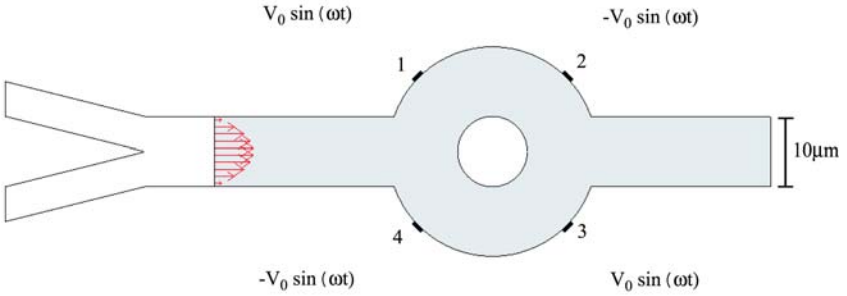


Figure 4-38: Geometry of the micromixer with four symmetric electrodes on the wall of the mixing chamber. This example does not model the two inlet channels. Here you assume a parabolic inflow at the beginning of the computational domain (the gray area).

The Navier-Stokes equations for incompressible flow describe the flow in the channels:

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

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

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

Because you do not model the two inlet channels, assume that the entrance channel starts at a position where the flow has a fully developed laminar profile. The mixed fluid flows freely out of the right end boundary, where you specify vanishing total stress components normal to the boundary:

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

When brought into contact with an electrolyte, most solid surfaces acquire a surface charge. In response to the spontaneously formed surface charge, a charged solution forms close to the liquid-solid interface. Known as an electric double layer, it forms because of the charged groups located on the surface that faces the solution. When the operator applies an electric field, the electric field generating the electroosmotic flow displaces the charged liquid in the electric double layer. This scheme imposes a force on the positively charged solution close to the wall surface, and the fluid starts to flow

in the direction of the electric field. The velocity gradients perpendicular to the wall give rise to viscous transport in this direction. In the absence of other forces, the velocity profile eventually becomes almost uniform in the cross section perpendicular to the wall.

This model replaces the thin electric double layer with the Helmholtz-Smoluchowski relation between the electroosmotic velocity and the tangential component of the applied electric field:

$$\mathbf{u} = \frac{\varepsilon_w \zeta_0}{\eta} \nabla_T V$$

In this equation, $\varepsilon_w = \varepsilon_0 \varepsilon_r$ denotes the fluid's electric permittivity (F/m), ζ_0 represents the zeta potential at the channel wall (V), and V equals the potential (V). This equation applies on all boundaries except for the entrance and the outlet.

Assuming that there are no concentration gradients in the ions that carry the current, you can express the current balance in the channel with Ohm's law and the balance equation for current density

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

where σ denotes conductivity (S/m) and the expression within parentheses represents the current density (A/m^2).

The electric potentials on the four electrodes are sinusoidal in time with the same maximum value ($V_0 = 0.1$ V) and the same frequency (8 Hz), but they alternate in polarity. Potentials on electrodes 1 and 3 are $V_0 \sin(2\pi f t)$, whereas potentials on electrodes 2 and 4 are $-V_0 \sin(2\pi f t)$ (see Figure 4-38).

Assume all other boundaries are insulated. The insulation boundary condition

$$-\sigma \nabla V \cdot \mathbf{n} = 0$$

sets the normal component of the electric field to zero.

At the upper half of the inlet (see Figure 4-38) the solute has a given concentration, c_0; at the lower half the concentration is zero. Thus, assume that the concentration changes abruptly from zero to c_0 at the middle of the inlet boundary. The mixed solution flows out from the right outlet by convection, and all other boundaries are assumed insulated.

Inside the mixer, the following convection-diffusion equation describes the concentration of the dissolved substances in the fluid:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - \mathbf{u} \cdot \nabla c \qquad (4\text{-}12)$$

Here c is the concentration, D represents the diffusion coefficient, R denotes the reaction rate, and $\mathbf{u}$ equals the flow velocity. In this model $R = 0$ because the concentration is not affected by any reactions.

TABLE 4-4: MODEL INPUT DATA

PARAMETER	VALUE	DESCRIPTION
ρ	1000 kg/m^3	Density of the fluid
η	10^{-3} Pa·s	Dynamic viscosity of the fluid
U_0	0.1 mm/s	Average velocity through the inlet
ε_r	80.2	Relative electric permittivity of the fluid
ζ	-0.1 V	Zeta potential on the wall-fluid boundary
σ	0.11845 S/m	Conductivity of the ionic solution
D	10^{-11} m^2/s	Diffusion coefficient
c_0	1 mol/m^3	Initial concentration

Results and Discussion

Figure 4-39 shows a typical instantaneous streamline pattern. It reveals that electroosmotic recirculation of the fluid vigorously stirs the flow, typically in the form of two rotating vortices near the electrodes.

The fundamental processes of effective mixing involve a combination of repeated stretching and folding of fluid elements in combination with diffusion at small scales. As the system applies the AC field (Figure 4-40), the resulting electroosmotic flow perturbs the laminar pressure-driven flow such that it pushes the combined stream pattern up and down at the beginning of the mixing chamber, causing extensive folding and stretching of material lines.

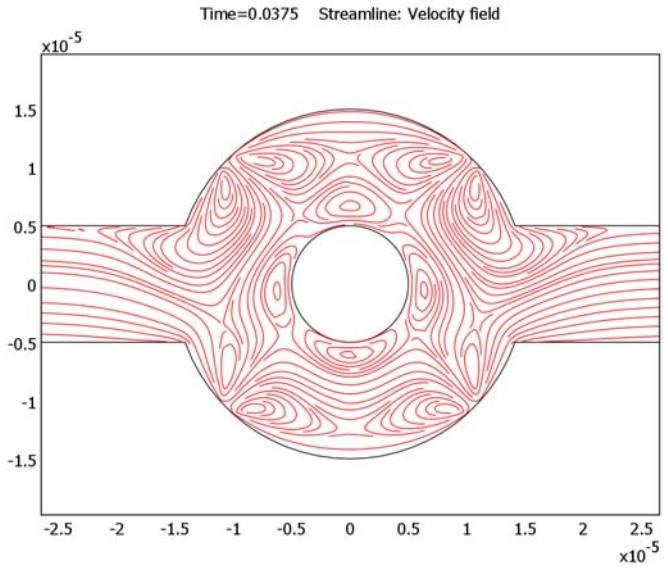


Figure 4-39: Fluid streamlines in an electroosmotic micromixer at t = 0.0375 s.

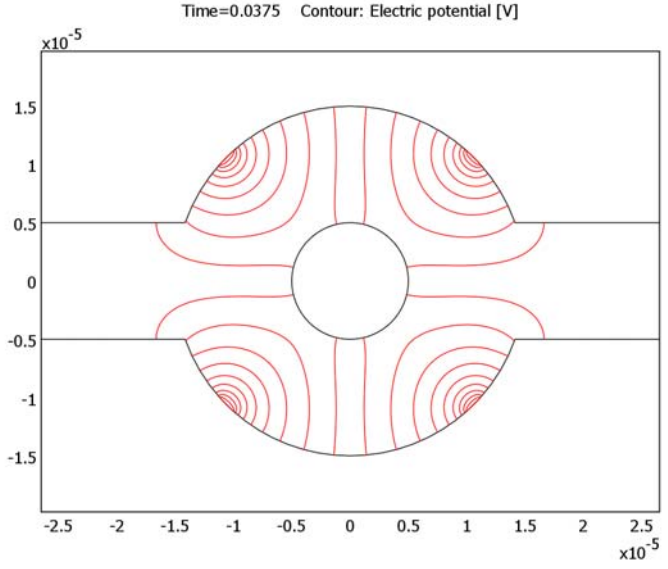


Figure 4-40: Electric potential lines for an electroosmotic micromixer. The contour lines show the shape when the device uses maximal potentials ($\pm V_0$).

The following plots further exemplify how the mixer operates. Figure 4-41 shows the concentration at steady state when the electric field is not applied. The flow is laminar and the diffusion coefficient is very small, so the two fluids are well separated also at the outlet. When the alternating electric field is applied, the mixing increases considerably owing to the alternating swirls in the flow. Figure 4-42 depicts the system at the instant when the electric field and the electroosmotic velocity have their largest magnitudes during the cycle (that is, when $|\sin \omega t| = 1$). From the plot you can estimate that the concentration at the output fluctuates with the same frequency as the electric field. Thus, this mixer should be further improved to get a steadier output.

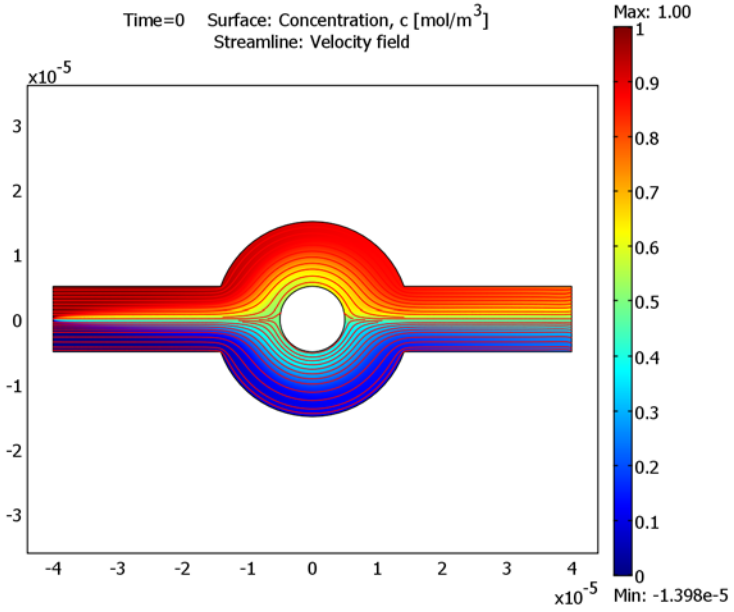


Figure 4-41: Steady-state solution in the absence of an electric field.

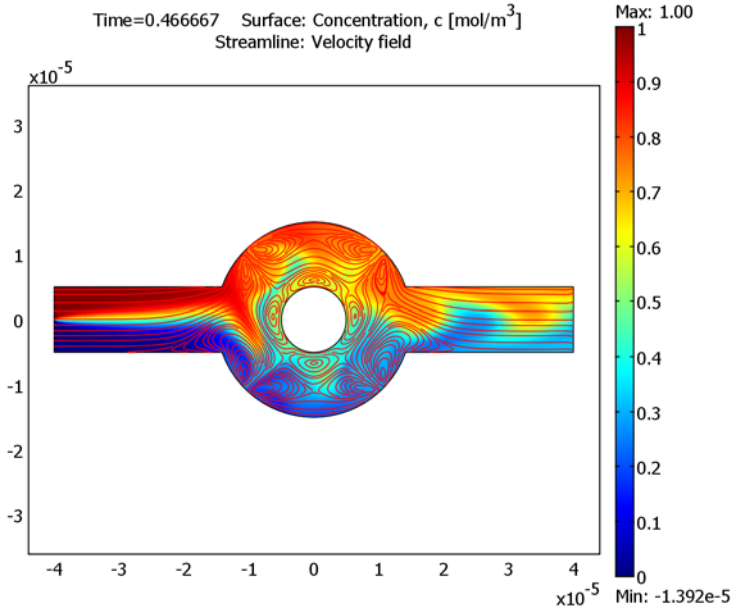


Figure 4-42: Time-dependent solution at the time when the alternating electric field has its largest magnitude.

This example demonstrates a rather simple and effective use of electrokinetic forces for mixing. The scheme is easy to implement, and you can easily control both the amplitude and the frequency. At low Reynold numbers the inertial forces are small, which makes it possible to calculate stationary streamlines patterns using the parametric solver to control amplitude.

Modeling in COMSOL Multiphysics

Cummings and others (Ref. 3) have shown that in order to use the Helmholtz-Smoluchowski equation at the fluid-solid boundaries, the electric field must be at least quasi-static to neglect transient effects. In other words, the time scale of the unsteady electric field must be much larger than that of the transient flow. Y. T. Zhang and others (Ref. 1) estimated that the time scale of the transient effect in the modeled micromixer (with a channel width of 10 microns) is roughly 0.0127 s. In this simulation the frequency of the applied electric potential is 8 Hz, which corresponds to a time scale of the electric field 10 times larger than that of the flow.

Because you can model the time-dependent electric field as a product of a stationary electric field and a time-dependent phase factor ($\sin\omega t$), it is possible to reduce the simulation time and memory requirements by dividing the solution into two stages. In the first, calculate the amplitude of the electric potential field and the initial state for the time-dependent flow model using a stationary solver. In the second stage, you deactivate the DC Conductive Media application mode and calculate the transient solution for the Incompressible Navier-Stokes and the Convection and Diffusion application modes. You obtain the tangential electric field components used in the electroosmotic velocity boundary condition by multiplying the stationary DC solution by $\sin\omega t$. This approach is permissible because there is only a one-way coupling between the electric field and the fluid fields.

References

1. H. Chen, Y.T. Zhang, I. Mezic, C.D. Meinhart, and L. Petzold, "Numerical simulation of an electroosmotic micromixer," *Proc Microfluidics 2003* (ASME IMECE), 2003.

2. Y.T. Zhang, H. Chen, I. Mezic, C.D. Meinhart, L. Petzold, and N.C. MacDonald, "SOI Processing of a Ring Electrokinetic Chaotic Micromixer," *Proc NSTI Nanotechnology Conference and Trade Show* (Nanotech 2004), vol. 1, pp. 292–295, 2004.

3. E. Cummings, S. Griffiths, R. Nilson, and P. Paul, "Conditions for similitude between the fluid velocity and the electric field in electroosmotic flow,", *Anal. Chem.*, vol. 72, pp. 2526–2532.

Model Library path: `MEMS_Module/Microfluidics_Models/electroosmotic_mixer`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, go to the **New** page and in the **Space dimension** list select **2D**.

2 Click the **Multiphysics** button.

3 In the **Application Modes** list, select **MEMS Module>Microfluidics>Incompressible Navier-Stokes>Transient analysis**. Click **Add**.

4 In the **Application Modes** list, select **MEMS Module>Electrostatics>Conductive Media DC**. Click **Add**.

5 In the **Application Modes** list, select **MEMS Module>Microfluidics>Convection and Diffusion>Transient analysis**. Click **Add**.

6 Click **OK**.

OPTIONS AND SETTINGS

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

2 In the dialog box that opens, define the following constants (the descriptions are optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
U0	0.1[mm/s]	Mean inflow velocity
sigma_w	0.11845[S/m]	Conductivity of the ionic solution
eps_r	80.2	Relative permittivity of the fluid
zeta	-0.1[V]	Zeta potential
V0	0.1[V]	Maximum value of the AC potential
freq	8[Hz]	Frequency of the AC potential
omega	2*pi[rad]*freq	Angular frequency of the AC potential
t	0[s]	Start time
D	1e-11[m^2/s]	Diffusion coefficient of the solution
c0	1[mol/m^3]	Initial concentration

You need the constant `t` (used in the scalar expressions below) when first solving the model using a stationary solver. In the time-dependent simulation, the internal time variable, `t`, overwrites this constant (the red color is just a warning signalling that `t` is an internal variable).

GEOMETRY MODELING

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

2 In the **Rectangle** dialog box that appears, enter these properties; when done, click **OK**.

PARAMETER	VALUE
Width	80e-6
Height	10e-6
Base	Center
x position	0
y position	0

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

4 Shift-click the **Ellipse/Circle (Centered)** button on the Draw toolbar.

5 In the **Circle** dialog box that appears, enter these properties; when done, click **OK**.

PARAMETER	VALUE
Radius	15e-6
Base	Center
x position	0
y position	0

6 Repeat Steps 4 and 5 for another circle centered at (0, 0) and with a radius of `5e-6`. Click **OK**.

7 Select all the geometry objects (for example by pressing Ctrl+A).

8 From the **Draw** menu, select **Create Composite Object**.

9 In the **Set formula** edit field, enter the expression `(R1+C1)-C2`.

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

11 Shift-click the **Rectangle/Square (Centered)** button in the Draw toolbar.

(Steps 12 to 15 create boundaries for the four electrodes.)

12 In the **Square** dialog box, enter these properties; when done, click **OK**.

PARAMETER	VALUE
Width	22.27e-6
Base	Center
x position	0
y position	0

13 Select all the geometry objects (press Ctrl+A).

14 From the **Draw** menu select **Create Composite Object**.

15 In the **Set formula** edit field, enter the expression `(CO1*SQ1)+CO1`. Verify that the **Keep interior boundaries** check box is cleared. Click **OK**.

16 Shift-click the **Point** button on the Draw toolbar. Specify values according to the following table; when finished, click **OK**.

PARAMETER	VALUE
Coordinate x	`-4e-5`
Coordinate y	0
Name	PT1

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

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

3 Select Subdomain 1.

4 On the **Physics** page, verify that the default values are as in the following table:

PROPERTY	VALUE
ρ	1e3
η	1e-3
F_x	0
F_y	0

5 On the **Microfluidic** page, type `eps_r` in the ε_r edit field; when done, click **OK**.

6 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

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

8 In the σ edit field, type `sigma_w`, then click **OK**.

9 From the **Multiphysics** menu, select **3 Convection and Diffusion (chcd)**.

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

11 Specify the following properties; when done, click **OK**.

PROPERTY	VALUE
D (isotropic)	D
R	0
u	u
v	v

Boundary Conditions

1 From the **Multiphysics** menu, choose **1 Incompressible Navier-Stokes (mmglf)**.

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

3 Enter the boundary conditions in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 3	BOUNDARIES 2, 4–6, 8–23	BOUNDARY 7
Boundary type	Inlet	Wall	Outlet
Boundary condition	Laminar inflow	Electroosmotic velocity	Normal stress
U_0	U0		
L_{entr}	1e-5		
Constrain end points to zero	Yes		
E_x		Ex_emdc*sin(omega*t)	
E_y		Ey_emdc*sin(omega*t)	
ζ		zeta	
f_0			0

4 From the **Multiphysics** menu, select **2 Conductive Media DC (emdc)**.

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

6 Specify the boundary conditions in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 10, 21	BOUNDARIES 11, 20	BOUNDARIES 1–9,12–19, 22, 23
Boundary condition	Electric potential	Electric potential	Electric insulation
V_0	-V0	V0	

7 From the **Multiphysics** menu, select **3 Convection and Diffusion (chcd)**.

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

9 Enter these boundary conditions; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 3	BOUNDARIES 2, 4–6, 8–23	BOUNDARY 7
Boundary condition	Concentration	Insulation/Symmetry	Convective flux
c_0	`c0*flc2hs(y[1/m],1e-7)`		

The concentration condition on Boundaries 1 and 3 give a sharp but smooth concentration gradient in the middle of the channel entrance.

MESH GENERATION

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

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

3 Click the **Custom mesh size** option button. Set the **Maximum element size scaling factor** to `0.25`.

4 Click the **Boundary** tab. Select Boundaries 10, 11, 20, and 21 (the electrodes).

5 In the **Boundary mesh parameters** area, set the **Maximum element size** to `0.2e-6` and the **Element growth rate** to `1.1`. These settings result in a finer mesh near the electrodes.

6 Click the **Point** tab. Select Point 2.

7 In the **Point mesh parameters** area, set the **Maximum element size** to `1e-7` and the **Element growth rate** to `1.1`. With these settings, the concentration gradient at the entrance is properly resolved.

8 Click **OK** to close the **Free Mesh Parameters** dialog box.

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

COMPUTING THE SOLUTION

Start by computing the stationary solution for velocity, pressure, concentration, and electric potential amplitude. In the transient simulation stage, you then solve only the Incompressible Navier-Stokes and the Convection and Diffusion application modes.

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

2 From the **Analysis** list, select **Stationary**, then click **Apply**.

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

4 Click the **Solve** button on the Main toolbar to compute the initial solutions for all application modes.

5 In the **Solver Parameters** dialog box, restore the **Analysis** list selection to **Transient**.

6 In the **Time stepping** area, type `0:0.125/60:0.5` in the **Times** edit field.

7 Click **OK**.

8 Click the **Solver Manager** button on the Main toolbar.

9 On the **Initial Value** page, click the **Store Solution** button.

10 In the **Initial value** area click the **Stored solution** option button.

11 On the **Solve For** page, select **Incompressible Navier-Stokes (mmglf)** and **Convection and Diffusion (chcd)** (first select one, then Ctrl-click the other).

12 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

First study the swirls in the flow (see Figure 4-39 on page 353):

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

2 In the **Plot type** area on the **General** page, select only **Streamline** and **Geometry edges**.

3 From the **Solution at time** list, select **0.0375**.

4 Click the **Streamline** tab. From the **Predefined quantities** list on the **Streamline Data** page, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

5 From the **Streamline plot type** list, select **Uniform density**.

6 Set the **Separating distance** to `0.01`, then click **Apply**.

Next visualize the electric potential (see Figure 4-40 on page 353):

1 Click the **General** tab. In the **Plot type** area, select only **Contour** and **Geometry edges**.

2 Click the **Contour** tab. On the **Contour Data**, page find the **Predefined quantities** list and select **Conductive Media DC (emdc)>Electric potential**.

3 In the **Contour levels** area, click the **Vector with isolevels** option button; in the associated edit field, type `linspace(-0.1,0.1,20)`.

4 In the **Contour color** area click the **Uniform color** option button.

5 Clear the **Color scale** check box.

6 Click **Apply**.

Finally examine the mixing of the fluid:

1 On the **General** page, select the **Surface** and **Streamline** check boxes and clear the **Contour** check box in the **Plot type** area.

2 From the **Solution at time** list, select the time you want: 0 corresponds to the steady state value, and at 0.46875 the electric field has it maximum amplitude.

3 Click the **Surface** tab. From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

4 Click **Apply** to generate the plot.

5 When you are done, click **OK** to close the **Plot Parameters** dialog box.

Star-Shaped Microchannel Chip

Lab-on-a-chip devices have become quite popular for analyses in fields such as biochemistry and bioengineering as well as MEMS in general. Through various techniques they incorporate all the equipment involved in a chemical process such as chemical reactors, heat exchangers, separators, and mixers.

This example involves the design of an infuser, a device that feeds a reactor or analysis equipment with a specific amount of fluid. Controlling pressure is an accurate way to introduce a set quantity of fluid at a certain velocity to some piece of equipment.

Flushing the equipment can also be important. Optimizing such an infuser to maximize its use would involve spending the least amount of time (and fluid) flushing the equipment. Modeling this process in the time domain can lead to an optimization of the infusing pressure, microchannel design, and time control.

This model demonstrates two useful tools in COMSOL Multiphysics modeling:

- The ability to easily define a time-dependent boundary condition
- The ability to easily extrude meshes into 3D to save memory

Model Definition

This exercise arbitrarily sets the geometry and conditions of the microchannel lab-on-a-chip (Figure 4-43). The differential pressure at the five inlets relative to the outlet pressure is time-controlled so that the inlet flow passes from one to the next in a smooth way. At any particular instant, one of the inlet flows dominates, although flow could be significant from more than one inlet. The pressure at the outlet is set to zero.

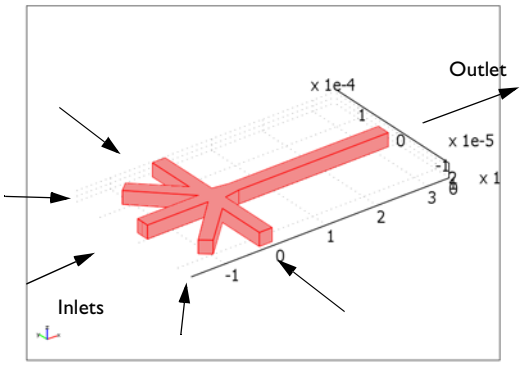


Figure 4-43: Model geometry for a star-shaped infuser with five inlets and one outlet. The model sets up a varying pressure differential at each inlet in the time domain in such a way that the dominant inlet flow alternates among them.

The example models only fluid flow whose velocity is of a magnitude that suggests laminar behavior. This implies that you can get a numerical solution of the full momentum balance and continuity equations for incompressible flow with a reasonable number of elements. The equations you must solve are the Navier-Stokes equations in the time domain

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

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

where ρ denotes density (kg/m^3), $\mathbf{u}$ is the velocity (m/s), η denotes dynamic viscosity (Pa·s), and p equals pressure (Pa). The fluid in this case is water, with the corresponding density and viscosity values.

The boundary conditions for the inlets and the outlet assume a set pressure; they also assume vanishing viscous stress:

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

$$p = p_i$$

Set the pressure at the outlet to zero; at the inlets, use the time-dependent expressions

$$p_i = 50 + 10\sin(\pi t + \alpha) \quad \text{Pa}$$

where t is time (s), and k is a value between zero and one. This simplified example sets the phase α to 0, $\pi/4$, $\pi/2$, $3\pi/4$, or π, depending on the inlet boundary.

Apply the no-slip condition to all other boundaries; it states that the velocity is zero in the x, y, and z directions at the wall:

$$\mathbf{u} = (0, 0, 0)$$

Results

Figure 4-44 shows the velocity field as a combined slice and arrow plot through the middle of the geometry at $t = 0.5$ s. The figure also displays the pressures at the walls. Setting up and observing this plot as an animation gives an informative qualitative description of the process as the largest pressure differential rolls from one inlet to the next.

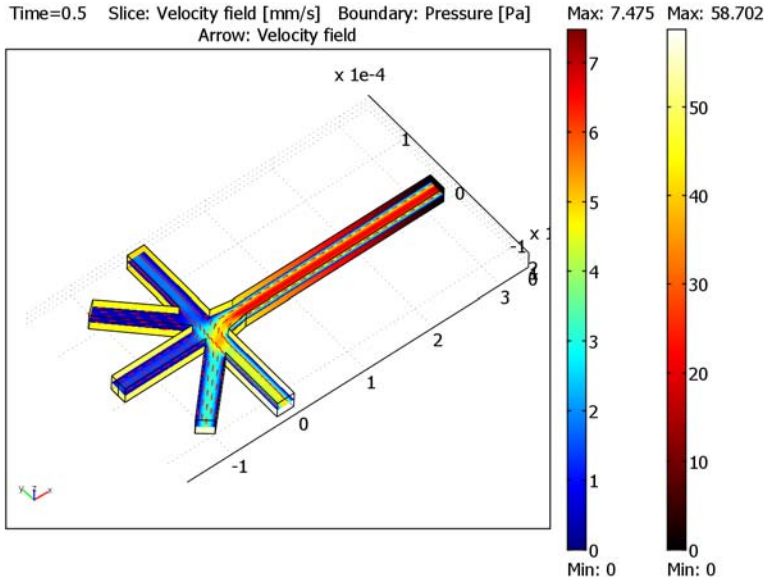


Figure 4-44: The velocity field in a microchannel infuser through the middle of the geometry. The plot also shows pressure at the walls.

Figure 4-45 and Figure 4-46 display the pressure and velocity field's x component (the direction of the long channel), respectively. The model includes a point in the middle of the geometry, just prior to the outlet, to investigate these two parameters. The figures show almost perfect sine curves (more frequent time sampling in the initial

stages would improve the graphs) for both of them. These results are close to those obtained with a refined mesh.

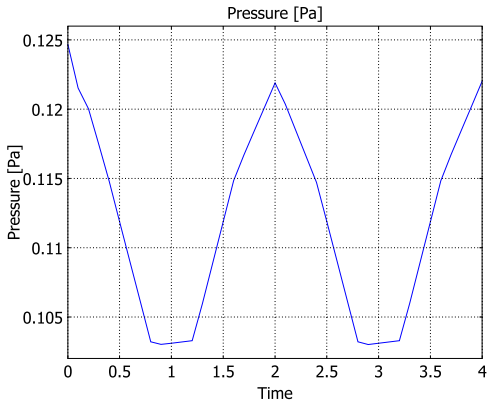


Figure 4-45: Pressure as a function of time at a point located just before the outlet.

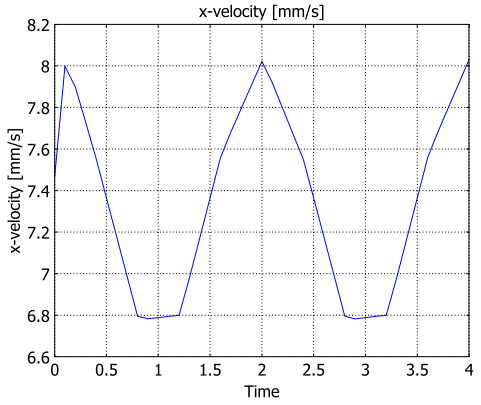


Figure 4-46: Velocity in the x direction as a function of time at a point located just before the outlet.

Modeling in COMSOL Multiphysics

This example illustrates how to use time-dependent boundary conditions to simulate a changing process. You can implement this scenario using a boundary condition that is a function of time. The user interface provides direct access to the built-in time variable (t) and the mathematical functions you need.

In 3D models, results at the walls are important but they can also hide what occurs within the geometry. This example also illustrates how to better display results with the help of suppressed (hidden) boundaries.

Finally, this model approaches meshing in a way that deviates from the default settings. In most cases COMSOL Multiphysics automatically generate a 3D mesh made completely of tetrahedrons. Here—as is the case in many other microchannels and minichannels—the top and the bottom boundaries are significant in modeling the flow profile because the distance between them is of the same magnitude as that between the two sides. This means that you must model the device in 3D. However, because the microchannel's height does not change along its length, the software does not require much meshing to resolve this dimension.

As an alternative to its default meshing, it is possible to extrude a mesh. To illustrate this concept, you create the mesh in this model by first taking a cross section of the full geometry to construct a 2D geometry. After meshing that, you then extrude both the geometry and the mesh in the height dimension. This approach allows for some mesh and memory conservation.

Model Library path: `MEMS_Module/Microfluidics_Models/star_chip`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics.

2 On the **New** page in the **Model Navigator**, select **3D** from the **Space dimension** list.

3 From the **Application Modes** list, select **MEMS Module>Microfluidics>Incompressible Navier-Stokes>Transient analysis**.

4 Click **OK**.

OPTIONS AND SETTINGS

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

2 Enter the following variable names, expressions, and (optionally) descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
eta	1e-3[Pa*s]	Dynamic viscosity
rho	1e3[kg/m^3]	Density
p0	50[Pa]	Pressure offset
p1	10[Pa]	Pressure amplitude
omega	pi[rad/s]	Angular velocity

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

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

NAME	EXPRESSION	DESCRIPTION
p_in_rm	p0+p1*sin(omega*t)	Pressure, rightmost inlet
p_in_ir	p0+p1*sin(omega*t+pi/4)	Pressure, inner right inlet
p_in_c	p0+p1*sin(omega*t+pi/2)	Pressure, central inlet
p_in_il	p0+p1*sin(omega*t+3*pi/4)	Pressure, inner left inlet
p_in_lm	p0+p1*sin(omega*t+pi)	Pressure, leftmost inlet

GEOMETRY MODELING

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

2 Click **OK** to use the default **Quick** work plane (the *xy*-plane at $z = 0$).

3 From the **Options** menu, select **Axes/Grid settings**.

4 On the **Axis** page, enter the following settings:

PROPERTY	VALUE
x min	-2e-4
x max	4e-4
y min	-1.5e-4
y max	2e-4

5 On the **Grid** page, clear the **Auto** check box. In the **x-y grid** area, specify the grid properties according to the following table; when done, click **OK**.

PROPERTY	VALUE
x spacing	`2.5e-5`
Extra x	`-11.5e-5 -9.7e-5 -3e-5 3e-5`
y spacing	`2.5e-5`
Extra y	`1.25e-5 3e-5 5.5e-5 11e-5`

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

7 Click on the points in the drawing area with the following (x, y) coordinate pairs in the given order:

ORDER	X-COORDINATE	Y-COORDINATE
1	`3.25e-4`	`0.125e-4`
2	`3.25e-4`	`0.25e-4`
3	`0.3e-4`	`0.25e-4`
4	0	`0.3e-4`
5	0	`1.5e-4`
6	`-0.25e-4`	`1.5e-4`
7	`-0.25e-4`	`0.55e-4`
8	`-0.97e-4`	`1.25e-4`
9	`-1.15e-4`	`1.1e-4`
10	`-0.3e-4`	`0.25e-4`
11	`-1.5e-4`	`0.25e-4`
12	`-1.5e-4`	`0.125e-4`
13	`-0.3e-4`	`0.125e-4`

8 Once you have clicked on the last point and have closed the geometry, right-click to create the 2D object.

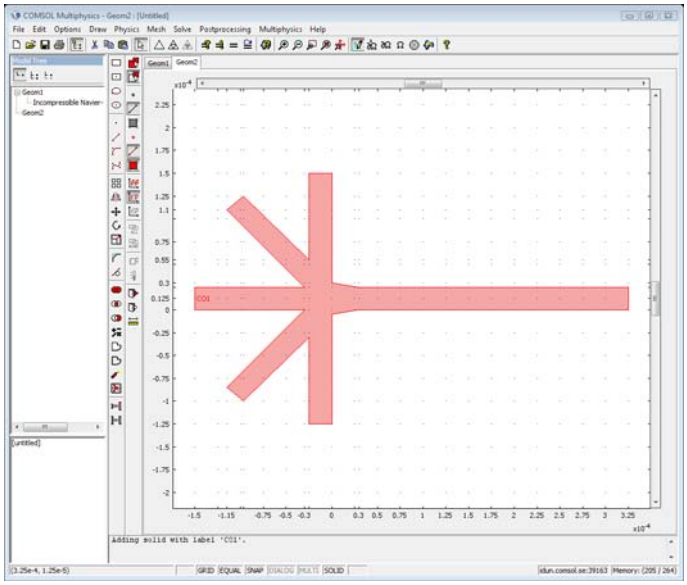
9 Click the **Mirror** button on the Draw toolbar.

10 In the **Point on line** edit fields, enter `0.825e-4` as the **x** value and `0.125e-4` as the **y** value. In the **Normal vector** edit fields, enter 0 as the **x** value and 1 as the **y** value. Click **OK**.

11 Select both objects by pressing Ctrl+A.

12 Click the **Union** button on the Draw toolbar.

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



The basic 2D geometry of the microchannel infuser.

MESH GENERATION

This step appears earlier in the modeling process than you might be accustomed to seeing it. This happens because you are extruding a 2D mesh into 3D to create a more structured mesh than the one the default procedure gives.

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

2 From the **Predefined mesh sizes** list, select **Finer**.

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

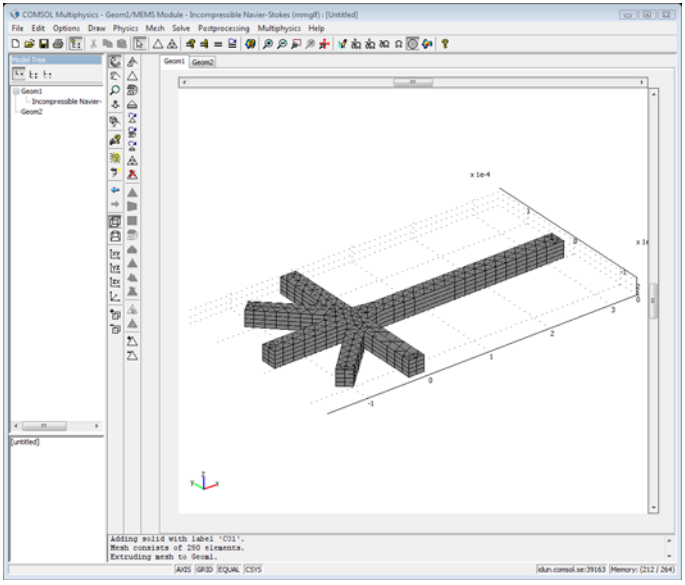
4 From the **Mesh** menu, choose **Extrude Mesh**.

5 On the **Geometry** page, type `2.5e-5` in the **Distance** edit field.

6 On the **Mesh** page, type `4` in the **Number of element layers** edit field.

7 Click **OK**.

This sequence automatically creates the 3D geometry and gives a view of the resulting mesh.



Extruding a 2D mesh into 3D.

PHYSICS SETTINGS

Boundary Conditions

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

2 Specify boundary conditions as in the following table (all external boundaries not listed use the default no-slip condition). When done, click **OK**.

SETTINGS	BOUNDARIES 1, 5	BOUNDARY 7	BOUNDARY 9	BOUNDARY 14	BOUNDARY 16	BOUNDARIES 23,24
Boundary type	Inlet	Inlet	Inlet	Inlet	Inlet	Outlet
Boundary condition	Pressure, no viscous stress	Pressure, no viscous stress	Pressure, no viscous stress	Pressure, no viscous stress	Pressure, no viscous stress	Pressure, no viscous stress
p	p_in_c	p_in_ir	p_in_il	p_in_rm	p_in_lm	0

Subdomain Settings

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

2 For Subdomain 1, specify the settings in the following table; when done, click **OK**.

PROPERTY	VALUE
ρ	rho
η	eta

COMPUTING THE SOLUTION

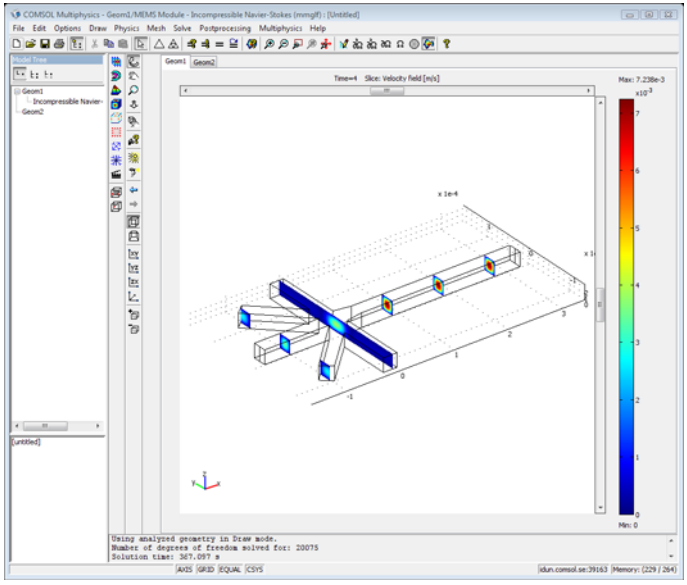
1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Analysis** list, select **Transient**.

3 In the **Times** edit field, type `0:0.1:4`. Click **OK**.

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

The default result plot in the user interface displays the velocity field.



A slice plot of the velocity field.

POSTPROCESSING AND VISUALIZATION

Reproduce the combined pressure and velocity plot in Figure 4-44 as follows:

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

2 On the **General** page, select the **Slice**, **Boundary**, **Arrow**, and **Geometry edges** check boxes.

3 From the **Solution at time** list, select **0.5**.

4 Clear **Auto** check box for the **Element refinement**. Type 8 in the associated edit field.

5 Click the **Slice** tab. From the **Predefined quantities** list in the **Slice data** area, select **Velocity field**. From the **Unit** list, select **mm/s**.

6 In the **Slice positioning** area, set **x levels** to 0, **y levels** to 0, and **z levels** to 1.

7 Click the **Boundary** tab. From the **Predefined quantities** list, select **Pressure**.

8 In the **Boundary color** area, select **hot** from the **Colormap** list.

9 Click the **Arrow** tab. Keep the default selection on the **Subdomain Data** page.

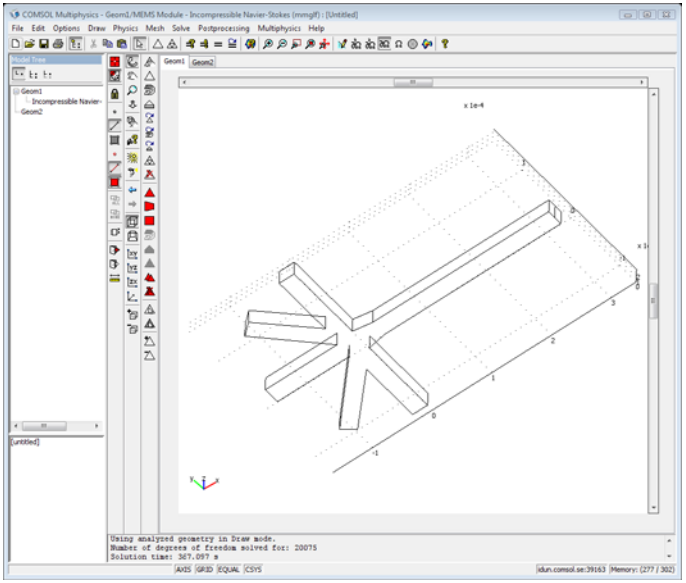
10 In the **Arrow positioning** area, set **x points** to 35, **y points** to 35, and **z points** to 1. In the **Arrow parameters** area, select **3D arrow** from the **Arrow type** list and **Normalized** from the **Arrow length** list. Clear the **Auto** check box and set the **Scale factor** to 0.3.

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

To see both the pressure and the velocity field you must suppress some boundaries:

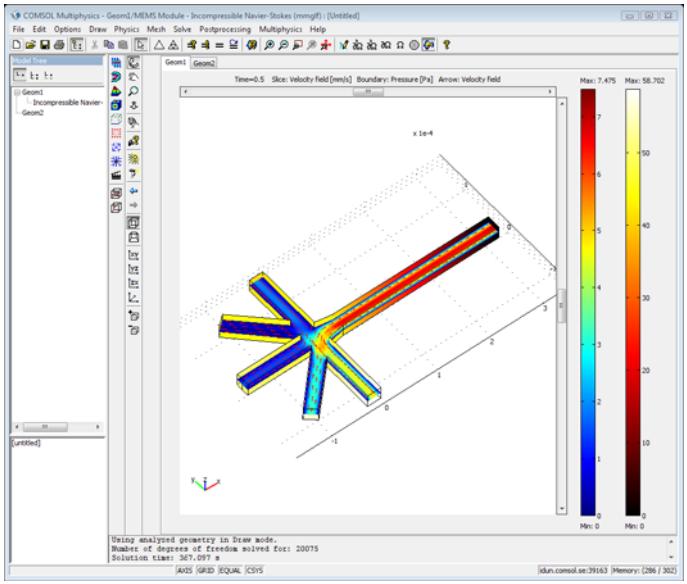
12 From the **Options** menu, select **Suppress>Suppress Boundaries**.

13 In the **Suppress Boundaries** dialog box, select Boundaries 1, 2, 4, 5, 7, 10, 11, 13, 14, 15, 18, and 21. Click **OK**.



Microchannel infuser geometry after suppressing selected boundaries.

I4 Click the **Postprocessing Mode** button on the Main toolbar to display the solution again. To adjust the camera angle, click and drag in the drawing area.



Velocity and pressure fields in the microchannel infuser.

To create the two figures showing the pressure and the velocity in the *x* direction at a point just near the outlet (Figure 4-45 and Figure 4-46), perform the following steps:

I5 From the **Postprocessing** menu, choose **Cross-Section Plot Parameters**.

I6 On the **Point** page, find the **Coordinates** area. In the **x** edit field type `3.24e-4`, in the **y** edit field type `0.125e-4`, and in the **z** edit field type `0.125e-4`.

I7 From the **Predefined quantities** list, select **Pressure**. Click **Apply** to plot the pressure.

I8 From the **Predefined quantities** list, select **x-velocity**. From the **Unit** list, select **mm/s**, then click **OK** to plot the velocity's *x* component.

Microchannel Cell

Introduction

This example was originally formulated by Albert Witarsa under Professor Bruce Finlayson's supervision at the University of Washington in Seattle. It was part of a graduate course in which the assignment consisted of using mathematical modeling to evaluate the potential of patents in the field of microfluidics.

This model treats a so-called H-microcell for separation through diffusion. The cell puts two different laminar streams in contact for a controlled period of time. The contact surface is well defined, and by controlling the flow rate it is possible to control the amount of species transported from one stream to the other through diffusion.

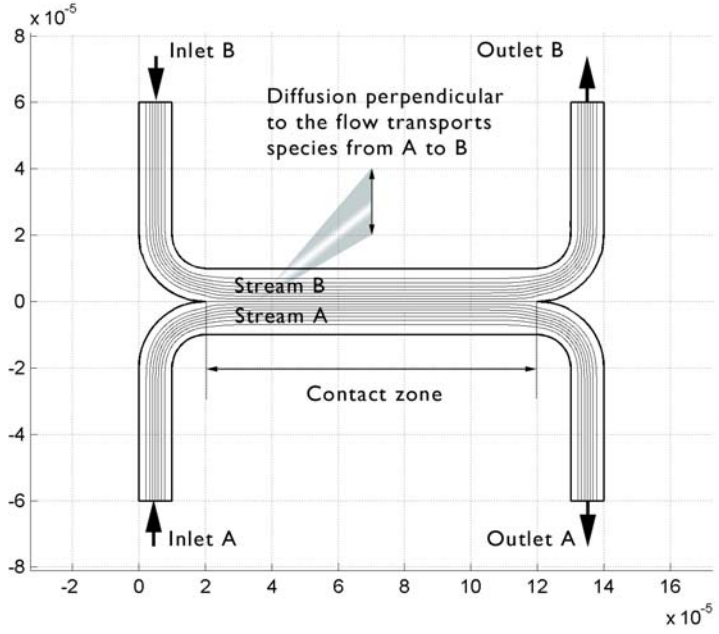


Figure 4-47: Diagram of the H-microcell.

Model Definition

The geometry of the microcell (Figure 4-43) is taken from Albert Witarsa's and Professor Finlayson's assignment. The cell geometry is divided in half because of symmetry. The design aims to avoid upsets in the flow field when the two streams, A and B, are united. This is to avoid the two streams mixing through convection, which would mix all species equally and lead to loss of control over the separation abilities. The transport of species between streams A and B should take place only by diffusion in order that species with low diffusion coefficients stay in their respective streams.

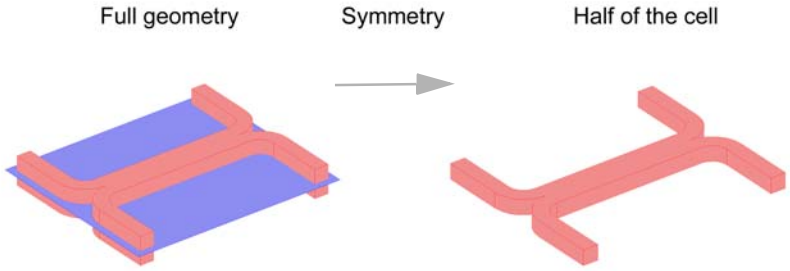


Figure 4-48: Model geometry. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

The simulations involve solving the fluid flow in the H-cell. According to the specifications, the flow rate at the inlet is roughly 0.1 mm/s. This implies a low Reynolds number, well inside the region of laminar flow:

$$\mathrm{Re} = \frac{d\rho u}{\eta} = \frac{1\cdot10^{-5}\cdot 1\cdot10^{3}\cdot 1\cdot10^{-4}}{1\cdot10^{-3}} \tag{4-13}$$

Equation 4-13 gives a Reynolds number of 0.001 for a water solution and the channel dimensions given in Figure 4-43, a value typical for microchannels. Thus it is easy to get a numerical solution of the full momentum balance and continuity equations for incompressible flow with a reasonable number of elements. The equations that you need to solve are the Navier-Stokes equations at steady state:

$$\begin{gathered} -\nabla\cdot\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p=0 \\ \nabla\cdot\mathbf{u}=0 \end{gathered} \tag{4-14}$$

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

Separation in the H-cell involves species in relatively low concentrations compared to the solvent, in this case water. This means that the solute molecules interact only with water molecules, and it is safe to use Fick's law to describe the diffusive transport in the cell. This mass-balance equation for a solute appears in the Convection and Diffusion application mode and reads

$$-\nabla \cdot (-D\nabla c + c\mathbf{u}) = 0 . \tag{4-15}$$

In this equation, D denotes the diffusion coefficient (m^2/s) and c represents the concentration (mol/m^3). In this model, you use the parametric solver to solve Equation 4-15 for three different values of D—$1 \cdot 10^{-11}$ m^2/s, $5 \cdot 10^{-11}$ m^2/s, and $1 \cdot 10^{-10}$ m^2/s—to simulate the mixing of different species.

You solve two versions of the model:

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

  $$\eta = \eta_0(1 + \alpha c^2) . \tag{4-16}$$

  Here α is a constant of dimension $(\text{concentration})^{-2}$. An influence of concentration on viscosity of this kind is usually observed in solutions of larger molecules.

Next, consider the boundary conditions, starting with the Navier-Stokes equations. For the relevant boundary groupings, refer to Figure 4-49.

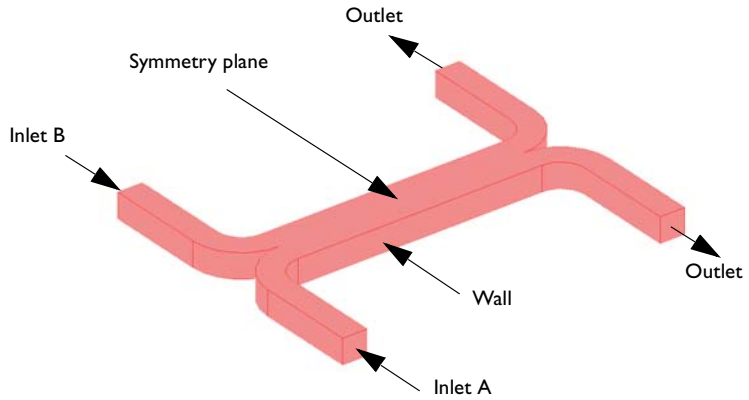


Figure 4-49: Model domain boundaries.

At the inlets and outlets, *Pressure* conditions apply along with vanishing viscous stress:

$$\begin{aligned} p &= p_0 \\ \mathbf{n} \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) &= 0 \end{aligned} \tag{4-17}$$

Setting the pressure at the outlets to zero, the pressure at the inlets represents the pressure drop over the cell. These inlet and outlet conditions comply with the H-cell being a part of a channel system of constant width, which justifies the assumption of developed flow.

At the symmetry plane, choosing the boundary type *Symmetry boundary* sets the velocity component in the normal direction of the surface to zero:

$$\begin{aligned} \mathbf{n} \cdot \mathbf{u} &= 0 \\ \mathbf{t} \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} &= 0 \end{aligned} \tag{4-18}$$

At the walls, *No slip* conditions state that the velocity is zero:

$$(u, v, w) = (0, 0, 0) \qquad \text{at the walls} \tag{4-19}$$

For the mass balances, the assumption that solute molecules interact only with water molecules implies that it is sufficient to consider a single species A of concentration c. At the inlets, use the *Concentration* boundary condition with the following values:

$$\begin{aligned} c &= c_0 \quad \text{at inlet A} \\ c &= 0 \quad \text{at inlet B} \end{aligned} \tag{4-20}$$

Model the symmetry plane and cell walls with the *Insulation/Symmetry* condition:

$$(-D\nabla c + c\mathbf{u}) \cdot \mathbf{n} = 0 \qquad \text{at the symmetry plane and walls} \tag{4-21}$$

This equation states that the flux of species perpendicular to the boundary equals zero. At the outlets, the *Convective flux* condition applies, stating that the diffusive transport perpendicular to the boundary normal is negligible:

$$(-D\nabla c) \cdot \mathbf{n} = 0 \qquad \text{at the outlets} \tag{4-22}$$

This condition eliminates concentration gradients in the flow direction.

Results

Figure 4-44 shows the velocity field. The flow is symmetric and is not influenced by the concentration field.

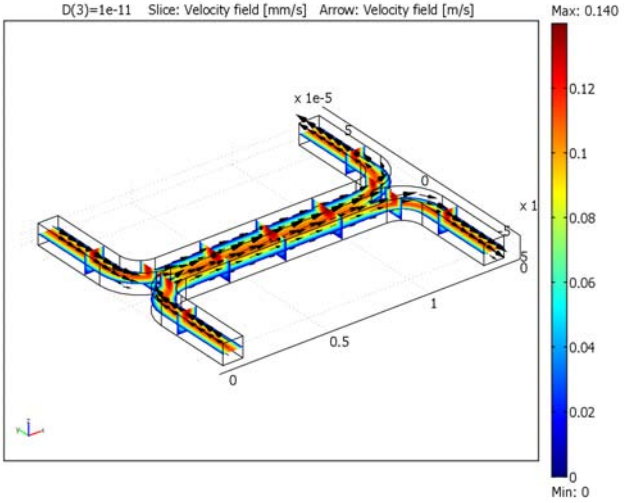


Figure 4-50: Flow velocity field.

Figure 4-45 shows the concentration distribution for the lightest species in this study.

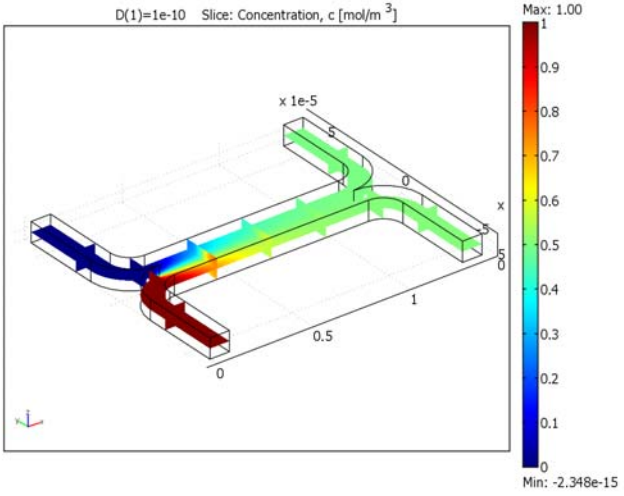


Figure 4-51: Concentration distribution for a species with diffusivity $1{\cdot}10^{-10} m^2/s$.

Because of the relatively large diffusion coefficient, the degree of mixing is almost perfect for the lightest species. The species with a diffusion coefficient ten times smaller than that of the lightest species shows a different result.

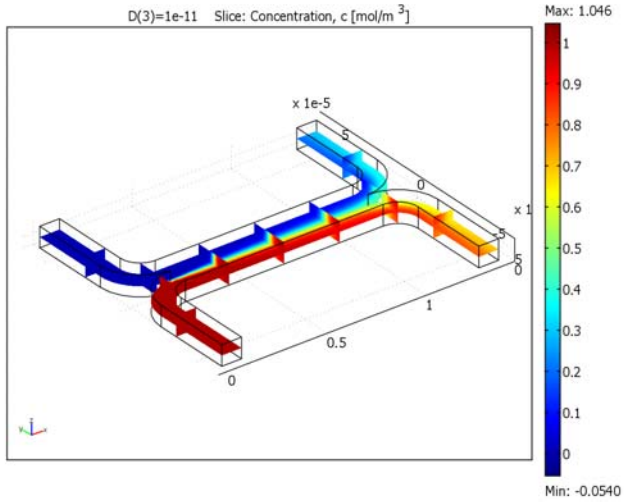


Figure 4-52: Concentration distribution for a species with diffusivity $1{\cdot}10^{-11} m^2/s$.

The concentration distribution in Figure 4-52 indicates that the diffusion coefficient for the species is low enough to avoid any significant mixing between streams A and B. The simulation clearly shows that the H-cell can separate lighter molecules from heavier ones. A cascade of H-cells can achieve a very high degree of separation.

In some cases, especially those involving solutions of macromolecules, the macromolecule concentration has a large influence on the liquid's viscosity. In such situations, the Navier-Stokes and the convection-diffusion become coupled, and they therefore must be solved simultaneously. Figure 4-53 shows the results of such a simulation, which you repeat in the second version of this model. You can see that changes in the concentration influence the flow field. It is clear from this plot that the velocity becomes asymmetric due to changes in viscosity. As a consequence of the modified flow field, the transport of molecules to the outlet B is also different from the result using a constant flow field. You can see the difference by comparing Figure 4-54 with Figure 4-52 on page 381.

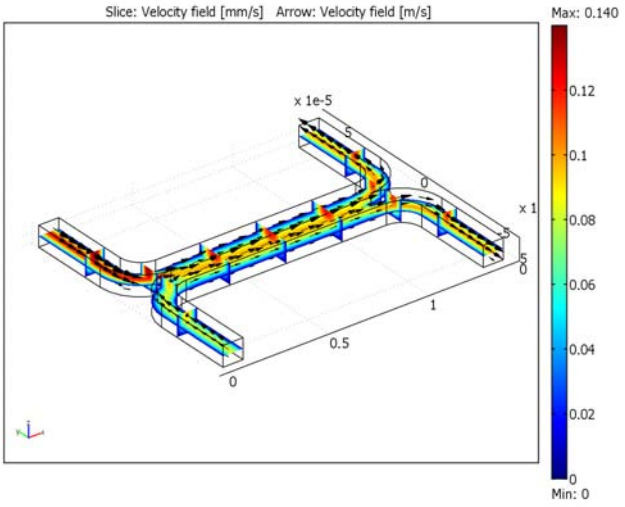


Figure 4-53: Velocity field. The viscosity varies with the concentration according to $\eta = \eta_0(1+\alpha c^2)$ *with* $\alpha = 0.5$ $(m^3/mol)^2$. *The figure shows that the velocity field is affected by variations in concentration. Compare it to the velocity field in Figure 4-44.*

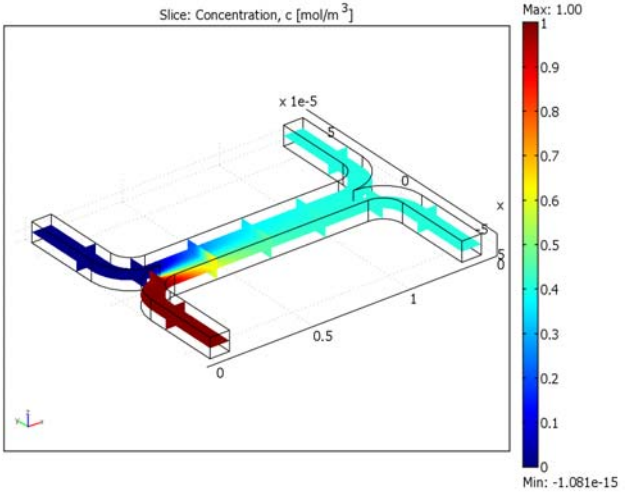


Figure 4-54: Concentration distribution for the species with diffusivity $1{\cdot}10^{-11}$ m^2/s *for the case where the fluid viscosity varies with concentration. Comparison with the plot in Figure 4-52 shows that fewer molecules of the species are transported to outlet B.*

Model Library path: `MEMS_Module/Microfluidics_Models/microchannel_h_cell`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

2 On the **New** page, set the **Space dimension** to **3D**.

3 From the list of application modes, select **MEMS Module>Microfluidics>Flow with Species Transport>Incompressible Navier-Stokes**.

4 Click the **Multiphysics** button, then click **Add**. As you can verify by inspection of the **Multiphysics** area on the right, this adds an Incompressible Navier-Stokes and a Convection and Diffusion application mode to the model. Later you will also see that a predefined coupling of the Navier-Stokes flow velocity has been included for the Convection and Diffusion application mode.

5 Click **OK**.

OPTIONS AND SETTINGS

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

2 Enter the following variable names, expressions, and (optionally) descriptions in the **Constants** dialog box; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1e3[kg/m^3]	Density
eta	1e-3[Pa*s]	Viscosity
D	1e-10[m^2/s]	Diffusion constant
p0	2[Pa]	Pressure drop
c0	1[mol/m^3]	Inlet concentration
alpha	0.5[(m^3/mol)^2]	Viscosity c^2-term prefactor

GEOMETRY MODELING

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

2 Use the default **Quick** work plane (the xy-plane at $z = 0$) by clicking **OK**.

3 From the **Options** menu, open the **Axes/Grid settings**.

4 On the **Axis** page, enter the following settings:

PROPERTY	VALUE
x min	-1
x max	15
y min	-7
y max	7

5 On the **Grid** page, clear the **Auto** check box and set both the **x spacing** and the **y spacing** to 1. Click **OK**.

6 Click the **Line** button on the Draw toolbar, then click the points with the x- and y-coordinates at (0, 6) and (0, 2).

7 Select the **2nd Degree Bezier Curve** tool on the Draw toolbar and click at the coordinate pairs (0, 0) and (2, 0).

8 Select the **Line** tool and click at the coordinates (12, 0).

9 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (14, 0) and (14, 2).

10 Select the **Line** tool and click at the coordinates (14, 6). Continue by clicking at the coordinates (13, 6) and (13, 2).

11 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (13, 1) and (12, 1).

12 Select the **Line** tool and click at the coordinates (2, 1).

13 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (1, 1) and (1, 2).

14 Select the **Line** tool and click at the coordinates (1, 6).

15 Click the right mouse button to close the set of lines and create a solid object, CO1.

You have now created half of the 2D cross section and can use copy, paste, and rotate operations to create the other half.

1 Click first the **Copy** button and then the **Paste** button, both on the Main toolbar. Let the **Displacements** remain at 0 and click **OK** to create the composite object CO2.

2 Click the **Scale** button on the Draw toolbar. Change the **y** component of the **Scale factor** to -1 (leave the other parameters at their default values).

3 Click **OK** to flip CO2 over the x-axis.

4 From the **Edit** menu, choose **Select All**. (Alternatively, press Ctrl+A.)

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

6 Clear the **Keep interior boundaries** check box. Click **OK**.

The cross section is now finished and you can extrude it to the full 3D geometry.

7 Select **Extrude** from the **Draw** menu. Let the **Distance** remain equal to `1`. Click **OK**.

The final geometry-modeling step is to scale the geometry to the correct scale.

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

9 Type `1e-5` in all three **Scale factor** edit fields. Click **OK**.

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

You do not need the 2D workplane any more, so you can remove it from the model:

1 From the **Multiphysics** menu, choose **Model Navigator**.

2 In the **Multiphysics** area to the right, select **Geom2 (2D)** and then click **Remove**.

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

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

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

3 Select Subdomain 1, then specify the settings in this table; when done, click **OK**.

PROPERTY	VALUE
ρ	`rho`
η	`eta`

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

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

6 Select Subdomain 1.

7 In the **D (isotropic)** edit field, type `D`. Note that the velocity variables from the Incompressible Navier-Stokes application mode appear as predefined couplings.

8 Click **OK** to confirm the settings and close the dialog box.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

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

3 Specify boundary conditions as in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 2, 8	BOUNDARIES 20, 22	BOUNDARY 4	ALL OTHERS
Boundary type	Inlet	Outlet	Symmetry boundary	Wall
Boundary condition	Pressure, no viscous stress	Pressure, no viscous stress		No slip
p_0	p0	0	-	-

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

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

6 Specify the boundary conditions in the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARY 8	BOUNDARIES 20, 22	ALL OTHERS
Type	Concentration	Concentration	Convective flux	Insulation/ Symmetry
c_0	c0	0	-	-

MESH GENERATION

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

2 From the **Predefined mesh sizes** list, select **Extra fine**.

3 Click the **Remesh** button.

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

COMPUTING THE SOLUTION

Start by first computing the solution for the velocity field and then use that solution for solving the mass transport problem.

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

2 On the **General** page, select **Direct (PARDISO)** from the **Linear system solver** list.

3 Click **OK**.

4 Click the **Solver Manager** button on the Main toolbar.

5 On the **Solve For** page, select **Incompressible Navier-Stokes (mmglf)**.

6 On the **Initial Value** page, click the **Initial value expression** option button in the **Initial value** area.

7 Click **OK**.

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

You have now computed the velocity field and can use that solution to make a parametric analysis for the mass transport problem with varying diffusivity.

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

2 On the **Solve For** page, select **Convection and Diffusion (chcd)**.

3 Click the **Initial Value** tab, then click the **Current solution** option button in the **Initial value** area.

4 Click **OK**.

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

6 From the **Solver** list, select **Parametric**.

7 In the **Parameter name** edit field, type `D`.

8 In the **Parameter values** edit field, type `1e-10 5e-11 1e-11`.

9 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION

To generate Figure 4-44 follow these steps:

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

2 On the **General** page, select the **Slice** and **Arrow** check boxes in the **Plot type** area.

3 Clear the **Element refinement Auto** check box and type `5` in the associated edit field.

4 Click the **Slice** tab.

5 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

6 From the **Unit** list, select **mm/s**.

7 In the **Slice positioning** area, set **x levels** to `5`, **y levels** to `2`, and **z levels** to `1`.

8 Click the **Arrow** tab.

9 On the **Subdomain Data** page, verify that **Velocity field** is selected in the **Predefined quantities** list.

10 In the **Arrow positioning** area, set the numbers of **x points**, **y points**, and **z points** to `14`, `21`, and `3`, respectively.

11 In the **Arrow parameters** area, click the **Color** button. Select the black swatch from the palette in the **Arrow Color** dialog box, then click **OK**.

12 Select **3D arrow** from the **Arrow type** list.

13 Click **Apply** to generate the plot.

To generate Figure 4-45, continue with the following steps:

1 Clear the **Arrow plot** check box, then click the **Slice** tab.

2 From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

3 On the **General** page, select **1e-10** from the **Parameter value** list. Click **OK**.

Generate Figure 4-52 the same way as Figure 4-45, except use the parameter value **1e-11**.

PHYSICS SETTINGS—STUDY 2

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

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

3 Change the viscosity expression to `eta*(1+alpha*c^2)`. Click **OK**.

COMPUTING THE SOLUTION—STUDY 2

When the viscosity is concentration dependent you must solve all equations simultaneously.

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

2 On the **Solve For** page, select **Geom1 (3D)** from the **Solve for variables** list. Click **OK**.

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

4 From the **Solver** list, select **Stationary**. Click **OK**.

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

POSTPROCESSING AND VISUALIZATION—STUDY 2

Finally, generate Figure 4-53 and Figure 4-54 with the following steps:

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

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

3 Click the **Slice** tab.

4 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)> Velocity field**.

5 In the **Unit** list, select **mm/s**, then click **Apply** to generate Figure 4-53.

6 In the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

7 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

8 Click **OK** to close the dialog box and generate Figure 4-54.

Inkjet Model

Inkjet printers are attractive tools for printing text and images because they combine low cost and high resolution with acceptable speed. The working principle behind inkjet technology is to eject small droplets of liquid from a nozzle onto a sheet of paper. Important properties of a printer are its speed and the resolution of the final images. Designers can vary several parameters to modify a printer's performance. For instance, they can vary the inkjet geometry and the type of ink to create droplets of different sizes. The size and speed of the ejected droplets are also strongly dependent on the speed at which ink is injected into the nozzle. Simulations can be very useful to improve the understanding of the fluid flow and to predict the optimal design of an inkjet for a specific application.

Although initially invented to produce images on paper, the inkjet technique has since been adopted for other application areas. Instruments for the precise deposition of microdroplets often employ inkjets. These instruments are used within the life sciences for diagnosis, analysis, and drug discovery. Inkjets have also been used as 3D printers to synthesize tissue from cells and to manufacture microelectronics. For all of these applications it is important to be able to accurately control the inkjet's performance.

This example demonstrates how to use the Level Set Two-Phase Flow, Laminar application mode available in the MEMS Module to model the fluid flow within an inkjet. The application mode uses the Navier-Stokes equations to describe the momentum transport and conservation of mass. Surface tension is included in the momentum equations. A reinitialized, conservative level set method represents and moves the interface between the air and ink.

Model Definition

Figure 4-55 shows the geometry of the inkjet studied in this example. Because of its symmetry you can use an axisymmetric 2D model. Initially, the space between the inlet and the nozzle is filled with ink. Additional ink is injected through the inlet during a period of 10 μs, and it consequently forces ink to flow out of the nozzle. When the injection stops, a droplet of ink snaps off and continues to travel until it hits the target.

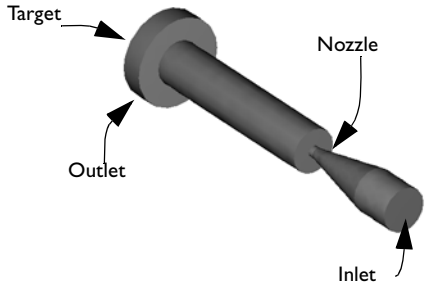


Figure 4-55: Geometry of the inkjet.

TRANSPORT OF MASS AND MOMENTUM

The Navier-Stokes equations describe the transport of mass and momentum for fluids of constant density. It is possible to model both ink and air as being incompressible as long as the fluid velocity is small compared to the speed of sound. In this model, you must add a term to account for surface tension. The Navier-Stokes equations with surface tension are

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - \nabla \cdot (\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)) + \nabla p = \mathbf{F}_{\mathrm{st}}$$

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

Here, ρ denotes density (kg/m^3), μ equals the dynamic viscosity (Ns/m^2), $\mathbf{u}$ represents the velocity (m/s), and p denotes pressure (Pa). $\mathbf{F}_{\mathrm{st}}$ is the surface tension force, which is

$$\mathbf{F}_{\mathrm{st}} = \nabla \cdot \mathbf{T}$$

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

where $\mathbf{I}$ is the identity matrix, $\mathbf{n}$ is the interface normal, σ equals the surface tension coefficient (N/m), and δ equals a Dirac delta function that is nonzero only at the fluid interface.

The following table gives the physical parameters of ink and air:

MEDIUM	DENSITY	DYNAMIC VISCOSITY	SURFACE TENSION
ink	10^3 kg/m^3	0.01 Ns/m^2	0.07 N/m
air	1.225 kg/m^3	$1.789 \cdot 10^{-5}$ Ns/m^2	

REPRESENTATION AND CONVECTION OF THE FLUID INTERFACE

In this model you use a reinitialized, conservative level set method to describe and convect the interface. The 0.5 contour of the level set function ϕ defines the interface, where ϕ equals 0 in air and 1 in ink. In a transition layer close to the interface, ϕ goes smoothly from 0 to 1. The normal to the interface is

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

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

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\phi\mathbf{u}) + \gamma\left[\left(\nabla \cdot \left(\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)\right) - \varepsilon\nabla \cdot \nabla\phi\right] = 0 \qquad (4\text{-}23)$$

The thickness of the transition layer is proportional to ε. For this model you can use $\varepsilon = 2h$, where h is the mesh size. You then obtain a sharper interface in the regions where the mesh is finer. In this example you use a structured mesh. For unstructured meshes, avoid letting ε depend on h.

The parameter γ determines the amount of reinitialization. If the velocity gradients are small at the fluid interface you can choose $\gamma = 1$. In this example the velocity gradients at the interface are significant, and you must therefore choose a larger value for γ to keep the thickness of the transition layer constant.

The application mode uses the level set function to smooth the density and viscosity jump across the interface by letting

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

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

To simplify the calculation of the surface tension force the delta function is approximated by

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

INITIAL CONDITIONS

Figure 4-56 shows ϕ at $t = 0$, that is, the initial distribution of ink and air. The velocity is initially 0.

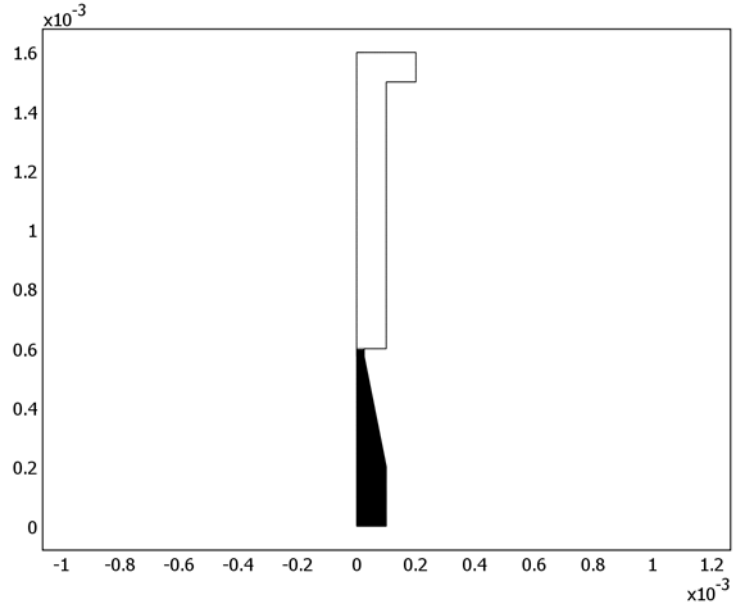


Figure 4-56: Initial distribution of ink. Black corresponds to ink and white corresponds to air.

BOUNDARY CONDITIONS

Inlet

The inlet velocity in the z direction increases from 0 to the parabolic profile

$$v(r) = 4.5\left(\frac{r + 1 \cdot 10^{-4}}{2 \cdot 10^{-4}}\right)\left(1 - \frac{r + 1 \cdot 10^{-4}}{2 \cdot 10^{-4}}\right)$$

during the first 2 µs. The velocity is then $v(r)$ for 10 µs and finally decreases to 0 for another 2 µs. You can obtain this effect by using the smooth step function $H(t - \delta_1, \delta_2)$, which is 0 for $t > \delta_1 - \delta_2$, increases from 0 to 1 as t goes from $\delta_1 - \delta_2$ to $\delta_1 + \delta_2$, and it is 1 for $t > \delta_1 + \delta_2$ as shown in Figure 4-57.

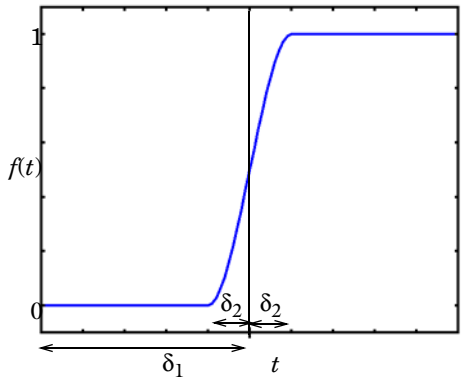


Figure 4-57: Smooth step function $f(t) = H(t - \delta_1, \delta_2)$.

The time-dependent velocity profile in the z direction can then be defined as

$$v(r,t) = (H(t - 1 \cdot 10^{-6}, 1 \cdot 10^{-6}) - H(t - 13 \cdot 10^{-6}, 1 \cdot 10^{-6})) \cdot v(r)$$

where t is given in seconds.

For the level set equation, use $\phi = 1$ as the boundary condition.

Outlet

Set a constant pressure at the outlet. The value of the pressure given here is not important because the velocity depends only on the pressure gradient. You thus obtain the same velocity field regardless of whether the pressure is set to 1 atm or to 0.

Walls

On all other boundaries except the target, set no-slip conditions. If you use a no-slip condition at the target, the interface cannot move along the boundary. Therefore, use instead the wetted wall condition. The wetted wall boundary conditions allows a small amount of slip, according to

$$u = -\lambda \frac{\partial u}{\partial z}$$

where λ is the slip length, in this example $1 \cdot 10^{-5}$ m. Where the fluid interface attaches to the wall, the angle between the fluid interface and the wall (the contact angle) is assumed to be $\pi/2$.

Figure 4-58 and Figure 4-59 show the ink surface and the velocity field at different times. The droplet hits the target after approximately 140 µs.

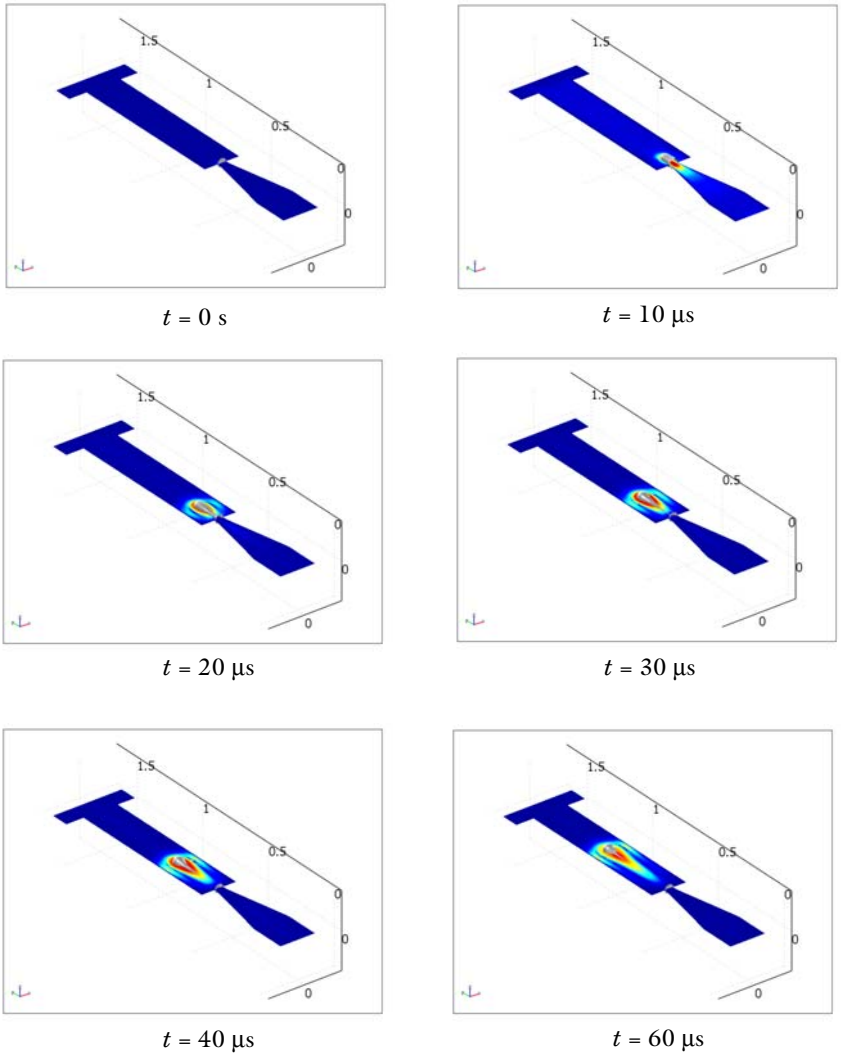


Figure 4-58: Position of air/ink interface and velocity field at various times.

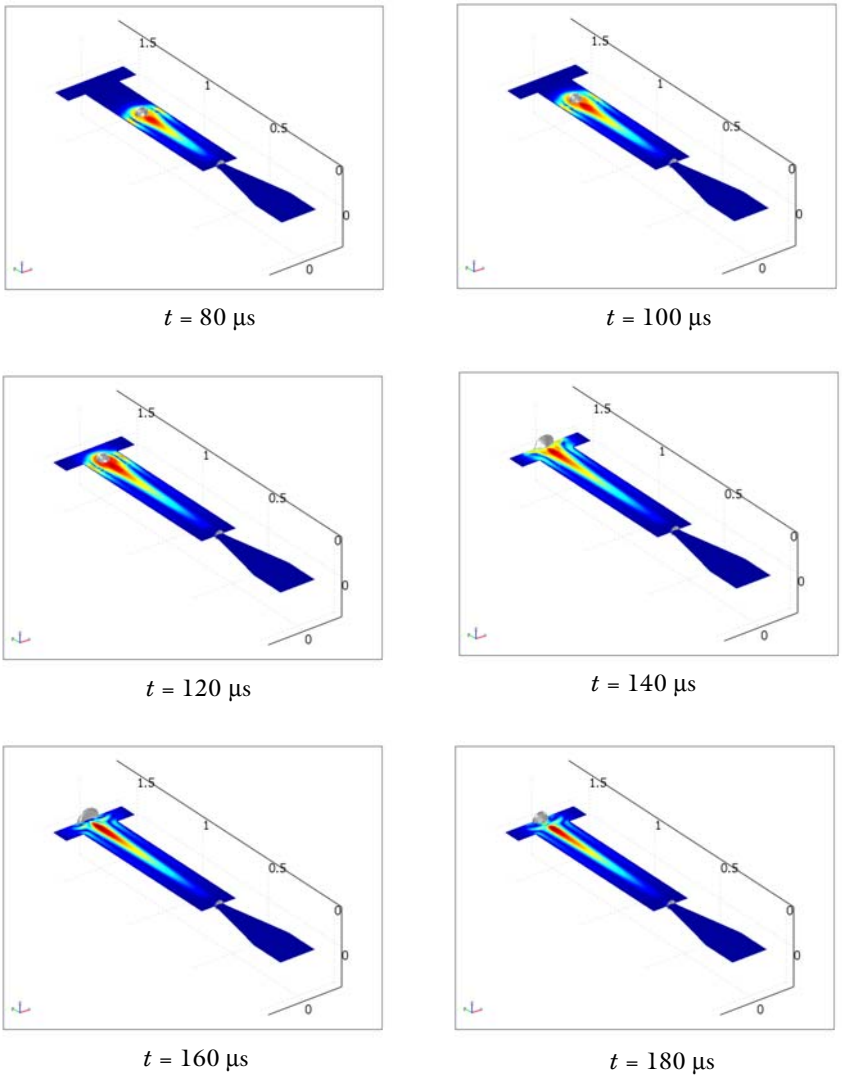


Figure 4-59: Position of air/ink interface and velocity field at various times.

Figure 4-60 illustrates the mass of ink that is further than $0.7 \cdot 10^{-3}$ m from the inlet. The figure shows that the mass of the ejected droplet is approximately $2.0 \cdot 10^{-10}$ kg.

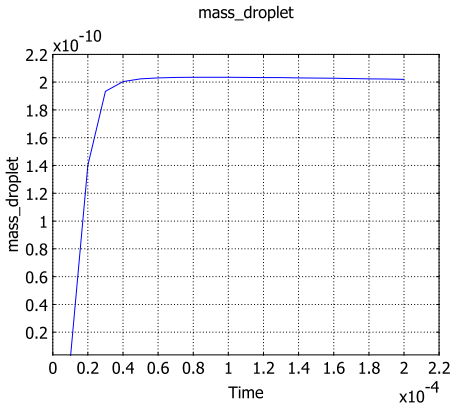


Figure 4-60: Amount of ink just above the nozzle.

This example studies only one inkjet model, but it is easy to modify the model in several ways. You can, for example, change properties such as the geometry or the inlet velocity and study the influence on the size and the speed of the ejected droplets. You can also investigate how the inkjet would perform if the ink were replaced by a different fluid. It is also easy to add forces such as gravitation to the model.

Modeling in COMSOL Multiphysics

You can easily set up the model using the application mode Level Set Two-Phase flow, Laminar. This application mode sets up the equations automatically, and you need only specify physical parameters of the fluids and initial and boundary conditions.

Use a structured mesh and refine it in the regions where the fluid interface passes.

The simulation involves two computations. First, you calculate the initial level set function. Then you store the solution, switch the Analysis Type to Transient, and start the time-dependent simulation of the fluid motion.

To calculate the droplet's mass, use an integration coupling variable. To visualize the droplet in 3D, revolve the 2D axisymmetric solution to a 3D geometry.

References

1. J.-T. Yeh, "A VOF-FEM Coupled Inkjet Simulation," *Proc. ASME FEDSM'01*, New Orleans, Louisiana, 2001.

2. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow," *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

Model Library path: `MEMS_Module/Microfluidics_Models/inkjet`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 From the list of application modes, select **MEMS Module>Microfluidics>Level Set and Laminar Flow**. Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu, select **Specify Objects>Line**.

2 Select **Closed polyline (solid)** from the **Style** list.

3 In the **r** edit field, enter `0 1e-4 1e-4 2.5e-5 2.5e-5 1e-4 1e-4 2e-4 2e-4 0`, and in the **z** edit field `0 0 2e-4 5.75e-4 6e-4 6e-4 1.5e-3 1.5e-3 1.6e-3 1.6e-3`.

4 Click **OK**.

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

6 Shift-click the **Rectangle/Square** button on the Draw toolbar. Type `1e-4` in the **Width** edit field, `2e-4` in the **Height** edit field, and `0` in both the **r** and the **z** edit field. Make sure **Corner** is selected in the **Base** list, then click **OK**.

7 Repeat the previous step three times to specify three more rectangles according to the following table:

WIDTH	HEIGHT	BASE	R	Z
2.5e-5	2.5e-5	Corner	0	5.75e-4
2.5e-5	9e-4	Corner	0	6e-4
7.5e-5	1e-4	Corner	2.5e-5	1.5e-3

OPTIONS AND SETTINGS

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

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

NAME	EXPRESSION	DESCRIPTION
rhoair	1.225[kg/m^3]	Density of air
rhoink	1e3[kg/m^3]	Density of ink
etaair	1.7894e-5[Pa*s]	Viscosity of air
etaink	1e-2[Pa*s]	Viscosity of ink
sigma	0.07[N/m]	Surface tension
lambdaslip	10[um]	Slip length

3 Click **OK**.

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

5 Define the following expressions:

NAME	EXPRESSION	DESCRIPTION
inletr	4.5[m/s]*((r[1/m]+1e-4)/2e-4)*(1-((r[1/m]+1e-4)/2e-4))	
inlett	flc2hs(t[1/s]-1e-6,1e-6)-flc2hs(t[1/s]-13e-6,1e-6)	
inletvel	inletr*inlett	Inlet velocity

6 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 In the **Model Tree**, right-click **Level Set and Laminar Flow (mmglf)** and select **Subdomain Settings**.

Note: There are a number of different ways to open the **Subdomain Settings** and the **Boundary Settings** dialog boxes. This description assumes that you have the **Model Tree** visible in **Overview** mode. To open the **Model Tree**, click the **Model Tree** button on the Main toolbar, then click the **Overview** button on the toolbar at the top of the **Model Tree**.

---

2 Select Subdomain 1 and press Ctrl+A to select all the subdomains. Enter physical parameters according to the following table.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ_1	rhoair	Density, fluid 1
η_1	etaair	Dynamic viscosity, fluid 1
ρ_2	rhoink	Density, fluid 2
η_2	etaink	Dynamic viscosity, fluid 2

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

4 Click the **Init** tab. Select Subdomains 1, 2, and 3 and click the **Fluid 2** button. These subdomains are initially filled with ink.

5 Click **OK**.

Boundary Conditions

1 In the **Model Tree** right-click **Level Set and Laminar Flow (mmglf)** and select **Boundary Settings**. Set boundary conditions according to the following table.

SETTINGS	BOUNDARIES 1, 3, 5, 7, 9	BOUNDARY 2	BOUNDARY 24	BOUNDARIES 11, 18, 23	BOUNDARIES 12, 13, 15, 19, 20, 22
Boundary type	Symmetry boundary	Inlet	Outlet	Wall	Wall
Boundary condition	Axial symmetry	Velocity	Pressure, no viscous stress	Wetted wall	No slip
U_0		inletvel			
P_0			0		
ϕ_0		1			
θ				pi/2	
β				lambdaslip	

2 Select Boundary 8, then select the **Interior boundaries** check box. From the **Boundary condition** list, select **Initial fluid interface**.

3 Click **OK**.

MESH GENERATION

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

2 Click the **Boundary** tab.

3 Select Boundaries 1, 2, 3, 5, 7, 9, 15, and 22, then select the **Constrained edge element distribution** check box. Next select each boundary separately and specify the **Number of edge elements** according to this table:

Boundary	1	2	3	5	7	9	15	22
Number of edge elements	10	10	8	10	180	20	20	10

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

COMPUTING THE SOLUTION

First reinitialize ϕ to obtain the correct shape of ϕ in the transition layer.

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

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

3 From the **Linear system solver** list, select **Direct (PARDISO)**. While the solution times are comparable, the PARDISO solver is more memory efficient than the default linear system solver, UMFPACK.

4 Click **OK**.

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

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

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

2 On the **Initial Value** page, click the **Store Solution** button. Select the time **2e-6**, then click **OK**.

3 In the **Initial value** area, select **Stored solution**.

4 From the **Solution at time** list, select **2e-6**. Click **OK**.

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

6 On the **General** page, type `0:1e-5:2e-4` in the **Times** edit field. Click **OK**.

7 From the **Physics** menu, select **Properties**. Change the **Analysis type** to **Transient**, then click **OK**.

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

Note: The calculations take at least 4 hours. If you do not obtain a solution because of memory limitations in your computer, perform Steps 1–4 in the following list. Skip these steps if you do obtain a solution.

1. Click the **Solver Parameters** button on the Main toolbar.
2. From the **Linear system solver** list, select **Direct (SPOOLES)**.

   This solver uses less memory but is slightly slower compared to the UMFPACK solver.
3. Click the **Advanced** tab, then select the **Store solution on file** check box. Click **OK**.
4. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To visualize the solution in 3D, perform these steps:

1. From the **Draw** menu, select **Revolve**.
2. In the **Objects to revolve** list, select all the elements (select any object and then press Ctrl+A). Click **OK**.
3. In the **Model Tree**, click **Geom1** to return to the 2D model.
4. Select **Options>Extrusion Coupling Variables>Subdomain Variables**.
5. Select any subdomain and then press Ctrl+A to select all the subdomains.
6. In the **Name** edit field, type `phi3d`, and in the **Expression** edit field type `phi`.
7. Click the **General transformation** option button.
8. Type `vel3d` in the **Name** edit field on the second row and `sqrt(u^2+v^2)` in the corresponding **Expression** edit field.
9. Select **General transformation** for this variable as well.
10. Click the **Destination** tab. In the **Geometry** list, select **Geom2**. In the **Level** list, select **Subdomain**.
11. Select any subdomain then press Ctrl+A to select all the subdomains.
12. Select the **Use selected subdomains as destination** check box.
13. In the **x** edit field, type `sqrt(x^2+z^2)`.
14. From the **Variable** list, select **phi3d**.
15. Select the **Use selected subdomains as destination** check box and type `sqrt(x^2+z^2)` in the **x** edit field. Click **OK**.

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

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

18 On the **General** page, clear the **Geometry edges** check box and select the **Isosurface** check box.

19 Clear the **Auto** check box for **Element refinement**, then type `4` in the associated edit field.

20 Click the **Slice** tab. In the **Expression** edit field, type `vel3d`; in the **x levels** edit field, type `0`; and in the **z levels** edit field, type `1`.

21 Click the **Isosurface** tab. In the **Expression** edit field, type `phi3d`. Select **Vector with isolevels**, then type `0.5` in the corresponding edit field.

22 Click the **Uniform color** option button, then click the **Color** button. Choose a gray color to plot the ink/air interface. Click **OK**.

23 Click the **General** tab. In the **Solution at time** list, select **0**. Click **OK** to plot the initial position of the interface.

24 Click the **Scene Light** button on the Camera toolbar.

25 To plot the solution at other times, click the **Plot Parameters** button and select other values from the **Solution at time** list. Click **Apply** to plot the solution at the corresponding time.

26 Click **OK**.

Go through the following steps to calculate the mass of the ejected droplet.

1 Click the **Geom1** tab.

2 Choose **Options>Integration Coupling Variables>Subdomain Variables**.

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

4 In the first **Name** edit field, type `mass_droplet`. In the corresponding **Expression** field, type `rhoink*phi*(z>7e-4)*2*pi*r`. Click **OK**.

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

6 From the **Postprocessing** menu, select **Global Variables Plot**.

7 In the **Expression** edit field, type `mass_droplet`, then click the **Add Entered Expression** button (the one marked **>**).

8 Click **OK** to generate the plot.

Filling of a Capillary Channel

Introduction

Surface tension and wall adhesive forces are often used to transport fluid through microchannels in MEMS devices or to measure, transport and position small amounts of fluid using micropipettes. Multiphase flow through a porous medium and droplets on solid walls are other examples where wall adhesion and surface tension strongly influence the dynamics of the flow.

To model the adhesive forces at the walls correctly, the treatment of the boundary conditions is important. If you fix the velocity to zero on the walls, the interface cannot move along the walls. Instead, you need to allow a non-zero slip velocity and to add a frictional force at the wall. With such a boundary condition, it is possible to explicitly set the contact angle, that is, the angle between the fluid interface and the wall. The correct value of the contact angle depends on properties of the fluids and the wall. You can determine the contact angle experimentally or calculate it from the surface energies related to the different phase interfaces using Young's law.

This example studies a narrow vertical cylinder placed on top of a reservoir filled with water. Because of wall adhesion and surface tension at the air/water interface, water rises through the channel. The model calculates the pressure field, the velocity field, and the water surface's shape and position. It uses a level set method to track the air/water interface and shows how to add friction and specify the contact angle at the channel walls.

Model Definition

The model consists of a capillary channel of radius 0.15 mm attached to a water reservoir. Water can flow freely into the reservoir. Because both the channel and the reservoir are cylindrical, you can use the axisymmetric model illustrated in Figure 4-61. Initially, the thin cylinder is filled with air. The wall adhesion causes water to creep up along the cylinder boundaries. The deformation of the water surface induces surface tension at the air/water interface, which in turn creates a pressure jump across the interface. The pressure variations cause water and air to move upward. The fluids continue to rise until the capillary forces are balanced by the gravity force that builds up as the water rises in the channel. In the present example, the capillary forces

dominate over gravity throughout the simulation. Consequently, the interface moves upwards during the entire simulation.

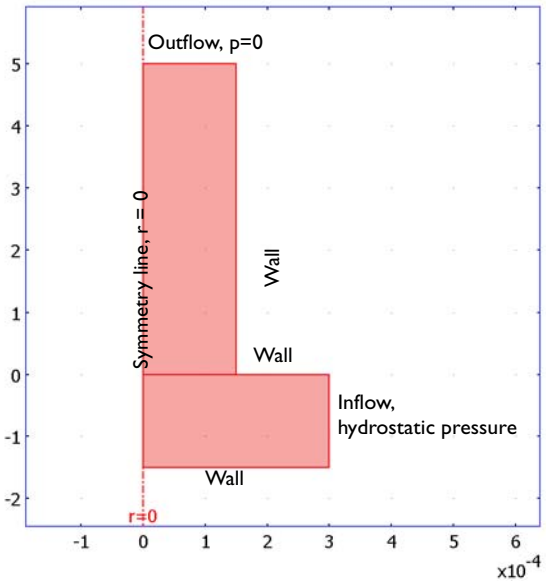


Figure 4-61: Axisymmetric geometry description.

MASS AND MOMENTUM TRANSPORT

The Navier-Stokes equations describe the transport of mass and momentum for fluids of constant density. In order to account for capillary effects, it is crucial to include surface tension in the model. The Navier-Stokes equations are then

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - \nabla \cdot (\eta(\nabla \mathbf{u} + \nabla \mathbf{u}^T)) + \nabla p = \mathbf{F}_{\text{st}} + \rho \mathbf{g}$$

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

Here, ρ denotes the density (kg/m^3), η equals the dynamic viscosity (Ns/m^2), $\mathbf{u}$ represents the velocity (m/s), p denotes the pressure (Pa), and $\mathbf{g}$ is the gravity vector (m/s^2). $\mathbf{F}_{\text{st}}$ is the surface tension force that acts at the air/water interface and is

$$\mathbf{F}_{\text{st}} = \nabla \cdot \mathbf{T}$$

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

Here, $\mathbf{I}$ is the identity matrix, $\mathbf{n}$ is the interface normal, σ equals the surface tension coefficient (N/m), and δ equals a Dirac delta function that is nonzero only at the fluid interface. When you use the finite element method to solve the Navier-Stokes equations, you multiply the equations by test functions and then integrate over the computational domain. If you use integration by parts, you can move derivatives of $\mathbf{T}$ to the test functions. This is used in the Level Set and Laminar Flow application mode and results in an integral over the computational domain plus a boundary integral of the form

$$\int_{\partial\Omega} \text{test}(\mathbf{u}) \cdot [\sigma(\mathbf{n}_{\text{wall}} - (\mathbf{n}\cos\theta))\delta] dS\,, \tag{4-24}$$

where θ is the contact angle (see Figure 4-62). If you apply a no-slip boundary condition, the boundary term vanishes because $\text{test}(\mathbf{u}) = 0$ on that boundary, and you cannot specify the contact angle. Instead, the interface remains fixed on the wall. However, if you allow a small amount of slip, it is possible to specify the contact angle. The Wetted wall boundary condition adds the term given by Equation 4-24 and consequently allows you to set the contact angle.

REPRESENTATION AND CONVECTION OF THE FLUID INTERFACE

The Level Set Two-Phase Flow, Laminar application mode automatically sets up the equations for the convection of the interface, calculates normal and curvature of the interface, and adds surface tension and gravitation to the Navier-Stokes equations.

The application mode represents the interface as the 0.5 contour of the level set function ϕ. In air, $\phi = 0$ and in water $\phi = 1$. You can thus think of the level set function as the volume fraction of water. The transport of the interface is given by

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\phi\mathbf{u}) + \gamma\left[\left(\nabla \cdot \left(\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)\right) - \varepsilon\nabla \cdot \nabla\phi\right] = 0$$

The application mode uses the level set function to smooth the density and viscosity jump across the interface by letting

$$\rho = \rho_{\text{air}} + (\rho_{\text{water}} - \rho_{\text{air}})\phi$$

$$\mu = \mu_{\text{air}} + (\mu_{\text{water}} - \mu_{\text{air}})\phi$$

The delta function is approximated by

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

and the interface normal is calculated from

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

INITIAL CONDITIONS

Initially, the reservoir is filled with water and the capillary channel is filled with air. The initial velocity is zero.

BOUNDARY CONDITIONS

Inlet

The hydrostatic pressure, $p = \rho g z$, gives the pressure at the inflow boundary. Only water enters through the inlet, so the level set function, that is, the volume fraction of water, is 1 here.

Outlet

At the outlet, the pressure is equal to zero, that is, equal to the pressure at the top of the inflow boundary. Because it is an outflow boundary, you do not have to set any condition on the level set function.

Walls

The boundary condition **Wetted wall** is suitable for solid walls in contact with a fluid interface. It sets the velocity component normal to the wall to zero, that is,

$$\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$$

and adds a frictional boundary force

$$\mathbf{F}_{\text{fr}} = -\frac{\eta}{\beta}\mathbf{u}$$

Here, β is the slip length. The boundary condition also allows you to specify the contact angle θ, that is, the angle between the wall and the fluid interface (see Figure 4-62 according to "Mass and Momentum Transport" on page 405). In this example, the contact angle is 67.5° and the slip length equals the mesh element size, h.

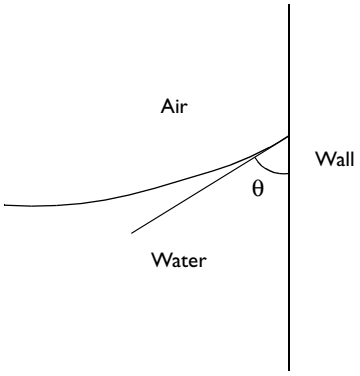


Figure 4-62: Definition of the contact angle θ.

Results and Discussion

Figure 4-63 shows the interface and the velocity field at different times. Initially, the shape of the interface changes dynamically (see Figure 4-64). After about 0.6 ms the shape of the water surface remains constant and forms a rising concave meniscus. Note that the slip velocity at the walls is almost zero, except close to the fluid interface/wall contact point.

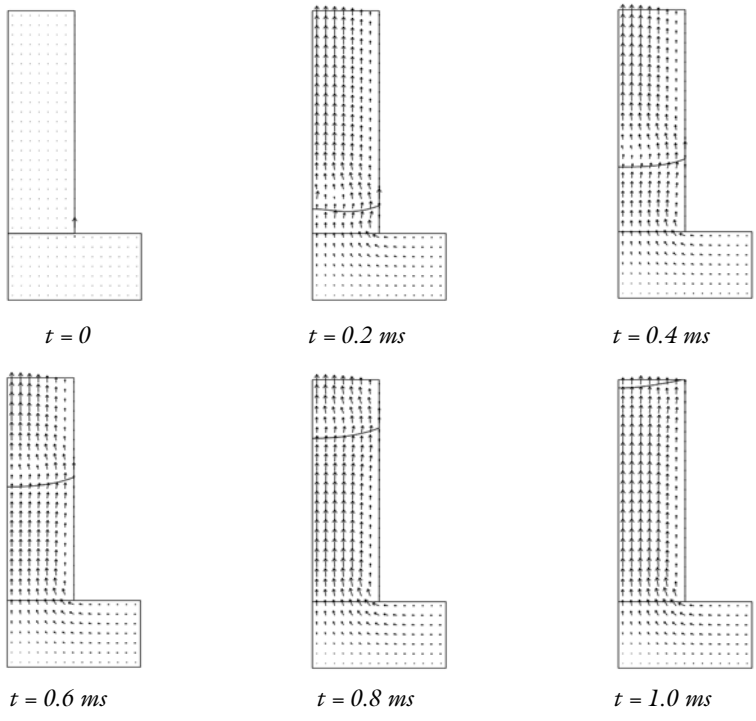


Figure 4-63: Interface and velocity field at different times.

Figure 4-64 shows how the interface dynamically deforms during the first 0.2 ms as a result of the surface tension at the water surface.

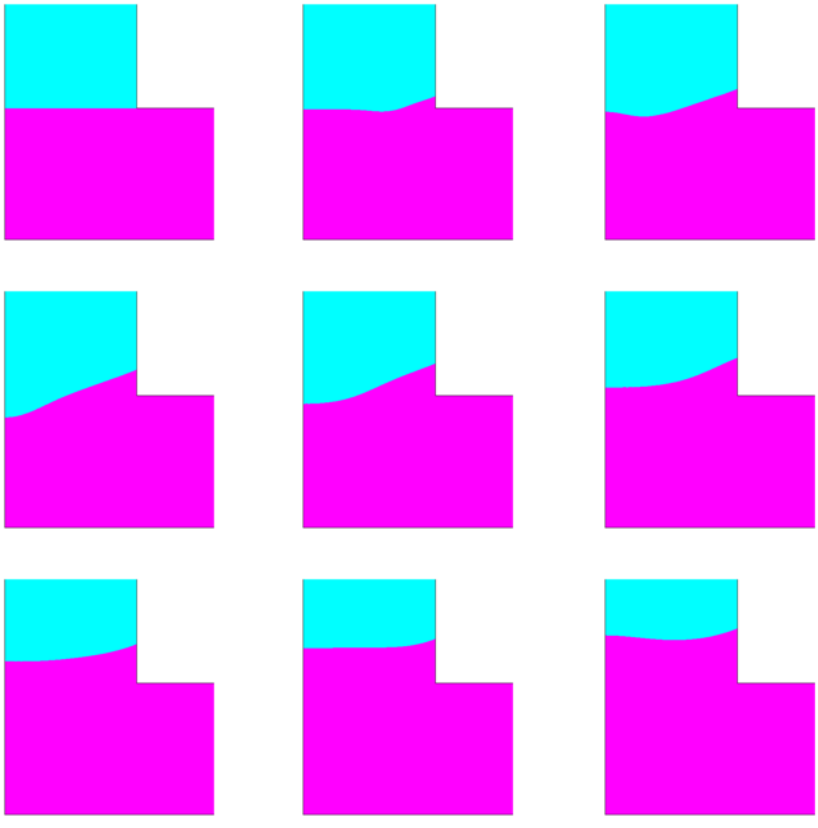


Figure 4-64: Snapshots of the position of the interface during the first 0.2 ms.

Figure 4-65 shows the pressure profile at $t = 0.6$ ms. At the fluid interface there is a pressure jump of roughly 300 Pa. The jump is caused by the surface tension, and forces water and air to rise through the channel.

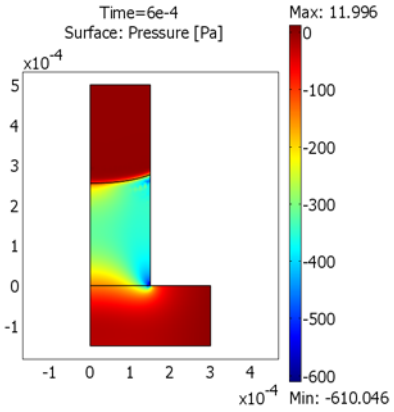


Figure 4-65: Pressure at t = 0.6 ms.

You can easily calculate the position of the interface/wall contact point by integrating the level set function along the thin cylinder wall. Figure 4-66 shows the position of the contact point as a function of time. After 0.6 ms, the contact point moves with an almost constant speed.

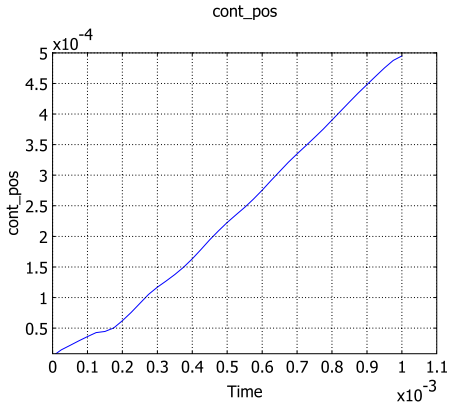


Figure 4-66: Position of the interface/wall contact point as a function of time. The velocity is approximately constant after t = 0.6 ms.

Finally, you can verify the obtained contact angle. It is defined by $\cos\theta = \mathbf{n}^T\mathbf{n}_{\text{wall}}$.

In this case, the normal to the wall is $\mathbf{n}_{\text{wall}} = (1, 0)$. The contact angle is thus $\theta = \text{acos}\, n_r$, where n_r is the radial component of the interface normal. At $t = 0.6$ ms, the contact angle is 1.16 rad $= 66°$, which can be compared with the imposed contact angle of $3\pi/8 = 1.18 = 67.5°$. The contact angle approaches the imposed value if you refine the mesh further.

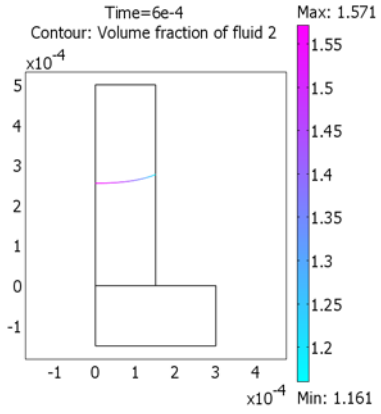


Figure 4-67: Plot of acos(n_r). At the wall, this gives the contact angle. In this case $\theta = 1.16$ *rad* $= 66°$.

Modeling in COMSOL Multiphysics

It is straightforward to set up the model with the Level Set Two-Phase Flow, Laminar application mode. At the walls in contact with the fluid interface, use the Wetted wall boundary condition.

Model Library path:
`MEMS_Module/Microfluidics_Models/capillary_filling`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

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

2 From the list of application modes, select
MEMS Module>Microfluidics>Level Set Two-Phase Flow, Laminar.

3 In the **Application mode name** edit field, type `twophase`, then click **OK**.

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button on the Draw toolbar. Type `3e-4` in the **Width** edit field, `1.5e-4` in the **Height** edit field, `0` in the ***r*** edit field, and `-1.5e-4` in the **z** edit field. Click **OK**. Click the **Zoom Extents** button on the Main toolbar.

2 Create another rectangle with these settings:

WIDTH	HEIGHT	BASE	R	Z
1.5e-4	5e-4	Corner	0	0

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

OPTIONS AND SETTINGS

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

2 Define the following constants:

NAME	EXPRESSION	DESCRIPTION
theta	(3*pi/8)[rad]	Contact angle
p_ref	1e5[Pa]	Reference pressure
T_ref	293[K]	Temperature
sigma	0.073[N/m]	Surface tension coefficient
g	9.81[m/s^2]	Acceleration due to gravity

3 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 In the **Model Tree**, right-click **Level Set Two-Phase Flow, Laminar (twophase)** and select **Subdomain Settings**.

Note: There are a number of different ways to open the **Subdomain Settings** and the **Boundary Settings** dialog boxes. This description assumes that you have the **Model Tree** visible in **Overview** mode. To open the **Model Tree** click the **Model Tree** button on the Main toolbar, then click the **Overview** button on the toolbar at the top of the **Model Tree**.

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2 Press Ctrl and select both subdomains. In the **Fluid 1** area, click the **Load** button. Select **Liquids and Gases>Gases>Air, 1 atm** from the **Materials** list and click **OK**.

3 Click the **Load** button in the **Fluid 2** area. Select **Liquids and Gases>Liquids>Water, liquid** and click **OK**.

4 For both fluids, replace `p` and `T` in the expressions for the **Dynamic viscosity** and **Density** by `p_ref` and `T_ref`.

5 Go to the **Sources/Sinks** page. Type `sigma` in the **Surface tension coefficient** edit field and `-g` in the **Gravity, z component** edit field.

6 Click the **Init** tab. Select Subdomain 1 and select the option button **Fluid 2**.

7 Click **OK**.

Boundary Conditions

1 In the **Model Tree** right-click **Level Set Two-Phase Flow, Laminar (twophase)** and select **Boundary Settings**.

2 Assign boundary conditions for the exterior boundaries according to the following table.

SETTINGS	BOUNDARIES 1, 3	BOUNDARY 8	BOUNDARY 5	BOUNDARIES 6, 7
Boundary type	Symmetry boundary	Inlet	Outlet	Wall
Boundary condition	Axial symmetry	Pressure, no viscous stress	Pressure, no viscous stress	Wetted wall
P_0		`rho_twophase*z*gz_twophase`	0	
ϕ_0		1		
θ				`theta`
β				`h`

3 Select Boundary 4 and select the **Interior boundaries** check box. Select the boundary condition **Initial fluid interface**.

4 Click **OK**.

MESH GENERATION

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

2 Select both subdomains and select **Extremely fine** from the **Predefined mesh sizes** list.

3 Click the **Mesh Selected** button, then click **OK**.

COMPUTING THE SOLUTION

First reinitialize ϕ to obtain the correct shape of ϕ in the transition layer.

1. From the **Solve** menu select **Solver Parameters**.
2. Click the **General** tab and enter `1e-3` in the **Times** edit field. Click **OK**.
3. Click the **Solve** button on the Main toolbar. This creates a good initial solution to the level set function.

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

1. Click the **Solver Manager** button on the Main toolbar.
2. Click the **Store Solution** button. Select the time **0.001**. Click **OK**.
3. In the **Initial value** area click the **Stored solution** option button.
4. Select **0.001** from the **Solution at time** list, then click **OK**.
5. Click the **Solver Parameters** button on the Main toolbar.
6. Click the **General** tab, then enter `0:0.25e-4:1e-3` in the **Times** edit field. Click **OK**.
7. From the **Physics** menu, select **Properties**.
8. Change the **Analysis type** to **Transient**, then click **OK**.
9. Click the **Solve** button on the Main toolbar.

Note: The calculations take 2–3 hours.

POSTPROCESSING AND VISUALIZATION

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, clear the **Surface** check box and select the **Contour** and **Arrow** check boxes.
3. On the **Contour** page, go to the **Contour levels** area and click the **Vector with isolevels** option button. Type `0.5` in the corresponding edit field.
4. Click the **Arrow** tab. From the **Predefined quantities** list on the **Subdomain Data** page, select **Velocity field**. In the **Number of points** edit field for **z points**, type `30`.
5. Click **Apply**.

6 On the **General** page, select a value from the **Solution at time** list and then click **Apply** to visualize the result at the corresponding value. Repeat to view the solution at other times.

7 Click **OK**.

8 To create a movie from the plots at the different times, click the **Animate** button on the Plot toolbar.

To create filled contour plots as in Figure 4-64, perform the following steps:

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

2 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

3 On the **Contour** page, select the **Filled** check box.

4 Click **OK**.

Next, create the pressure plot in Figure 4-65.

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

2 On the **General** page, clear the **Contour** check box and select the **Surface** check box in the **Plot type** area. In the **Solution to use** area, select `6e-4` from the **Solution at time** list.

3 Click the **Surface** tab. From the **Predefined quantities** list on the **Surface Data** page, select **Pressure**.

4 Click **OK**.

Follow the next steps to calculate and plot the position of the contact point as in Figure 4-66.

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

2 Select Boundary 6. Type `cont_pos` in the **Name** edit field on the first row of the table and `phi` in the corresponding **Expression** edit field. Click **OK**.

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

4 From the **Postprocessing** menu, select **Global Variables Plot**.

5 Type `cont_pos` in the **Expression** edit field, then click the **Add Entered Expression** button next to the edit field. Click **OK** to generate the plot.

Finally, check the obtained contact angle.

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

2 On the **General** page, clear the **Surface** check box and select the **Contour** check box in the **Plot type** area.

3 Click the **Contour** tab. On the **Color Data** page, click the **Color data** option button.

4 Clear the **Filled** check box.

5 In the **Expression** edit field, type `acos(normr_twophase)`, then click **OK**.

Hydrocarbon Dehalogenation in a Tortuous Microreactor

Introduction

Removing halogen groups from hydrocarbons is an important reaction step in several chemical processes. One application is water purification. Other examples involve organic synthesis, where the removal of halogen groups serves as a starting point for carbon-carbon coupling reactions. Typically, the carbon-halogen bond scission is activated by precious metal catalysts based on platinum or palladium.

The model presented here shows hydrocarbon dehalogenation as it occurs in a microreactor. The reactants are transported from the fluid bulk to the catalytic surfaces at the reactor walls, where they react. A first model is set up in Reaction Engineering Lab, where two competing reactions are analyzed. Subsequently, the reaction kinetics are exported to the MEMS Module, where a space-dependent model of the microreactor is set up and solved.

Note: This model requires the COMSOL Reaction Engineering Lab and the MEMS Module.

Model Definition

The adsorption of halogenated hydrocarbons onto the surface of a platinum catalyst leads to cleavage of the carbon halogen bond. The hydrocarbon fragments then undergo either hydrogenation or coupling reactions. Figure 4-68 illustrates the overall reactions for a brominated hydrocarbon species.

$$\begin{aligned} \text{R-Br} &\xrightarrow[\text{[Pt]}]{k_1} \text{R-H} \\ 2\text{R-Br} &\xrightarrow[\text{[Pt]}]{k_2} \text{R-R} \end{aligned} \tag{4-25}$$

Figure 4-68: The dehalogenation of RBr can result either in hydrogenation or coupling of the hydrocarbon fragments.

The reaction rates are:

$$r_1 = k_1 c_{RBr} \tag{4-26}$$

and

$$r_2 = k_2 c_{RBr}^2 \tag{4-27}$$

where the rate constants are given by the Arrhenius expression:

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T}\right) \tag{4-28}$$

In Equation 4-28, A is the frequency factor, and E the activation energy (J/mol). The table below lists the values of the Arrhenius parameters for the two reactions.

TABLE 4-5: ARRHENIUS PARAMETERS

	FREQUENCY FACTOR	ACTIVATION ENERGY
Reaction 1	2e-3	10e3
Reaction 2	1e-3	30e3

IDEAL REACTOR MODEL

The mass balance equation for a flow-through reactor is given by

$$\frac{dF_i}{dV} = R_i \tag{4-29}$$

where F is the molar flow rate (mol/s), V the reactor volume (m^3), and R_i the net reaction term (mol/($m^3 \cdot$ s)). If the reactor has constant cross-section and constant flow velocity, the left hand side of Equation 4-29 can be rewritten as

$$\frac{dF_i}{dV} = u\frac{dc_i}{dx} = \frac{dc_i}{d\tau} \tag{4-30}$$

The reactor mass balance thus becomes

$$\frac{dc_i}{d\tau} = R_i \tag{4-31}$$

where τ represents the residence time (s). The assumption of constant flow velocity is valid for incompressible liquids or liquids where the effect of temperature on the density is small. Equation 4-31 is identical to the balance equation of the batch reactor,

except that residence time replaces the reaction time. You can therefore make use of the Batch reactor type when solving the model in the Reaction Engineering Lab.

The ideal reactor model assumes by default that reactions take place in the entire reactor volume. In the 3D microreactor model, reactions occur at catalytic surfaces located at the reactor walls. In order to make the ideal model represent a reactor with surface reactions, Equation 4-31 has to be scaled by the reactive area per reactor volume. Scaling the ideal reactor equations by the dimensions of the microreactor makes the 1D and 3D models comparable. The area to volume ratio is

$$\frac{WL}{WLH} = \frac{1}{H} \tag{4-32}$$

where W is the width of the channel (m), H the channel height (m), and L the length of a reactive section (m). The scaled ideal reactor equation is then

$$\frac{dc_i}{d\tau} = \frac{R_i}{H} \tag{4-33}$$

Note that the net reaction term (R_i) in this case represents surface reactions (mol/(m^2· s)).

SPACE-DEPENDENT MODEL

The microreactor considered in this example consists of a tortuous channel, fitted with inlet and outlet adapter sections, as illustrated in Figure 4-69.

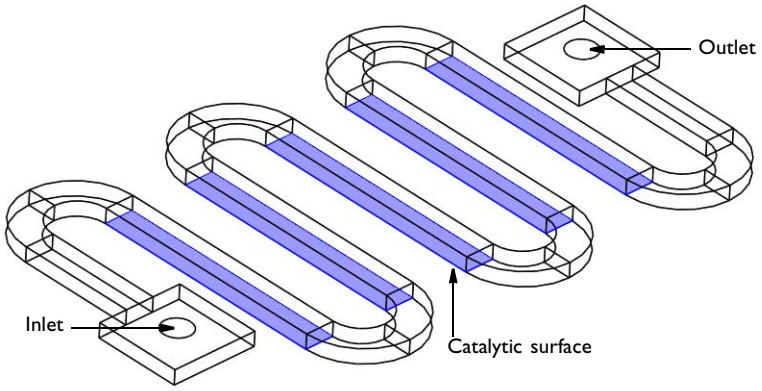


Figure 4-69: Microreactor geometry.

In the straight sections of the reactor, the channel walls are in part coated with platinum catalyst. As water with small amounts of a brominated hydrocarbon flows through the reactor, dehalogenation reactions occur at the catalytic surfaces.

MOMENTUM BALANCES

The flow in the channel is described by the Navier-Stokes equations:

$$\begin{gathered}\nabla \cdot [-\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p\mathbf{I}] = -\rho(\mathbf{u} \cdot \nabla)\mathbf{u} \\ \nabla \cdot \mathbf{u} = 0\end{gathered} \tag{4-34}$$

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

A pressure difference drives the flow through the reactor, as indicated by the boundary conditions

$$\begin{aligned} p &= p_{\text{inlet}} && \text{inlet} \\ p &= 0 && \text{outlet} \end{aligned} \tag{4-35}$$

Each pressure condition is specified along with a vanishing viscous stress condition at the boundary

$$\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

At the wall the velocity is zero

$$\mathbf{u} = 0 \qquad \text{walls} \tag{4-36}$$

MASS BALANCES

The mass balances set up and solved are the diffusion-convection equations at steady state:

$$\nabla \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = 0 \tag{4-37}$$

where D_i denotes the diffusion coefficient (m^2/s), c_i is the species concentration (mol/m^3), and $\mathbf{u}$ equals the velocity vector (m/s).

No reactions take place in the fluid bulk. Rather, the reactions take place on the catalytic surfaces. The boundary fluxes at the catalytic surfaces thus become

$$\mathbf{n} \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = R_i \tag{4-38}$$

where R_i represents the reaction term. Note that these boundary conditions are set up automatically as you export the reaction kinetics from the Reaction Engineering Lab to COMSOL Multiphysics.

Inlet conditions are equal to the inlet concentrations

$$c = c_{\text{in}} \tag{4-39}$$

At the outlet, you can set the convective flux condition, assuming that the transport of mass across the boundary is dominated by convection

$$\mathbf{n} \cdot (-D\nabla c) = 0 \tag{4-40}$$

All other boundaries use the insulating condition

$$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = 0 \tag{4-41}$$

Results

First review the results of the ideal reactor model, which you set up and solve in the Reaction Engineering Lab.

Figure 4-70 through Figure 4-72 show concentration profiles of reactant and products as function of residence time, evaluated at 288 K, 343 K, and 363 K.

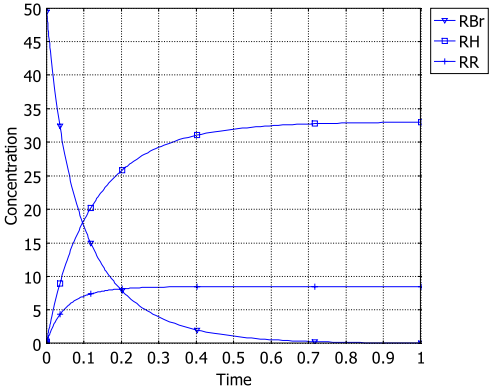


Figure 4-70: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 288 K.

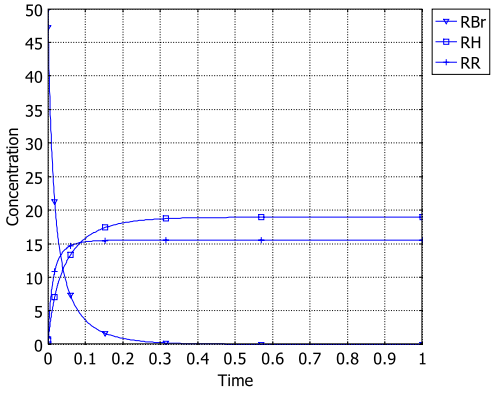


Figure 4-71: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 343 K.

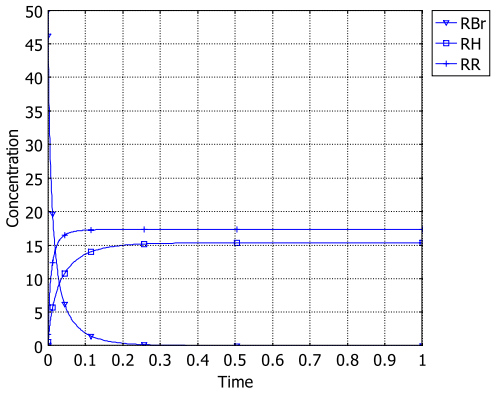


Figure 4-72: Concentration of the RBr, RH, and RR species as function of residence time. Reactions occur at 363 K.

The hydrocarbon coupling reaction has the higher activation energy and is hence more temperature sensitive than the hydrogenation reaction (see Table 4-5). The concentration plots of the ideal reactors outline the effect quite clearly. At 288 K, the hydrogenation product RH is dominant, while at 363 K the coupling product is the more prominent. Notably, at 343 K, the concentration dependency on the reaction rates becomes accentuated, so that RBr dominates only at shorter τ and RH at longer τ.

Although the primary goal may be to remove the halogenated reactant, RBr, it may also be important to set reaction conditions in such a way that the most favorable by-product is formed. The present model shows how such design aspects can readily be investigated in the Reaction Engineering Lab.

The next set of results refer to the space-dependent model of a tortuous microreactor, set up and solved in COMSOL Multiphysics.

Figure 4-73 shows the velocity of the laminar flow field in the reactor. The flow is driven by a pressure difference of 1500 Pa between inlet and outlet. The resulting maximum velocity is close to 5 mm/s.

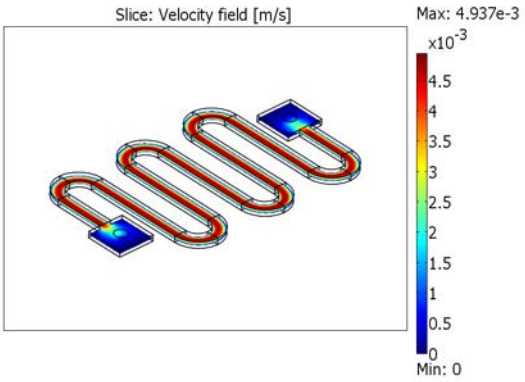


Figure 4-73: Velocity field in the reactor where the pressure difference between inlet and outlet is 1500 Pa.

Figure 4-74 shows the concentration distribution of the reactant RBr in the reactor. At relatively low temperature, 288 K, the outlet concentration is 10.6 mol/m^3.

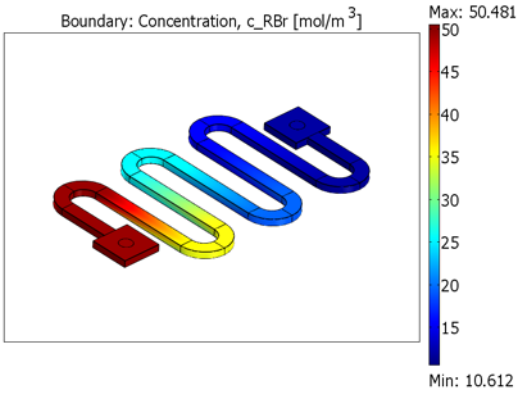


Figure 4-74: Concentration distribution of the halogenated reactant RBr. Fluid properties and reaction rates are evaluated at 288 K.

Running the reactor at 363 K, the outlet concentration of RBr is still 6.7 mol/m^3.

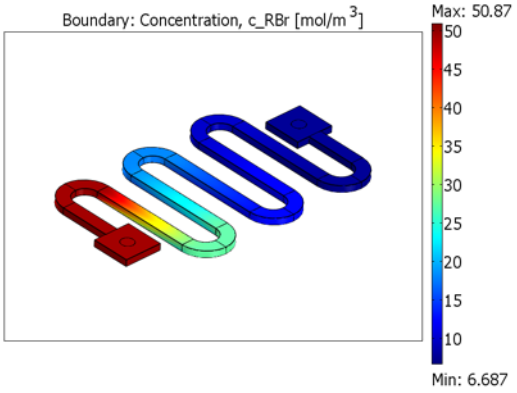


Figure 4-75: Concentration distribution of the halogenated reactant RBr. Fluid properties and reaction rates are evaluated at 363 K.

Judging from the results of the ideal reactor models, a more pronounced temperature effect would be expected. The reason for this apparently moderate influence on conversion is that the increased temperature also affects the flow.

Raising the temperature from 282 K to 363 K decreases the viscosity of water from $1.36 \cdot 10^{-3}$ to $3.17 \cdot 10^{-4}$. This is automatically taken into account by the temperature dependent fluid properties. As the flow through the reactor is driven by a constant pressure difference, the velocity will increase as viscosity decreases. Results show that the maximum fluid velocity at 363 K is ~3.6 times greater than at 282 K, resulting in a shorter residence time.

The following path shows the location of the COMSOL Multiphysics model:

Model Library path: `MEMS_Module/Microfluidics_Models/tortuous_reactor`

Modeling Using COMSOL Multiphysics

MODEL NAVIGATOR

1 Start COMSOL Multiphysics by clicking the desktop icon.

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

3 In the list of application modes select **MEMS Module>Microfluidics>Incompressible Navier-Stokes**.

4 Click **OK**.

GEOMETRY MODELING

Select the menu item **File>Import CAD Data From File**. Browse to the file `tortuous_reactor.mphbin` and click **Import**.

PHYSICS SETTINGS

Subdomain Settings—Incompressible Navier-Stokes

1 Choose **Physics>Subdomain Settings**.

2 In the **Subdomain selection** list, select all subdomains by pressing Ctrl+A and clicking the list.

3 Go to the **Material/Coefficients Library** by clicking the **Load** button.

4 Browse to **Liquids and Gases>Liquids>Water, liquid** and click **OK** to load the properties.

5 Click **OK**.

Boundary Conditions—Incompressible Navier-Stokes

1 Choose **Physics>Boundary Settings**.

2 Enter the following boundary conditions:

SETTINGS	BOUNDARY 6	BOUNDARY 104
Boundary type	Inlet	Outlet
Boundary condition	Pressure, no viscous stress	Pressure, no viscous stress
p_0	delta_p	0

Leave all other boundaries at their default setting (Wall, No slip).

3 Click **OK**.

OPTIONS AND SETTINGS

1 Choose **Options>Constants** then enter the following data:

NAME	EXPRESSION	DESCRIPTION
delta_p	1.5[kPa]	Inlet overpressure
T	288[K]	Temperature

2 Click **OK**.

MESH GENERATION

1 Select the menu item **Mesh>Free Mesh Parameters**.

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

3 Click the **Boundary** page, select Boundary 8, and click the **Mesh Selected** button.

4 Choose **Mesh>Swept Mesh Parameters**.

5 Select Subdomains 2–19 and 21 from the **Subdomain selection** list by pressing Ctrl and clicking the list.

6 Click the **Mesh Selected** button.

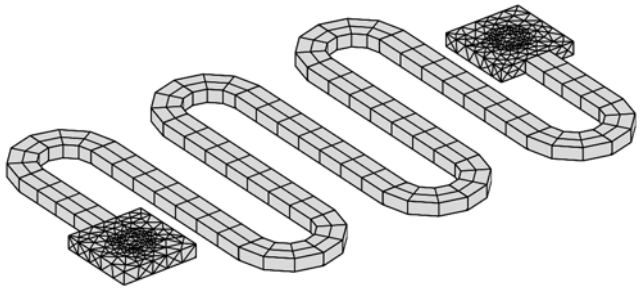
7 Click **OK** to close the **Swept Mesh Parameters** dialog.

8 Go to the **Free Mesh Parameters** dialog, and click the Subdomain page.

9 Select Subdomains 1 and 20 from the **Subdomain selection** list by pressing Ctrl and clicking the list.

10 Click the **Mesh Selected** button.

11 Click **OK** to close the **Free Mesh Parameters** dialog box.



COMPUTING THE SOLUTION

1 Solve the problem by clicking the **Solve** button (**=**) on the Main toolbar.

2 Select the menu item **Solve>Solver Manager**.

3 Press the **Store Solution** button and the click **OK**.

POSTPROCESSING THE SOLUTION

The following steps reproduce Figure 4-73:

1 Choose **Postprocessing>Plot Parameters**.

2 On the **Slice** page, select the **Slice plot** check box.

3 Type `0` in the **x-levels** edit field and `1` in the **z-levels** edit field.

4 Click **OK**.

Modeling Using the COMSOL Reaction Engineering Lab

1 In the main user interface of COMSOL Multiphysics, choose **File>Reaction Engineering Lab**.

The main user interface of COMSOL Reaction Engineering Lab opens up.

2 Click the **COMSOL Reaction Engineering Lab** window.

OPTIONS AND SETTINGS

1 Click the **Model Settings** button on the Main toolbar.

2 On the **General** page type `288` in the **Temperature** edit field.

3 Click **Close**.

4 Choose **Model>Constants** then enter the following data:

NAME	EXPRESSION	DESCRIPTION
H	5e-6	Reactor channel height (m)

5 Click **OK**.

REACTIONS INTERFACE

1 Click the **Reaction Settings** button on the Main toolbar.

2 Make sure the **Reactions** page is active. Create two entries in the **Reaction selection** list by clicking the **New** button twice.

3 Enter the following reaction formulas by first selecting the appropriate row in the **Reaction selection** list and then entering the corresponding text in the **Formula** edit field.

REACTION ID #	REACTION FORMULA
1	RBr=>RH
2	2RBr=>RR

4 Select row 1 from the **Reaction selection** list.

5 Select the **Use Arrhenius expression** check box.

6 Enter `2e-3` in the **A** edit field and `10e3` in the **E** edit field.

7 Select row 2 from the **Reaction Selection** list.

8 Select the **Use Arrhenius expression** check box.

9 Enter `1e-1` in the **A** edit field and `30e3` in the **E** edit field.

10 Select Reaction 1 from the **Reaction selection** list and type `kf_1*c_RBr/H` in the **r** edit field.

11 Select Reaction 2 from the **Reaction selection** list and type `kf_2*c_RBr^2/H` in the **r** edit field.

You have now modified the automatically generated reaction rates by dividing with the scale factor H, according to Equation 4-33.

SPECIES INTERFACE

1 Click the **Species** tab.

2 Select **RBr** from the **Species selection** list and type `50` in the c_0 edit field.

3 Click **Close**.

COMPUTING THE SOLUTION

1. Open the **Simulation>Solver Parameters** dialog box.
2. Type `1` in the **Times** edit field.
3. Click **OK**.
4. Click the **Solve Problem** button (**=**) on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The results of Figure 4-70 are shown in the default plot. To generate the results shown in Figure 4-71 follow these steps.

1. Click the **Model Settings** button on the Main toolbar.
2. On the **General** page type `343` in the **Temperature** edit field.
3. Click **Close**.
4. Click the **Solve Problem** button.

To generate the results shown in Figure 4-72:

1. Click the **Model Settings** button on the Main toolbar.
2. On the **General** page type `363` in the **Temperature** edit field.
3. Click **Close**.
4. Click the **Solve Problem** button.

EXPORT SETTINGS

You will now proceed to export the reaction kinetics to the reacting boundaries in the Multiphysics model. Recall that the rate constants are temperature dependent. To export a temperature variable while only exporting mass balances, follow these steps:

1. Click the **Model Settings** button on the Main toolbar.
2. On the **General** page type `Temp` in the **Temperature** edit field.
3. Click **Close**.

This will export a variable name `Temp` rather than a constant temperature, which would otherwise be the case.

Recall also that the reaction rates were scaled in order to make the 1D ideal reactor comparable to the 3D microreactor. As you are about to export the reaction kinetics to the 3D model, the effect of the scaling should first be removed.

1 Choose **Model>Constants** then set the scaling factor H to 1:

NAME	EXPRESSION	DESCRIPTION
H	1	reactor channel height (m)

2 Click **OK**.

Now, move on to export the reaction model.

1 Click the **Export to COMSOL Multiphysics** button on the Main toolbar.

2 The **Export to COMSOL Multiphysics** dialog box appears.

3 Select **Boundary** in the **Domain level** drop down list.

4 Go to the **Export mass balance** area, and in the **Application mode** list select **Convection and Diffusion: New**.

5 In the **Group name** edit field type `reactions`.

6 Move to the **Export energy balance** area and clear the check box in the upper left corner.

7 Click the **Export** button at the bottom of the dialog box.

Modeling Using COMSOL Multiphysics

It is now time to investigate the chemistry taking place in a space-dependent model.

Click the **COMSOL Multiphysics** window.

Subdomain Settings—Convection and Diffusion

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

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

3 In the **Subdomain selection** list, select all subdomains by pressing Ctrl+A and clicking the list.

4 On the **c_RBr** page type the following:

EDIT FIELD	VALUE
Diffusion coefficient	D
x-velocity	u
y-velocity	v
z-velocity	w

5 Type in the same entries on the **c_RH** page and the **c_RR** page.

6 Click **OK**.

Boundary Conditions—Convection and Diffusion

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

2 In the **Boundary selection** list, select **27**, **41**, **57**, **71**, and **87** by pressing Ctrl and clicking the entries. These boundaries represent the reactive surfaces.

3 Select **reactions** from the **Group** list.

This associates the exported kinetics from Reaction Engineering Lab with the catalytic surfaces. The **Flux** boundary condition is automatically set on all mass balance pages, and the appropriate reaction terms appear in the **Inward flux** edit fields.

4 Enter the remaining boundary conditions for each of the species **c_RBr**, **c_RH**, and **c_RR** according to the following table:

SETTINGS	BOUNDARY 6	BOUNDARY 104	ALL OTHERS
Boundary condition	Concentration	Convective flux	Insulation/Symmetry
c_RBr_0	50		
c_RH_0	0		
c_RR_0	0		

5 Click **OK**.

OPTIONS AND SETTINGS

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

2 Add entries to complete the list of constants as follows:

NAME	EXPRESSION	DESCRIPTION
delta_p	1.5[kPa]	Inlet overpressure
T	288[K]	Temperature
D	1e-6[m^2/s]*exp(-2000[K]/T)	Diffusivity
Temp	T	Temperature

3 Click **OK**.

COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Manager**.

2 In the **Values of variables not solved for and linearization point**, click the **Stored solution** option button.

3 Click the **Solve For** tab.

4 Select only the **Convection and Diffusion (chcd)** folder in the **Solve for variables** tree.

5 Click **OK**.

6 Solve the problem by clicking the **Solve** button (**=**) on the Main toolbar.

POSTPROCESSING THE SOLUTION

The following steps reproduce Figure 4-74:

1 Choose **Postprocessing>Plot Parameters**.

2 On the **Boundary** page, select the **Boundary plot** check box.

3 Type `c_RBr` in the **Expression** edit field.

4 Click **OK**.

To reproduce the results in Figure 4-75, change the variable `T` in the **Constants** dialog box to `363[K]`, and solve for the flow and mass balances as outlined above.

5

Models of Piezoelectric Devices

The piezoelectric effect is a transfer of electric energy to mechanical energy and vice versa. It arises in many crystalline materials, and some of them—for example, quartz, Rochelle salt, and lead titanate zirconate ceramics—display the phenomenon strongly enough that it can be useful.

The *direct* piezoelectric effect consists of an electric polarization in a fixed direction when the piezoelectric crystal is deformed. The polarization is proportional to the deformation and causes an electric potential difference over the crystal.

The *inverse* piezoelectric effect, on the other hand, constitutes the opposite of the *direct* effect. This means that an applied electric field induces a deformation of the crystal.

The following models show the application of the MEMS Module for modeling piezoelectric effects in a static linear analysis:

- An axisymmetric example of a piecoceramic tube that models both the direct and the inverse piezoelectric effect
- A 3D shear bender example modeling the inverse piezoelectric effect
- A 3D model of a composite piezoelectric transducer

Piezoceramic Tube

Introduction

This example performs a static 2D axisymmetric analysis of a piezoelectric actuator using the 2D Piezo Axial Symmetry application mode. It models a radially polarized piezoelectric tube as described by S. Peelamedu and others (Ref. 1). One application area where radially polarized tubes are employed is in nozzles for fluid control in inkjet printers.

Model Definition

GEOMETRY

The tube has a height of 0.62 mm and an inner and outer radius of 0.38 mm and 0.62 mm, respectively.

MATERIAL

The material properties for the piezoceramic (PZT-5H) are:

$$c = \begin{bmatrix} 127 & 80.2 & 84.7 & 0 & 0 & 0 \\ & 127 & 84.7 & 0 & 0 & 0 \\ & & 117 & 0 & 0 & 0 \\ & & & 23.0 & 0 & 0 \\ & \text{sym} & & & 23.0 & 0 \\ & & & & & 23.5 \end{bmatrix} \text{GPa}$$

$$e = \begin{bmatrix} 0 & 0 & 0 & 0 & 17.03448 & 0 \\ 0 & 0 & 0 & 17.03448 & 0 & 0 \\ -6.22812 & -6.22812 & -23.2403 & 0 & 0 & 0 \end{bmatrix} \text{C/m}^2$$

$$\varepsilon = \begin{bmatrix} 1.5 & 0 & 0 \\ 0 & 1.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \cdot 10^{-8} \text{ F/m}$$

BOUNDARY CONDITIONS

This model studies two cases, each of which studies different boundary conditions. Case 1 represents the inverse piezoelectric effect, and case 2 represents the direct piezoelectric effect.

Case 1:

- Structural mechanics boundary condition—constrain the bottom surface from moving axially (in the z-direction).
- Electrostatics boundary condition—apply a 1 V potential difference between the tube's inner and outer surfaces.

Case 2:

- Structural mechanics boundary condition—constrain the bottom surface from moving axially (in the z direction), but also add an internal fluid pressure of 0.1 MPa.
- Electrostatics boundary condition—ground the inner and outer surfaces.

Results and Discussion

The image in Figure 5-1 shows the deformation due to the applied voltage difference in Case 1. For the same case, Figure 5-2 shows the radial displacement as a function of the tube thickness at the top boundary.

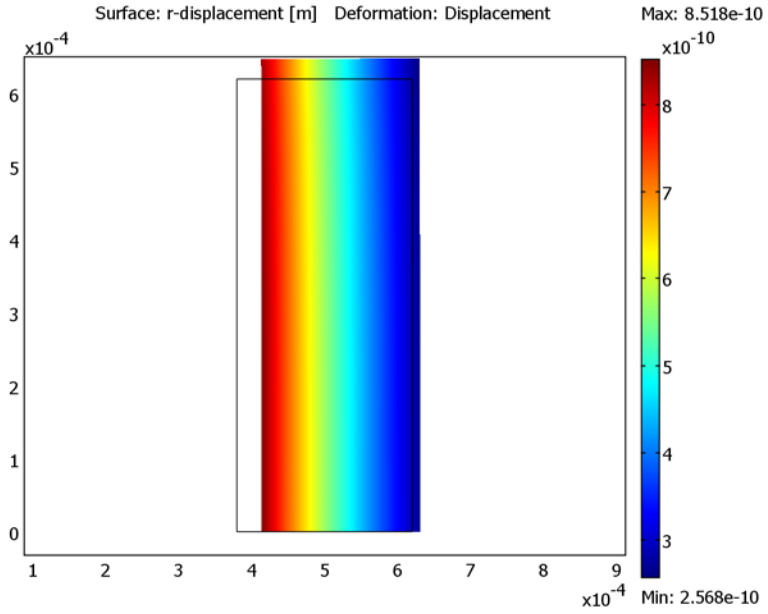


Figure 5-1: The deformed shape and radial displacement of a piezoceramic-tube actuator due to the radial electric field for Case 1.

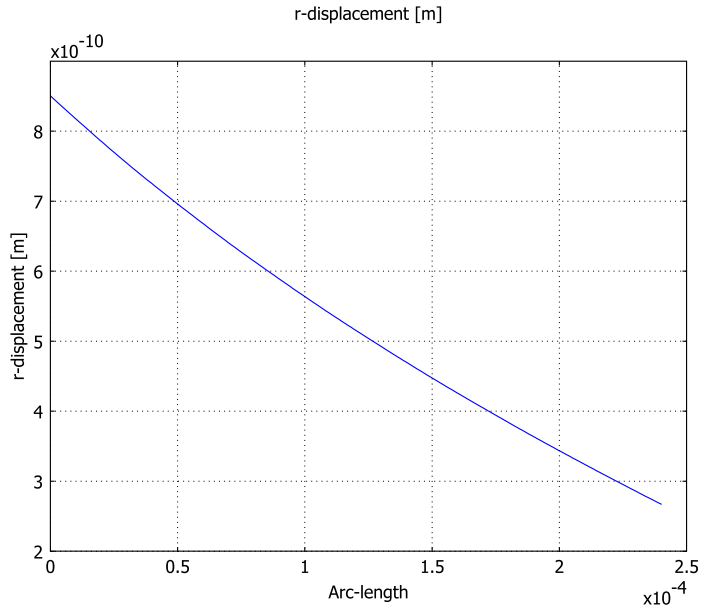


Figure 5-2: The radial displacement as a function of the tube thickness due to the radial electric field (Case 1).

For the second case, Figure 5-3 shows the deformed shape in Case 2. For that same case, Figure 5-4 shows the radial displacement as a function of tube thickness. These results show good agreement with those from S. Peelamedu (Ref. 1).

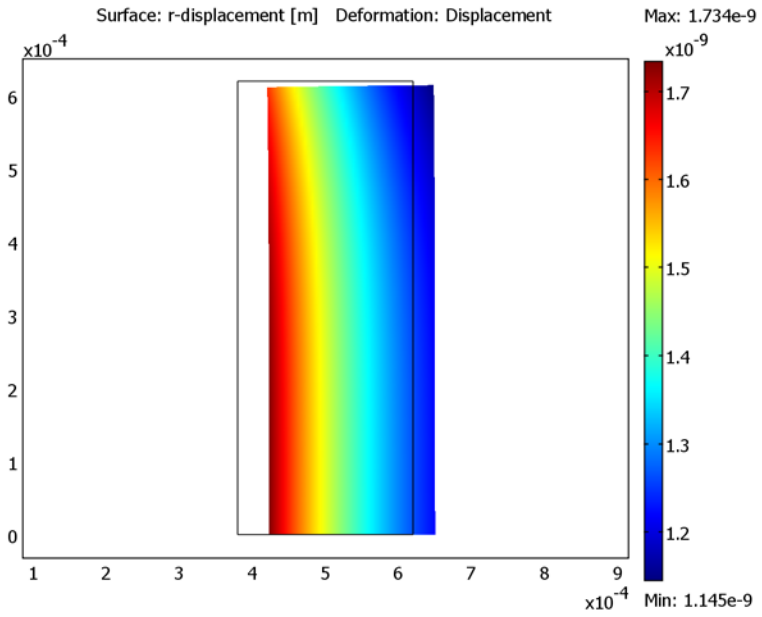


Figure 5-3: The deformed shape and radial displacement in a piezoceramic-tube actuatordue to an internal pressure of 0.1 MPa (Case 2).

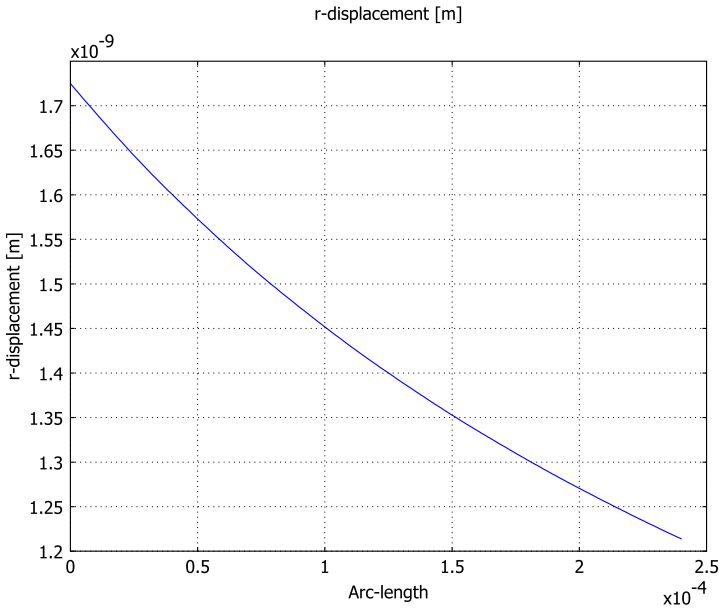


Figure 5-4: The radial displacement as function of the tube thickness due to an internal pressure of 0.1 MPa (Case 2).

Modeling in COMSOL Multiphysics

CONSTITUTIVE EQUATION AND MATERIAL DATA

You specify the material parameters for the piezoelectric material in the **Subdomain Settings** dialog box in the piezoelectric application mode. Then select the stress-charge form for the constitutive equation because this suits the form in which you give the material data. Further, enter the elasticity matrix into the c_e matrix, enter the piezoelectric coupling matrix into the e matrix, and enter the relative permittivities into the ε_{rS} matrix.

You enter the material properties in this example such that the polarization is in the z direction (in a 3D Cartesian coordinate system), which is a common orientation for published material data. This orientation means that you must rotate the material so that its polarization direction is aligned with the r-direction (radially polarized). To do so, use the material-orientation feature in the Piezo Axial Symmetry application mode. By selecting the material orientation as the zx-plane, you rotate the material so that its

z direction is aligned with the r direction of the model, and the material's x direction is aligned with the model's z direction.

The piezoceramic material in this example (PZT-5H) is a transversely isotropic material, which is a special class of orthotropic materials. Such a material has the same properties in one plane (isotropic behavior) and different properties in the direction normal to this plane. Thus you can use either the zx-plane material orientation or the zy-plane material orientation; both give the same solution.

MESHING

The rectangular geometry is well suited for quadrilaterals, and the model uses a 6-by-6-element grid.

Reference

1. S. Peelamedu et al., *Numerical Approach for Axisymmetric Piezoceramic Geometries towards Fluid Control Applications*, Univ. Toledo, OH, Mechanical, Industrial and Manufacturing Engineering Dept., 2000.

Model Library path: `MEMS_Module/Piezo_Models/piezoceramic_tube`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Start COMSOL Multiphysics. This invokes the **Model Navigator**, which you can also open from an already running COMSOL Multiphysics session by choosing **New** from the **File** menu.
2. Select **Axial Symmetry (2D)** from the **Space dimension** list.
3. Select **MEMS Module>Structural Mechanics>Piezo Axial Symmetry>Static analysis** from the list of application modes.
4. Click **OK** to close the **Model Navigator**. Note that this gives you second-order elements, **Lagrange - Quadratic**, by default.

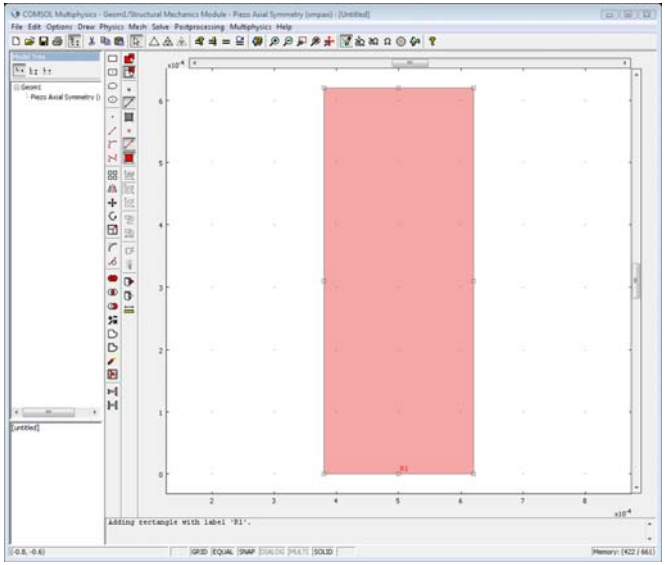
GEOMETRY MODELING

Define the model geometry in Draw mode.

1 Shift-click the **Rectangle/Square** button in the Draw toolbar to open the **Rectangle** dialog box.

2 Type `0.24e-3` in the **Width** edit field and `0.62e-3` in the **Height** edit field. In the **Position** area, type `0.38e-3` in the **r** edit field and `0` in the **z** edit field. This creates a rectangle with opposite corners at (0.38e-3, 0) and (0.62e-3, 0.62e-3).

3 Click the **Zoom Extents** button.



PHYSICS SETTINGS FOR MODEL CASE 1

Boundary Conditions

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

2 Select Boundary 2 from the **Boundary selection** list.

3 Select **Roller** from the **Constraint condition** list on the **Constraint** page.

4 Select all boundaries by pressing Ctrl+A.

5 Select **Zero charge/Symmetry** from the **Boundary condition** list on the **Electric BC** page.

6 Select Boundary 1 and then select **Ground** from the **Boundary condition** list.

7 Select Boundary 4 and then select **Electric potential** from the **Boundary condition** list and type `1` in the **Electric potential** edit field.

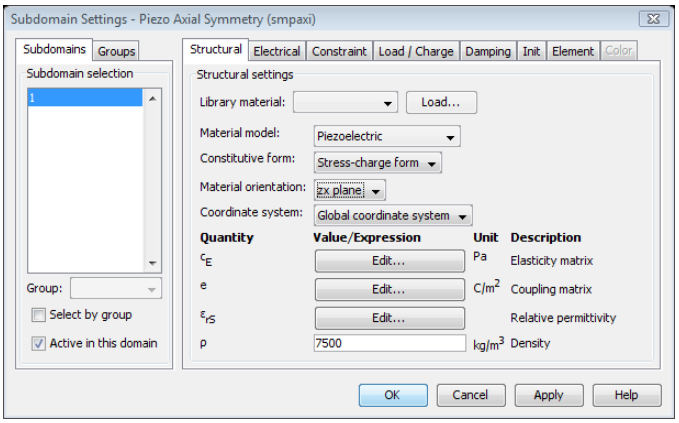
8 Click **OK** to close the dialog box.

Subdomain Settings

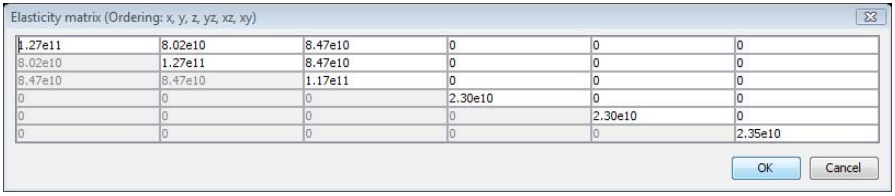
1 Open the **Subdomain Settings** dialog box by selecting **Subdomain Settings** from the **Physics** menu.

2 Select Subdomain 1 and click the **Structural** tab.

3 Select **zx plane** from the **Material orientation** list.



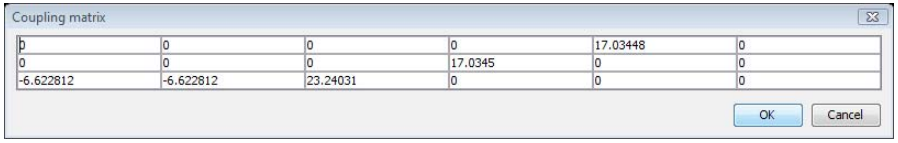
4 Click the **Edit** button associated with $\mathbf{c_E}$ and enter the following values into the **Elasticity matrix** dialog box; when done, click **OK**.



1.27e11	8.02e10	8.47e10	0	0	0
	1.27e11	8.47e10	0	0	0
		1.27e11	0	0	0
			2.30e10	0	0
				2.30e10	0
					2.30e10

Entries for the elasticity matrix.

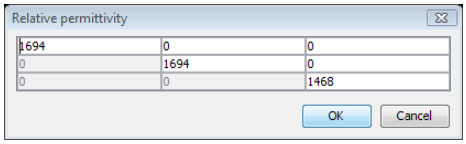
5 Click the **Edit** button associated with **e** and enter the following values into the **Coupling matrix** dialog box; when done, click **OK**.



0	0	0	0	17.03448	0
0	0	0	17.03448	0	0
-6.22812	-6.22812	-23.2403	0	0	0

Entries for the coupling matrix.

6 Click the **Edit** button associated with ε_{rS} and enter the following values into the **Relative permittivity matrix** dialog box; when done, click **OK**.



1694		
	1694	
		1468

Entries for the relative permittivity matrix.

7 Click **OK** again to close the **Subdomain Settings** dialog box.

MESH GENERATION

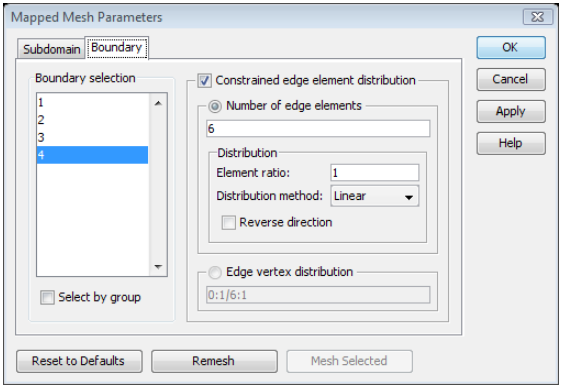
1 From the **Mesh** menu choose **Mapped Mesh Parameters**.

2 Click the **Boundary** tab.

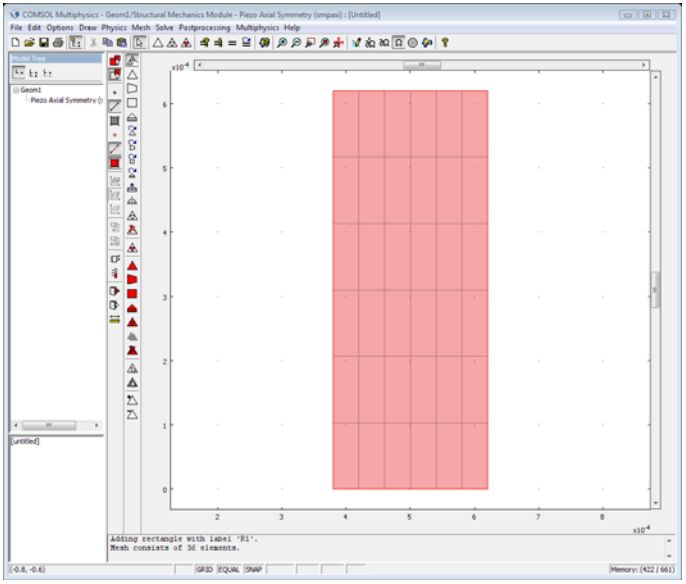
3 Select Boundary 1 and click the **Constrained edge element distribution** button.

4 Enter 6 in the **Number of edge elements** edit field.

5 Repeat this for the remaining three boundaries.



6 Click the **Remesh** button.



The meshed geometry for the piezoceramic-tube actuator.

7 Click **OK**.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

1. Choose **Plot Parameters** from the **Postprocessing** menu to open the **Plot Parameters** dialog box.
2. On the **General** page, find the **Plot type** area, then select the **Deformed shape** and **Surface** check boxes.
3. Click the **Surface** tab.
4. Select ***r*-displacement** from the **Predefined quantities** list and click **OK** (this step reproduces Figure 5-1).
5. Choose **Cross-Section Plot Parameters** from the **Postprocessing** menu.
6. Click the **Line/Extrusion** tab.
7. Select ***r*-displacement** from the **Predefined quantities** list.
8. Go to the **Cross-section line data** area. In the **r0** edit field enter `3.8e-4`. Similarly set **r1** to `6.2e-4` and then both **z0** and **z1** to `3e-4`.
9. Click **OK** (this step reproduces Figure 5-2).

PHYSICS SETTINGS FOR MODEL CASE 2

Boundary Conditions

1. Open the **Boundary Settings** dialog box by selecting **Boundary Settings** from the **Physics** menu. In this dialog box you can select boundaries and enter expressions for boundary conditions.
2. Select Boundary 1 from the **Boundary selection** list.
3. Enter `0.1e6` in the $\mathbf{F_r}$ edit field on the **Load** page.
4. Select Boundaries 1 and 4 and then select **Ground** from the **Boundary condition** list on the **Electric BC** page.
5. Select Boundaries 2 and 3 and then select **Zero charge/Symmetry** from the **Boundary condition** list on the **Electric BC** page.
6. Click **OK** to close the dialog box.

COMPUTING THE SOLUTION

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

POSTPROCESSING AND VISUALIZATION

1. Choose **Plot Parameters** from the **Postprocessing** menu to open the **Plot Parameters** dialog box.

2 On the **General** page select the **Deformed shape** and **Geometry edges** check boxes in the **Plot type** area.

3 Click the **Surface** tab and select **r-displacement** from the **Predefined quantities** list and click **OK** (this reproduces Figure 5-3).

4 Choose **Cross-Section Plot Parameters** from the **Postprocessing** menu.

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

6 Select **r-displacement** from the **Predefined quantities** list.

7 Go to the **Cross-section line data** area. In the **r0** edit field enter `3.8e-4`. Similarly set **rl** to `6.2e-4` and then both **z0** and **zl** to `3e-4`.

8 Click **OK** (this reproduces Figure 5-4).

Piezoelectric Shear Actuated Beam

Introduction

This example performs a static analysis on a piezoelectric actuator based on the movement of a cantilever beam, using the static 3D Piezo Solid application mode. Inspired by work done by V. Piefort (Ref. 1) and A. Benjeddou (Ref. 2), it models a sandwich beam using the shear mode of the piezoelectric material to deflect the tip.

Model Definition

GEOMETRY

The model consists of a sandwiched cantilever beam 100 mm long; it consists of a rigid foam core 2 mm thick sandwiched by two 8-mm thick aluminum layers. Further, the device replaces part of the foam core with a 10-mm long piezoceramic actuator that is positioned between z = 55 mm and z = 65 mm (Figure 5-5). The cantilever beam is orientated along the x-axis.

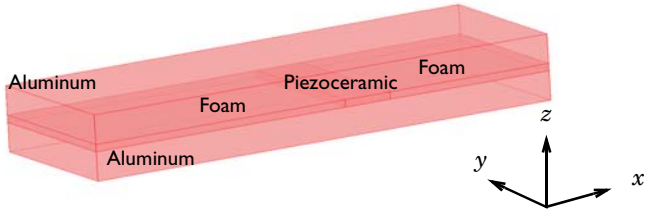


Figure 5-5: In this geometry for the shear bender note that a piezoceramic material replaces part of the foam core.

BOUNDARY CONDITIONS

- The structural mechanics boundary conditions for this model are that the cantilever beam is fixed at its surfaces at x = 0 and that all other surfaces are free.
- The electrostatic boundary conditions for this model are that the system applies a 20 V potential difference between the top and bottom surfaces of the piezoceramic subdomain. This gives rise to an electric field perpendicular to the poling direction (x-direction) and thus induces a transverse shear strain.

MATERIAL PROPERTIES

The following table lists the material properties for the aluminum layers and the foam core:

PROPERTY	ALUMINUM	FOAM
E	70 GPa	35.3 MPa
ν	0.345	0.383
ρ	2690 kg/m^3	32 kg/m^3

The matrices later in the section contain the material properties for the piezoceramic (PZT-5H): c_E is the elasticity matrix, e is the piezoelectric coupling matrix, and ε is the absolute permittivity matrix.

Note that it is necessary to recalculate the absolute permittivity matrix using the permittivity of vacuum ε_0 to the relative permittivity matrix.

Note also that the order of the material properties is such that the polarization direction is in the z direction. The polarization direction of the piezoceramic material in this model is however aligned with the x-axis and thus a local coordinate system must be used in the material settings to rotate the piezoceramic material.

$$c_E = \begin{bmatrix} 126 & 79.5 & 84.1 & 0 & 0 & 0 \\ & 126 & 84.1 & 0 & 0 & 0 \\ & & 117 & 0 & 0 & 0 \\ & & & 23.0 & 0 & 0 \\ & \text{sym} & & & 23.0 & 0 \\ & & & & & 23.3 \end{bmatrix} \text{ GPa}$$

$$e = \begin{bmatrix} 0 & 0 & 0 & 0 & 17 & 0 \\ 0 & 0 & 0 & 17 & 0 & 0 \\ -6.5 & -6.5 & 23.3 & 0 & 0 & 0 \end{bmatrix} \text{ C/m}^2$$

$$\varepsilon = \begin{bmatrix} 1.503 & 0 & 0 \\ 0 & 1.503 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \cdot 10^{-8} \text{ F/m}$$

Results

The shear deformation of the piezoceramic core layer and the flexible foam layer induce the bending action. Figure 5-6 shows the resulting tip deflection. The model calculates this deflection as 83 nm, which is in good agreement with the work in Ref. 1 and Ref. 2.

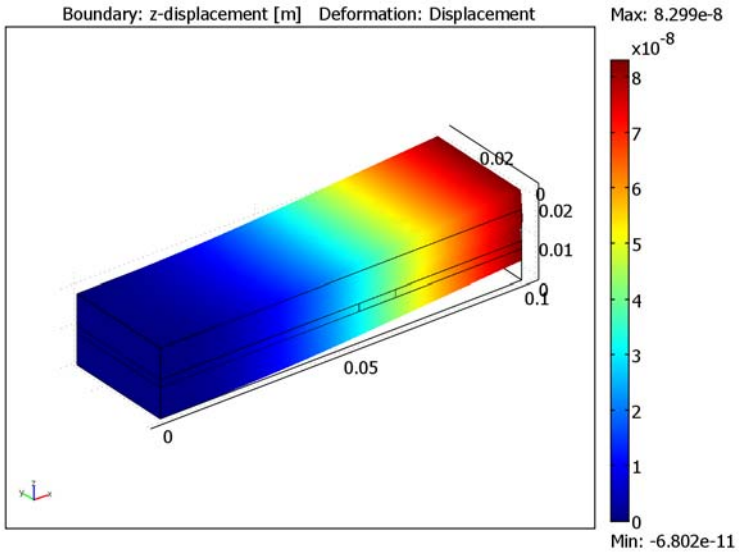


Figure 5-6: Tip deflection with the piezoceramic positioned at z = 60 mm.

Modeling in COMSOL Multiphysics

CONSTITUTIVE EQUATION AND MATERIAL DATA

You specify the material parameters for the piezoelectric material in the **Subdomain Settings** dialog box in the corresponding piezoelectric application mode. You select the stress-charge form for the constitutive equation because it suits the form in which you give the material data. Enter data for the elasticity matrix into the c_e matrix; enter data for the piezoelectric coupling matrix into the e matrix; and enter the relative permittivities into the ε_{rs} matrix.

You must also define a local coordinate system that is rotated 90 degrees about the y-axis. Then use this coordinate system n the piezoelectric material settings in order to rotate the material so that the poling direction is aligned with the x-axis.

MESHING

The thin central core that holds the piezoelectric actuator and the foam normally creates a relatively dense isotropic mesh. You can avoid this situation by scaling the mesh in the z direction with a factor of three. Doing so reduces the degrees of freedom from approximately 85,000 to 23,000 (by a factor of approximately 3.7) and hence it reduces both the solution time and memory requirements.

References

1. V. Piefort, *Finite Element Modelling of Piezoelectric Active Structures*, Ph.D. thesis, Université Libre de Bruxelles, Belgium, Dept. Mechanical Engineering and Robotics, 2001.

2. A. Benjeddou and others, *A Unified Beam Finite Element Model for Extension and Shear Piezoelectric Actuation Mechanisms*, CNAM (Paris, France), Structural Mechanics and Coupled Systems Laboratory, 1997.

Model Library path: `MEMS_Module/Piezo_Models/shear_bender`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start COMSOL Multiphysics. This invokes the **Model Navigator**, which you can also open from an already running COMSOL Multiphysics session by choosing **New** from the **File** menu.

2 On the **New** page select **3D** from the **Space dimension** list.

3 Click the **Multiphysics** button, then select **MEMS Module>Structural Mechanics>Piezo Solid>Static analysis** from the list of application modes.

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

Note that this gives you second-order elements, **Lagrange - Quadratic**, by default.

GEOMETRY MODELING

Define the model geometry in draw mode:

1 Draw a block by first clicking the **Block** button on the Draw toolbar and then entering the following parameters in the **Block** dialog box:

LENGTH	EXPRESSION
X	0.1
Y	0.03
Z	0.018

2 Draw a second block by clicking the **Block** button and entering the following parameters:

LENGTH	EXPRESSION
X	0.1
Y	0.03
Z	0.002

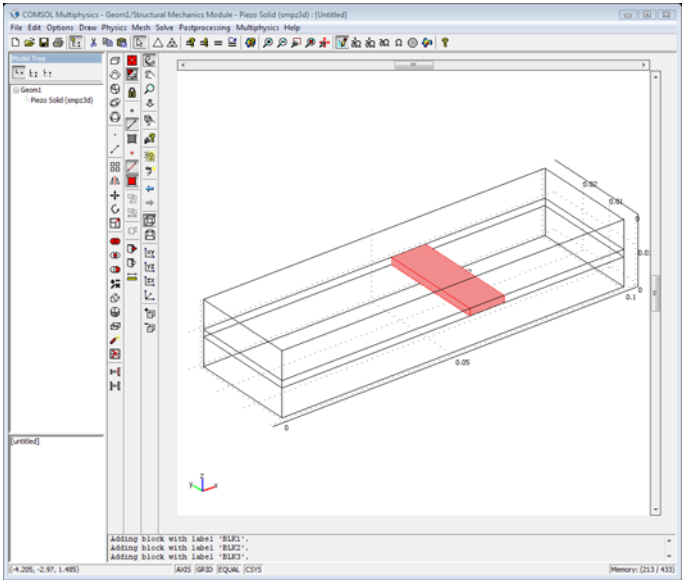
AXIS BASE POINT	EXPRESSION
x	0
y	0
z	0.008

3 Draw a third block by clicking the **Block** button and entering the following parameters:

LENGTH	EXPRESSION
X	0.01
Y	0.03
Z	0.002

AXIS BASE POINT	EXPRESSION
x	0.055
y	0
z	0.008

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



The basic geometry of the shear-actuated beam consisting of three blocks.

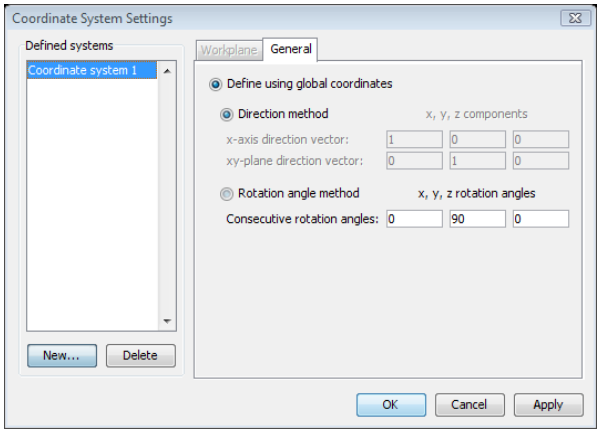
OPTIONS AND SETTINGS

1 From the **Options** menu choose **Coordinate Systems**.

2 In the **Coordinate System Settings** dialog box click the **New** button, then click **OK** in the **New Coordinate System** dialog box to use the default coordinate name.

3 Click the **General** tab. Click the **Define using global coordinates** option button, then click the **Rotation angle method** option button.

4 In the **x, y, z rotation angles** edit fields type `0`, `90`, and `0`, respectively, then click **OK** to close the dialog box.



Configuring the coordinate system.

The material properties for the foam and the aluminum are specified in the **Materials/ Coefficients Library** dialog box:

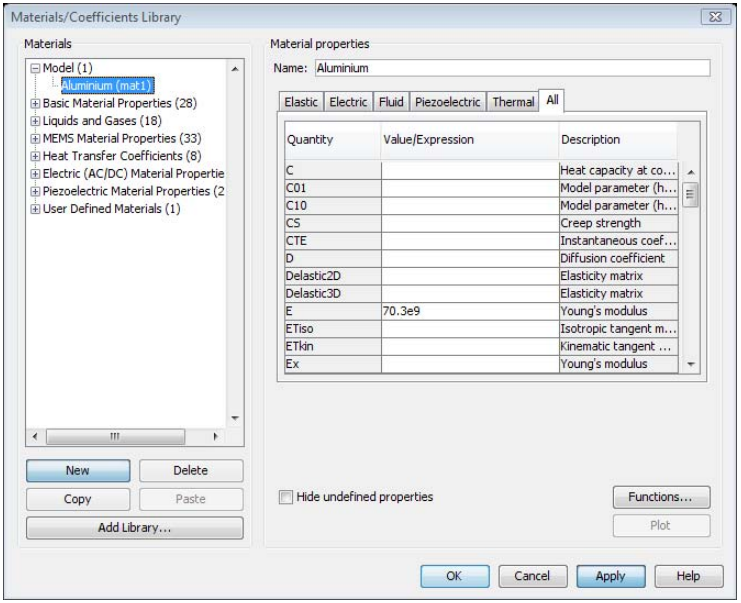
1 From the **Options** menu choose **Materials/Coefficients Library**.

2 Click the **New** button.

3 Change the **Name** to `Aluminum` and specify the following set of material parameters:

PARAMETER	EXPRESSION/VALUE	DESCRIPTION
E	70e9	Young's modulus
nu	0.345	Poisson's ratio
rho	2690	Density

4 Click **Apply**.

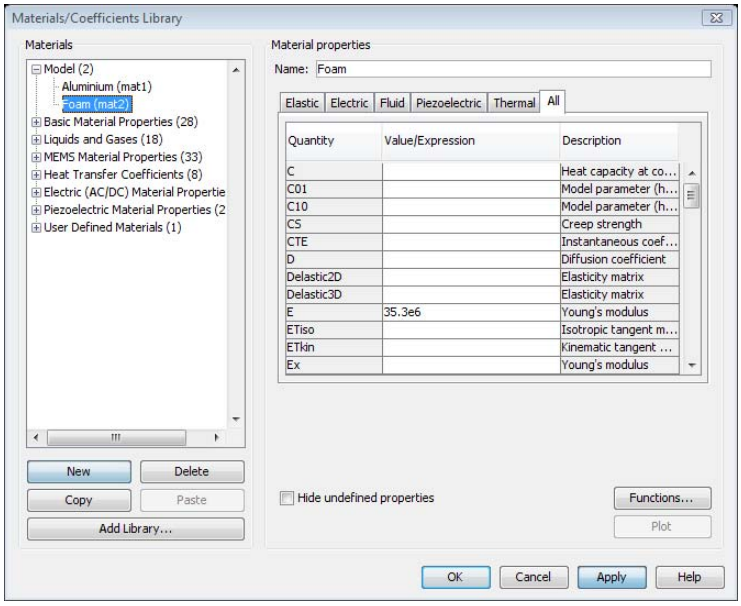


Material property values for aluminum.

5 Click the **New** button.

6 Change the **Name** to `Foam` and specify the following set of material parameters:

PARAMETER	EXPRESSION/VALUE	DESCRIPTION
E	35.3e6	Young's modulus
nu	0.383	Poisson's ratio
rho	32	Density



Material property values for foam.

7 Click **OK**.

PHYSICS SETTINGS

Subdomain Settings

1 Open the **Subdomain Settings** dialog box by choosing **Subdomain Settings** from the **Physics** menu. Go to the **Structural** page.

2 Select Subdomains 1 and 3 from the **Subdomain selection** list.

3 Select **Decoupled, isotropic** from the **Material model** list.

4 Select **Aluminum** from the **Library material** list; then click **Apply**.

5 Select Subdomains 2 and 5 from the **Subdomain selection** list.

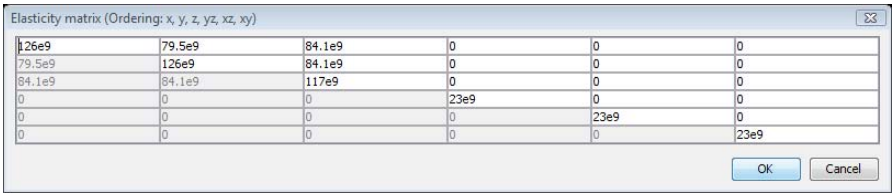
6 Select **Decoupled, isotropic** from the **Material model** list.

7 Select **Foam** from the **Library material** list; then click **Apply**.

8 Select Subdomain 4.

9 Select **Coordinate system 1** from the **Coordinate system** list.

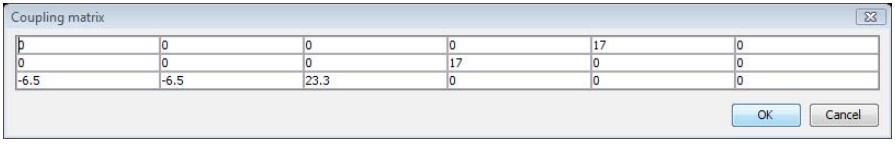
10 Click the **Edit** button associated with $\mathbf{c_E}$ and enter the following values into the **Elasticity matrix** dialog box; when complete, click **OK**.



126e9	79.5e9	84.1e9	0	0	0
	126e9	84.1e9	0	0	0
		117e9	0	0	0
			23e9	0	0
				23e9	0
					23e9

Entries for the elasticity matrix.

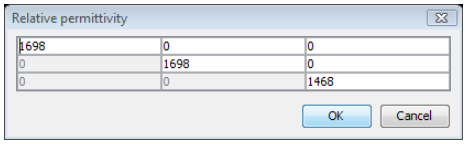
11 Click the **Edit** button associated with **e** and enter the following values into the **Coupling matrix, stress-charge form** dialog box; when complete, click **OK**.



0	0	0	0	17	0
0	0	0	17	0	0
-6.5	-6.5	23.3	0	0	0

Entries for the coupling matrix.

12 Click the **Edit** button associated with ε_{rs} and enter the following values into the **Relative permittivity matrix, stress-charge form** dialog box; when complete, click **OK**.



1698	0	0
	1698	
		1468

Entries for the relative permittivity matrix.

13 Click **OK**.

Boundary Conditions

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

2 Activate the **Interior boundaries** check box.

3 Fix the beam by selecting the following boundary condition on the **Constraint** page:.

SETTING	BOUNDARIES 1, 4, 7
Constraint condition	Fixed

4 Select Boundaries 14–19 from the **Boundary selection** list.

5 Go to the **Electric BC** page and select **Zero charge/Symmetry** from the **Boundary condition** list on the **Electric BC** page.

6 Select Boundary 16 and **Electric potential** from the **Boundary condition** list and enter 20 in the **Electric potential** edit field.

7 Select Boundary 17 and **Ground** from the **Boundary condition** list.

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

MESH GENERATION

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

2 Click the **Advanced** tab.

3 Type 3 in the **z-direction scale factor** edit field.

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

POSTPROCESSING AND VISUALIZATION

Before computing the solution change the default plot to display a boundary plot using the deformed shape:

1. From the **Postprocessing** menu choose **Plot Parameters**.
2. On the **General** page clear the **Slice** check box, then select the **Boundary** check box and the **Deformed shape** check box.
3. Click the **Boundary** tab and select **Piezo Solid (smpz3d)>z-displacement** from the **Predefined quantities** list.
4. Click **OK**.

COMPUTING THE SOLUTION

To start computing the solution, click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION, CONTINUED

Figure 5-6 on page 451 shows the resulting plot.

Composite Piezoelectric Transducer

Introduction

This example shows how to set up a piezoelectric transducer problem following the work of Y. Kagawa and T. Yamabuchi (Ref. 1). The composite piezoelectric ultrasonic transducer has a cylindrical geometry that consists of a piezoceramic (NEPEC 6) layer, two aluminum layers, and two adhesive layers. The layers are organized as follows: aluminum layer—adhesive layer—piezoceramic layer—adhesive layer—aluminum layer.

The system applies an AC potential on the electrode surfaces of both sides of the piezoceramic layer. The potential in this example has a peak value of 1V in the frequency range 20 kHz to 106 kHz. The goal is to compute the susceptance (the imaginary part of the admittance) $Y = I/V$, where I is the total current and V is the potential, for a frequency range around the four lowest eigenfrequencies of the structure.

The first step finds the eigenmodes, and the second step runs a frequency sweep across an interval that encompasses the first four eigenfrequencies. Both analyses are fully coupled, and COMSOL Multiphysics assembles and solves both the electric and mechanical parts of the problem simultaneously.

The problem is axially symmetric, and you could analyze it using an axisymmetric application mode in 2D. However, in order to illustrate the modeling principles for more complicated problems, this example is in 3D.

When creating the model geometry, you make use of the symmetry by first making a cut along a midplane perpendicular to the central axis and then cutting out a 10 degree wedge. Doing so reduces memory requirements significantly.

Results

Figure 5-7 shows the input admittance in the transducer as a function of the excitation frequency.

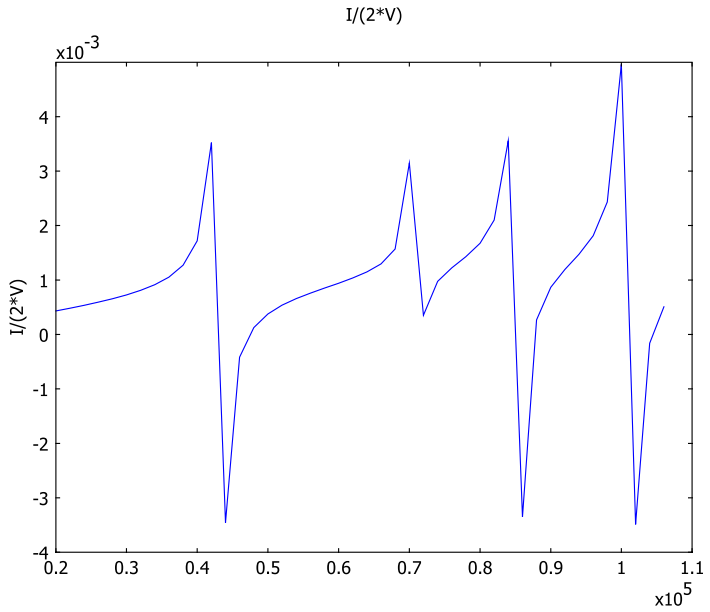


Figure 5-7: Input admittance as a function of excitation frequency

The result is in agreement with the work in Ref. 1. A small discrepancy close to the eigenfrequencies appears because the simulation uses no damping.

Reference

1. Y. Kagawa and T. Yamabuchi, "Finite Element Simulation of a Composite Piezoelectric Ultrasonic Transducer," *IEEE Transactions on Sonics and Ultrasonics*, vol. SU-26, no. 2, pp. 81–88, 1979.

Model Library path: `MEMS_Module/Piezo_Models/composite_transducer`

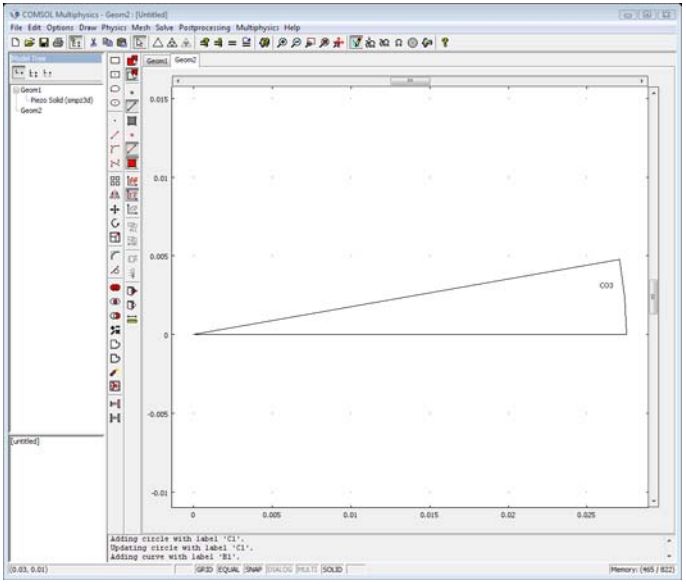
MODEL NAVIGATOR

1. Open the **Model Navigator** and click the **New** tab. From the **Space dimension** list select **3D**.
2. In the list of application modes select **MEMS Module>Structural Mechanics>Piezo Solid>Eigenfrequency analysis**.
3. Click **OK**.

GEOMETRY MODELING

1. From the **Draw** menu choose **Work Plane Settings**.
2. This model uses the default work plane at $z = 0$, so simply click **OK**. Doing so creates the work plane and opens a 2D drawing area.
3. Click the **Ellipse/Circle (Centered)** button on the Draw toolbar. Use the right mouse button to create a circle centered on the origin and with a radius of approximately 1 (the exact size is not important).
4. Double-click the circle. In the **Radius** edit field enter `27.5e-3`. Click **OK**.
5. Click the **Zoom Extents** button on the Main toolbar.
6. Click the **Line** button on the Draw toolbar. Draw a line from $(0, 0)$ to $(0.03, 0)$. Use the right mouse button to finish drawing lines.
7. Copy and paste the line onto itself with no displacements (either use Ctrl+C and Ctrl+V or use the **Edit** menu items).
8. Select the **Rotate** toolbar button from the Draw toolbar. In the **Rotation angle** edit field enter `10`. Click **OK**.
9. Select all objects (press Ctrl+A).
10. Click the **Coerce to Solid** button on the Draw toolbar.
11. Click the **Split Object** button on the Draw toolbar.
12. Select the larger object and press the Delete key.

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



Geometry for the composite piezoelectric transducer.

MESH GENERATION

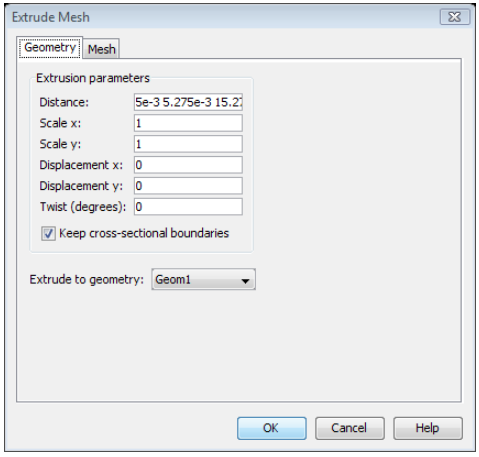
This model uses prism elements by extruding a triangular mesh.

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

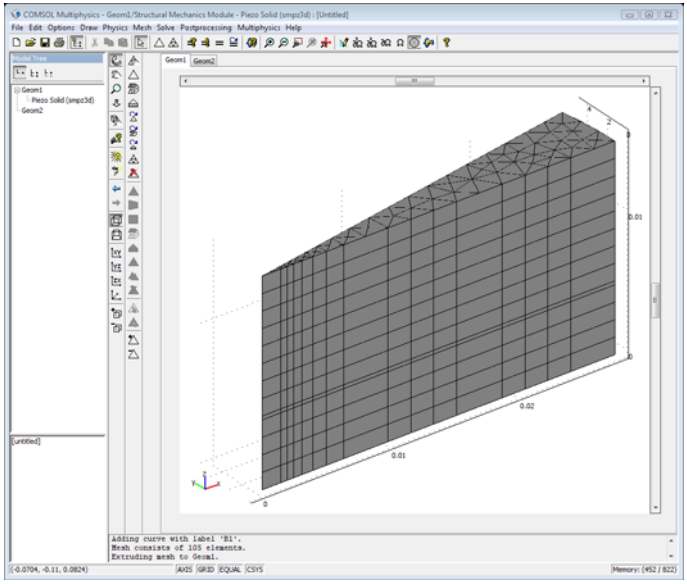
2 From the **Mesh** menu select **Extrude Mesh**.

3 In the **Distance** edit field enter `5e-3 5.275e-3 15.275e-3` (being careful to separate the entries with a space). Click **OK**. This step extrudes a mesh with three

domains corresponding to the piezoceramic (Subdomain 1), the adhesive layer (Subdomain 2), and the aluminum layer (Subdomain 3).



Extruding the mesh to create three subdomains.



The finalized mesh with the three subdomains.

OPTIONS AND SETTINGS

1 From the **Options** menu select **Materials/Coefficients Library**.

2 Click **New**.

3 Change the **Name** to `Adhesive`.

4 Enter these material properties; when done, click **Apply**.

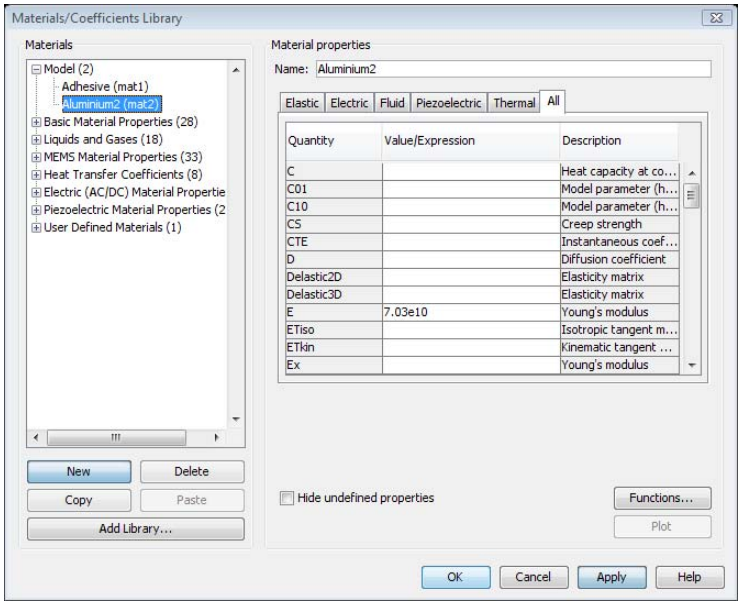
PARAMETER	EXPRESSION/VALUE	DESCRIPTION
E	1e10	Young's modulus
nu	0.38	Poisson's ratio
rho	1700	Density

5 Click the **New** button.

6 Change the name to `Aluminum2`.

7 Enter these material properties; when done, click **OK**.

PARAMETER	EXPRESSION/VALUE	DESCRIPTION
E	7.03e10	Young's modulus
nu	0.345	Poisson's ratio
rho	2690	Density



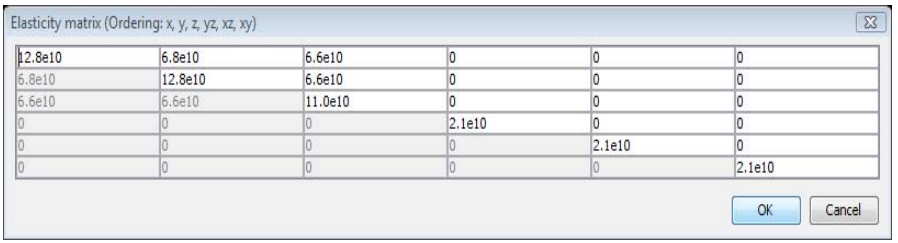
Material values to enter for the aluminum.

PHYSICS SETTINGS

Subdomain Settings

1. From the **Multiphysics** menu select **1 Geom1: Piezo Solid (smpz3d)**.
2. From the **Physics** menu select **Subdomain Settings** and go to the **Structural** page.
3. From the **Subdomain selection** list choose **1**.
4. See that the **Material Model** list has value **Piezoelectric**, then in the **Density** edit field enter 7730.

5 Click the **Edit** button associated with $\mathbf{c_E}$ and enter the following values into the **Elasticity matrix** dialog box; when finished, click **OK**:



12.8e10	6.8e10	6.6e10	0	0	0
	12.8e10	6.6e10	0	0	0
		11.0e10	0	0	0
			2.1e10	0	0
				2.1e10	0
					2.1e10

Entries for the elasticity matrix.

6 Click the **Edit** button associated with **e** and enter the following values into the **Coupling matrix, stress-charge form** dialog box; when finished, click **OK**:

0	0	0	0	0	0
0	0	0	0	0	0
-6.1	-6.1	15.7	0	0	0

Entries for the coupling matrix.

7 Click the **Edit** button associated with ε_{rS} and enter the following values into the **Relative permittivity, stress-charge form** dialog box; when finished, click **OK**:

993.53	0	0
	993.53	0
		993.53

Entries for the relative permittivity matrix.

8 In the **Subdomain selection** list choose Subdomains 2 and 3.

9 From the **Material Model** list select **Decoupled, isotropic**.

10 In the **Subdomain selection** list choose **2**.

11 Select **Adhesive** from the **Library material** list.

12 In the **Subdomain selection** list choose **3**.

13 Select **Aluminium2** from the **Library material** list.

14 Click **OK**.

Boundary Conditions

The total potential difference between the two electrodes (only one modeled here) is 1 V, but symmetry dictates that the potential is 0 V on the symmetry plane and 0.5 V on the electrode.

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

2 Activate the **Interior boundaries** check box.

3 In the **Boundary selection** list select all the boundaries (press Ctrl+A).

4 Go to the **Electric BC** page, find the **Boundary condition** list and select **Zero charge/ Symmetry**.

5 From the **Boundary selection** list choose Boundary 6.

6 In the **Boundary condition** list select **Electric potential**, and in the V_0 edit field type `0.5`.

7 Select Boundary 3.

8 Change the boundary condition on the **Electric BC** page to **Ground**.

9 From the **Boundary selection** list choose Boundaries 1, 2, 3, 4, 5, 7, and 8.

10 Go to the **Constraint** page, and in the **Constraint condition** list select **Symmetry plane**.

The outer boundary is free to move, so you do not set any constraints.

11 Click **OK**.

COMPUTING THE EIGENFREQUENCY SOLUTION

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

POSTPROCESSING AND VISUALIZATION OF THE EIGENFREQUENCIES

The lowest eigenfrequency is at approximately 43 kHz.

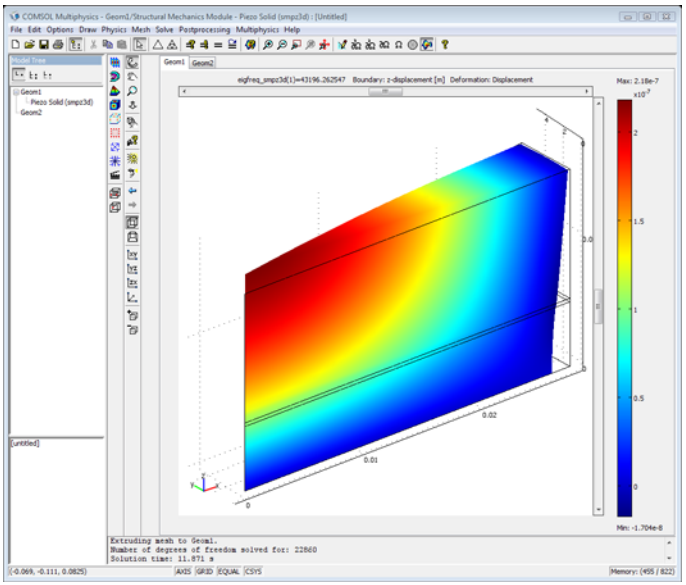
1 To visualize the solution of the lowest eigenfrequency, open the **Plot Parameters** dialog box from the **Postprocessing** menu.

2 On the **General** page, clear the **Slice** check box.

3 On the **Boundary** page, select the **Boundary plot** check box and select **Piezo Solid (smpz3d)>z-displacement (smpz3d)** in the **Predefined quantities** list.

4 On the **Deform** page, select the **Deformed shape plot** check box and see **Piezo Solid (smpz3d)>Displacement** in selected the **Predefined quantities** list.

5 Click **OK** to generate the visualization where you can see that the lowest eigenfrequency is at approximately 43 kHz.



Visualization of the lowest eigenfrequency for the piezoelectric transducer.

COMPUTING THE FREQUENCY RESPONSE SOLUTION

Next sweep over a frequency range from 20 kHz to 106 kHz in steps of 2 kHz.

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

2 In the **Analysis type** list select **Frequency response**. Click **OK**.

3 From the **Solve** menu select **Solver Parameters**.

4 On the **General** page see that the **Parameter name** edit field shows `freq_smpz3d`.

5 In the **Parameter values** edit field enter `20e3:2e3:106e3`.

6 Click **OK**.

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

POSTPROCESSING AND VISUALIZATION OF THE FREQUENCY RESPONSE

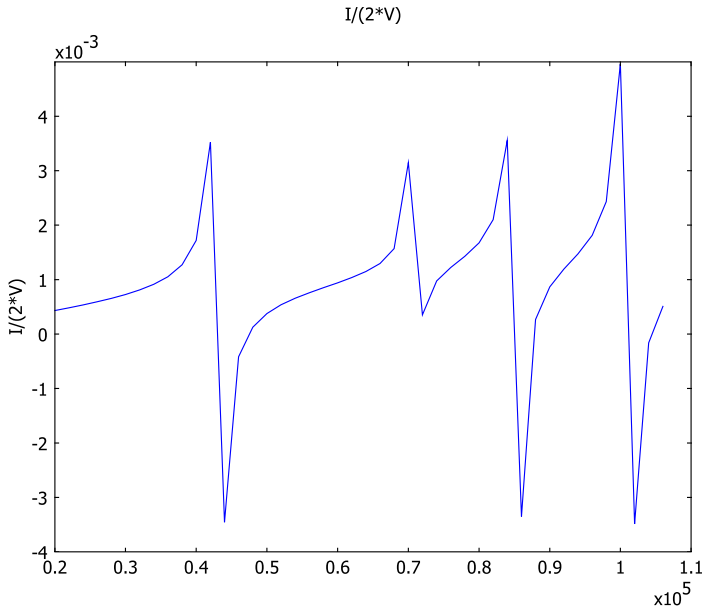
To compute the input admittance, use the current-density outflow variable, nJ, on the electrode surface. The total input current for the 10-degree wedge is then the surface integral of $-\text{imag}(nJ)$ over one of the electrode surfaces. To obtain the total current for the entire structure, multiply the result by 360/10 = 36.

1. From the **Options** menu select **Integration Coupling Variables>Boundary Variables**.
2. In the **Boundary selection** list choose Boundary 6 (corresponding to the electrode surface).
3. In the top row enter `I` as the name of the integration variable, then in the **Expression** column enter `-imag(nJ_smpz3d)*36`. Click **OK**.
4. From the **Solve** menu select **Update Model**.

The coupling variable `I` has global scope, and you can access it anywhere in the geometry model (the mesh). Use a domain plot to plot the value of Y versus frequency.

1. From the **Postprocessing** menu select **Domain Plot Parameters**.
2. Go to the **Point** page.
3. In the **Point selection** area choose a point on the electrode surface (for this exercise, select **2**).

4 In the **Expression** edit field enter `I/(2*V)`. Click **OK** to close the dialog box and plot the susceptance.



Plot of susceptance versus frequency for the piezoelectric transducer.

Recall that this example uses 0.5 V for the electrode potential but the overall potential difference is 1 V. Thus, to take symmetry into account, you must multiply the potential by 2.

INDEX