Exercise 1: Intro to COMSOL

Transport in Biological Systems

Fall 2015

Overview

In this course, we will consider transport phenomena in biological systems. Generally speaking, biological systems of interest have interesting geometries and we are interested in things happening in time and space. This means that analytical solutions can be challenging to find. Therefore, a modeling and simulation approach is often useful. Towards this, we will employ COMSOL in this course. It takes a little bit to get up to speed but it's a very powerful tool.

You will work on this in class (AC318) on September 3rd, the first day of class. Alisha will not be present, but you should all work as a group on this. Please try to complete the first 3 training items before class.

Training

- 1. Install COMSOL on your computer if you haven't (http://wikis.olin.edu/it/doku.php?id=comsol).
- 2. Read: http://cdn.comsol.com/documentation/5.1.0.180/IntroductionToCOMSOLMultiphysics.pdf
- 3. Watch: https://www.comsol.com/blogs/how-to-use-comsol-multiphysics-a-tutorial-video/
- 4. Attend the COMSOL training from 9:30-12:30 on September 17th. (Note: I know a few of you have class before this one. Please come as soon as you can. If it is acceptable for your other class to leave early on that day, it would be great, but I also understand if you can't.)

Exercises

1. Make a smiley face (Figure 1). Hint: think about using ellipses and intersections, not lines for the smile.

2. Make a hollow sphere with holes in it (Figure 2). Don't worry about dimensions, just the general concept.



Figure 2: A hollow sphere with holes.

3. Do the 3 exercises attached at the end of this document. (credit: COMSOL)

Objectives and Deliverables

The objective of this course is for you to apply concepts and skills in modeling and simulation to problems in biological transport. The objectives of this particular exercise are to gain practice using COMSOL. Complete the exercises and provide figures showing the final results for the exercises you have completed. It doesn't have to be anything pretty. Your results are due by September 21st.

Heat Sink

Introduction

This example is intended as a first introduction to simulations of fluid flow and conjugate heat transfer. It shows the following important points:

- How to draw an air box around a device in order to model convective cooling in this box.
- How to set a total heat flux on a boundary using automatic area computation.
- How to display results in an efficient way using selections in data sets.

The application is also described in detail in the book *Introduction to the Heat Transfer Module*. An extension of the application that takes surface-to-surface radiation into account is also available; see Heat Sink with Surface-to-Surface Radiation.



Figure 1: The application set-up including channel and heat sink.

Model Definition

The modeled system consists of an aluminum heat sink for cooling of components in electronic circuits mounted inside a channel of rectangular cross section (see Figure 1).

Such a set-up is used to measure the cooling capacity of heat sinks. Air enters the channel at the inlet and exits the channel at the outlet. The base surface of the heat sink receives a 1 W heat flux from an external heat source. All other external faces are thermally insulated.

The cooling capacity of the heat sink can be determined by monitoring the temperature of the base surface of the heat sink.

The model solves a thermal balance for the heat sink and the air flowing in the rectangular channel. Thermal energy is transported through conduction in the aluminum heat sink and through conduction and convection in the cooling air. The temperature field is continuous across the internal surfaces between the heat sink and the air in the channel. The temperature is set at the inlet of the channel. The base of the heat sink receives a 1 W heat flux. The transport of thermal energy at the outlet is dominated by convection.

The flow field is obtained by solving one momentum balance for each space coordinate (x, y, and z) and a mass balance. The inlet velocity is defined by a parabolic velocity profile for fully developed laminar flow. At the outlet, the normal stress is equal the outlet pressure and the tangential stress is canceled. At all solid surfaces, the velocity is set to zero in all three spatial directions.

The thermal conductivity of air, the heat capacity of air, and the air density are all temperature-dependent material properties.

You can find all of the settings mentioned above in the predefined multiphysics coupling for Conjugate Heat Transfer in COMSOL Multiphysics. You also find the material properties, including their temperature dependence, in the Material Browser.

Results

In Figure 2, the hot wake behind the heat sink visible in the plot is a sign of the convective cooling effects. The maximum temperature, reached at the heat sink base, is about 380 K.





Figure 2: The surface plot shows the temperature field on the channel walls and the heat sink surface, while the arrow plot shows the flow velocity field around the heat sink.

Application Library path: Heat_Transfer_Module/ Tutorials,_Forced_and_Natural_Convection/heat_sink

Modeling Instructions

From the File menu, choose New.

NEW

I In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 3D.
- 2 In the Select physics tree, select Heat Transfer>Conjugate Heat Transfer>Laminar Flow.
- 3 Click Add.
- 4 Click Study.
- 5 In the Select study tree, select Preset Studies for Selected Physics Interfaces>Stationary.
- 6 Click Done.

GEOMETRY I

The model geometry is available as a parameterized geometry sequence in a separate MPH-file. If you want to build it from scratch, follow the instructions in the section Appendix: Geometry Modeling Instructions. Otherwise load it from file with the following steps.

- I On the Geometry toolbar, click Insert Sequence.
- 2 Browse to the application's Application Library folder and double-click the file heat_sink_geom_sequence.mph.

The application's Application Library folder is shown in the **Application Library path** section immediately before the current section. Note that the path given there is relative to the COMSOL Application Library root, which for a standard installation on Windows is C:\Program

Files\COMSOL\COMSOL50\Multiphysics\applications.

Import I (imp1)

- I Click the Go to Default 3D View button on the Graphics toolbar.
- 2 On the Geometry toolbar, click Build All.

To facilitate face selection in the next steps, use the **Wireframe rendering** option (skip this step if you followed the instructions in the appendix):



3 Click the Wireframe Rendering button on the Graphics toolbar.

LAMINAR FLOW (SPF)

Since the density variation is not small, the flow can not be regarded as incompressible. Therefore set the flow to be compressible.

- I In the Model Builder window, under Component I (compl) click Laminar Flow (spf).
- 2 In the Settings window for Laminar Flow, locate the Physical Model section.
- 3 From the Compressibility list, choose Compressible flow (Ma<0.3).

Create a selection for the air domain used the physics interfaces to define the fluid.

- 4 Locate the Domain Selection section. In the Selection list, choose 2 and 3.
- **5** Click Create Selection.
- 6 In the Create Selection dialog box, type Air in the Selection name text field.
- 7 Click OK.

HEAT TRANSFER (HT)

On the Physics toolbar, click Laminar Flow (spf) and choose Heat Transfer (ht).

Heat Transfer in Fluids 1

- I In the Model Builder window, under Component I (compl)>Heat Transfer (ht) click Heat Transfer in Fluids I.
- **2** In the **Settings** window for Heat Transfer in Fluids, locate the **Domain Selection** section.
- 3 From the Selection list, choose Air.

MATERIALS

Next, add materials.

ADD MATERIAL

- I On the Home toolbar, click Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-In>Air.
- 4 Click Add to Component in the window toolbar.

MATERIALS

Air (mat1)

- I In the Model Builder window, under Component I (compl)>Materials click Air (matl).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Air.

ADD MATERIAL

- I Go to the Add Material window.
- 2 In the tree, select Built-In>Aluminum 3003-H18.
- 3 Click Add to Component in the window toolbar.

MATERIALS

Aluminum 3003-H18 (mat2)

- I In the Model Builder window, under Component I (compl)>Materials click Aluminum 3003-H18 (mat2).
- **2** Select Domain 2 only.

ADD MATERIAL

I Go to the Add Material window.

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- 2 In the tree, select Built-In>Silica glass.
- 3 Click Add to Component in the window toolbar.

MATERIALS

Silica glass (mat3)

- I In the Model Builder window, under Component I (compl)>Materials click Silica glass (mat3).
- **2** Select Domain 3 only.
- 3 On the Home toolbar, click Add Material to close the Add Material window.

Material 4 (mat4)

- I In the Model Builder window, right-click Materials and choose Blank Material.
- 2 In the Settings window for Material, type Thermal Grease in the Label text field.
- **3** Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 34 only.
- 5 Click to expand the Material properties section. Locate the Material Properties section. In the Material properties tree, select Basic Properties>Thermal Conductivity.
- 6 Click Add to Material.
- 7 Locate the Material Contents section. In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	2[W/m/K]	W/(m·K)	Basic

GLOBAL DEFINITIONS

Parameters

- I In the Model Builder window, expand the Global Definitions node, then click Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
UO	5[cm/s]	0.05 m/s	Mean inlet velocity

Name	Expression	Value	Description
Т0	20[degC]	293.2 K	Inlet temperature
P0	1[W]	IW	Total power dissipated by the electronics package

Now define the physical properties of the model. Start with the fluid domain.

LAMINAR FLOW (SPF)

On the Physics toolbar, click Heat Transfer (ht) and choose Laminar Flow (spf).

The no-slip condition is the default boundary condition for the fluid. Define the inlet and outlet conditions as described below.

Inlet 1

- I On the Physics toolbar, click Boundaries and choose Inlet.
- **2** Select Boundary 121 only.
- 3 In the Settings window for Inlet, locate the Boundary Condition section.
- 4 From the list, choose Laminar inflow.
- **5** Locate the Laminar Inflow section. In the U_{av} text field, type U0.

Outlet I

- I On the Physics toolbar, click Boundaries and choose Outlet.
- 2 Click the Zoom Extents button on the Graphics toolbar.
- **3** Select Boundary 1 only.

HEAT TRANSFER (HT)

Thermal insulation is the default boundary condition for the temperature. Define the inlet temperature and the outlet condition as described below.

Temperature 1

- I On the Physics toolbar, click Boundaries and choose Temperature.
- **2** Select Boundary 121 only.
- 3 In the Settings window for Temperature, locate the Temperature section.
- **4** In the T_0 text field, type T0.

Outflow I

- I On the Physics toolbar, click Boundaries and choose Outflow.
- **2** Select Boundary 1 only.

Next, use the P0 parameter to define the total heat source in the electronics package.

Heat Source 1

- I On the Physics toolbar, click Domains and choose Heat Source.
- **2** Select Domain 3 only.
- 3 In the Settings window for Heat Source, locate the Heat Source section.
- 4 Click the **Overall heat transfer rate** button.
- **5** In the P_0 text field, type P0.

Finally, add the thin thermal grease layer.

Thin Layer I

- I On the Physics toolbar, click Boundaries and choose Thin Layer.
- **2** Select Boundary 34 only.
- 3 In the Settings window for Thin Layer, locate the Thin Layer section.
- 4 In the d_s text field, type 50[um].

MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Mesh Settings section.
- 3 From the Element size list, choose Extra coarse.
- 4 Click the **Build All** button.

To get a better view of the mesh, hide some of the boundaries.

- 5 Click the Click and Hide button on the Graphics toolbar.
- 6 Click the Select Boundaries button on the Graphics toolbar.

7 Select Boundaries 1, 2, and 4 only.

The finished mesh should look like that in the figure below.



To achieve more accurate numerical results, this mesh can be refined by choosing another predefined element size. However, doing so requires more computational time and memory.

STUDY I

On the Home toolbar, click Compute.

RESULTS

Temperature (ht)

Four default plots are generated automatically. The first one shows the temperature on the wall boundaries, the third one shows the velocity magnitude on five parallel slices, the last one shows the pressure field and. Add an arrow plot to visualize the velocity field with temperature field.

I In the Model Builder window, under Results right-click Temperature (ht) and choose Arrow Volume.

- In the Settings window for Arrow Volume, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component l>Laminar Flow>u,v,w Velocity field.
- **3** Locate the **Arrow Positioning** section. Find the **x grid points** subsection. In the **Points** text field, type **40**.
- 4 Find the y grid points subsection. In the Points text field, type 20.
- 5 Find the z grid points subsection. From the Entry method list, choose Coordinates.
- 6 In the **Coordinates** text field, type 5[mm].
- 7 Right-click Results>Temperature (ht)>Arrow Volume I and choose Color Expression.
- 8 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Laminar Flow>spf.U Velocity magnitude.
- 9 On the Temperature (ht) toolbar, click Plot.

Derived Values

- I On the Results toolbar, click Global Evaluation.
- 2 In the Settings window for Global Evaluation, type Net Energy Rate in the Label text field.
- 3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Heat Transfer>Global>Net powers>ht.ntefluxInt - Total net energy rate.
- 4 Click the **Evaluate** button.

TABLE

Go to the **Table** window.

RESULTS

Derived Values

- I On the Results toolbar, click Global Evaluation.
- 2 In the Settings window for Global Evaluation, type Heat Source in the Label text field.
- 3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Heat Transfer>Global>Heat source powers>ht.Qlnt Total heat source.
- 4 Click the **Evaluate** button.

TABLE

I Go to the **Table** window.

The total rate of net energy and heat generation should be close to 1 W.

Appendix: Geometry Modeling Instructions

ROOT

On the Home toolbar, click Add Component and choose 3D.

GLOBAL DEFINITIONS

First define the geometry parameters.

Parameters

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

Name	Expression	Value	Description
L_channel	7[cm]	0.07 m	Channel length
W_channel	3[cm]	0.03 m	Channel width
H_channel	1.5[cm]	0.015 m	Channel height
L_chip	1.5[cm]	0.015 m	Chip size
H_chip	2[mm]	0.002 m	Chip height

GEOMETRY I

Build the geometry in three steps. First, import the heat sink geometry from a file.

Import I (imp1)

- I On the Home toolbar, click Import.
- 2 In the Settings window for Import, locate the Import section.
- 3 Click Browse.
- **4** Browse to the application's Application Library folder and double-click the file heat_sink.mphbin.
- 5 Click Import.

6 Click the Wireframe Rendering button on the Graphics toolbar.

Next, define a work plane containing the bottom surface of the heat sink to draw the imprints of the chip and of the air channel.

Work Plane I (wp1)

- I On the Geometry toolbar, click Work Plane.
- 2 In the Settings window for Work Plane, locate the Plane Definition section.
- 3 From the Plane type list, choose Face parallel.
- 4 Find the Planar face subsection. Select the Active toggle button.
- **5** Select the surface shown in the figure below.



6 Locate the Unite Objects section. Clear the Unite objects check box.

Square 1 (sq1)

- I On the Work Plane toolbar, click Primitives and choose Square.
- 2 In the Settings window for Square, locate the Size section.
- 3 In the Side length text field, type L_Chip.
- 4 Locate the Position section. From the Base list, choose Center.

- 5 Right-click Component I (comp1)>Geometry I>Work Plane I (wp1)>Plane Geometry>Square I (sq1) and choose Build Selected.
- 6 Click the Zoom Extents button on the Graphics toolbar.

Rectangle 1 (r1)

- I On the Work Plane toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size section.
- 3 In the Width text field, type L_channel.
- 4 In the **Height** text field, type W_channel.
- **5** Locate the **Position** section. In the **xw** text field, type -45[mm].
- 6 In the **yw** text field, type -W_channel/2.
- 7 Right-click Component I (compl)>Geometry I>Work Plane I (wpl)>Plane Geometry>Rectangle I (rl) and choose Build Selected.

Now extrude the chip imprint to define the chip volume.

Extrude I (extI)

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

Distances (m)

H chip

- 5 Right-click Component I (compl)>Geometry l>Extrude I (extl) and choose Build Selected.
- 6 Click the **Zoom Extents** button on the **Graphics** toolbar.

To finish the geometry, extrude the channel imprint in the opposite direction to define the air volume.

Extrude 2 (ext2)

- I On the Geometry toolbar, click Extrude.
- 2 Select the object wpl.rl only.
- 3 In the Settings window for Extrude, locate the Distances from Plane section.

4 In the table, enter the following settings:

Distances (m)

H_channel

5 Select the **Reverse direction** check box.

6 Click the **Build All Objects** button.

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

The model geometry is now complete.

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Cooling and Solidification of Metal

Introduction

This example is a model of a continuous casting process. Liquid metal is poured into a mold of uniform cross section. The outside of the mold is cooled and the metal solidifies as it flows through the mold. When the metal leaves the mold, it is completely solidified on the outside but still liquid inside. The metal then continues to cool and eventually solidify completely, at which point it can be cut into sections. This tutorial simplifies the problem somewhat by not computing the flow field of the liquid metal and assuming there is no volume change at solidification. It is also assumed that the velocity of the metal is constant and uniform throughout the modeling domain. The phase transition from molten to solid state is modeled via the apparent heat capacity formulation. Issues of convergence and mesh refinement are addressed for this highly nonlinear model.

The Continuous Casting application is similar to this one, except that the velocity is computed from the Laminar Flow interface instead of being considered constant and uniform. For a detailed description of the application, see Continuous Casting.



Figure 1: A continuous casting process. The section where the metal is solidifying is being modeled.

Model Overview

The model simplifies the 3D geometry of the continuous casting to a 2D axisymmetric model composed of two rectangular regions: one representing the strand within the mold, and one the spray cooled region outside of the mold, prior to the saw cutoff. In the second section, there is also significant cooling via radiation to the ambient. In this region it is assumed that the molten metal is in a hydrostatic state, that the only motion in the fluid is due to the bulk downward motion of the strand. This simplification allows the assumption of bulk motion throughout the domain.

Since this is a continuous process, the system can be modeled at steady state. The heat transport is described by the equation:

$$\nabla \cdot (-k\nabla T) = -\rho C_n \mathbf{u} \cdot \nabla T$$

where k and C_p denote thermal conductivity and specific heat, respectively. The velocity, **u**, is the fixed casting speed of the metal in both liquid and solid states.

As the metal cools down in the mold, it solidifies. During the phase transition, a significant amount of latent heat is released. The total amount of heat released per unit mass of alloy during the transition is given by the change in enthalpy, ΔH . In addition, the specific heat capacity, C_p , also changes considerably during the transition. The difference in specific heat before and after transition can be approximated by

$$\Delta C_p = \frac{\Delta H}{T}$$

As opposed to pure metals, an alloy generally undergoes a broad temperature transition zone, over several Kelvin, in which a mixture of both solid and molten material co-exist in a "mushy" zone. To account for the latent heat related to the phase transition, the Apparent Heat capacity method is used through the Heat Transfer with Phase Change domain condition. The objective of the analysis is to make ΔT , the half-width of the transition interval small, such that the solidification front location is well defined.

Table 1 reviews the material properties in this tutorial.

TABLE I: MATERIAL PROPERTIES

PROPERTY	SYMBOL	MELT	SOLID
Density	$\rho \text{ (kg/m}^3\text{)}$	8500	8500

2 | COOLING AND SOLIDIFICATION OF METAL

PROPERTY	SYMBOL	MELT	SOLID
Heat capacity at constant pressure	C_p (J/(kg·K))	531	380
Thermal conductivity	$k \; (W/(m \cdot K))$	150	300

The melting temperature, $T_{\rm m}$, and enthalpy, ΔH , are 1356 K and 205 kJ/kg, respectively.

This example is a highly nonlinear problem and benefits from taking an iterative approach to finding the solution. The location of the transition between the molten and solid state is a strong function of the casting velocity, the cooling rate in the mold, and the cooling rate in the spray cooled region. A fine mesh is needed across the solidification front to resolve the change in material properties. However, it is not known where this front will be.

By starting with a gradual transition between liquid and solid, it is possible to find a solution even on a relatively coarse mesh. This solution can be used as the starting point for the next step in the solution procedure, which uses a sharper transition from liquid to solid. This is done using the continuation method. Given a monotonic list of values to solve for, the continuation method uses the solution to the last case as the starting condition for the next. Once a solution is found for the smallest desired ΔT , the adaptive mesh refinement algorithm is used to refine the mesh to put more elements around the transition region. This finer mesh is then used to find a solution with an even sharper transition. This can be repeated as needed to get better and better resolution of the location of the solidification front.

In this example, the parameter ΔT is first ramped down from 300 K to 75 K, then the adaptive mesh refinement is used such that a finer mesh is used around the solidification front. The resultant solution and mesh are then used as starting points for a second study, where the parameter ΔT is further ramped down from 50 K to 25 K. The double-dogleg solver is used to find the solution to this highly nonlinear problem. Although it takes more time, this solver converges better in cases when material properties vary strongly with respect to the solution.

Results and Discussion

The solidification front computed with the coarsest mesh, and for $\Delta T = 75$ K, is shown in Figure 2. A wide transition between the molten and solid state is observed. The adaptive mesh refinement algorithm then refines the mesh along the solidification front because this is the region where the results are strongly dependent upon mesh size. This solution, and refined mesh, is used as the starting point for the next solution, which ramps the ΔT parameter down to 25 K. These results are shown in Figure 3.

The point of complete solidification moves slightly as the transition zone is made smaller. As the transition zone becomes smaller, a finer mesh is needed, otherwise the model might not converge. If it is desired to get an even better resolution of the solidification front, the solution procedure used here should be repeated to get an even finer mesh, and further ramp down the ΔT parameter.

The liquid phase fraction is plotted along the *r*-direction at the line at the bottom of the mold in Figure 4, and Figure 5 shows the liquid fraction along the centerline of the strand. For smaller values of ΔT , the transition becomes sharper, and the model gives confidence that the metal is completely solidified before the strand is cut.



Figure 2: The fraction of liquid phase for $\Delta T = 75$ K shows a gradual transition between the liquid and solid phase.



Figure 3: The fraction of liquid phase for $\Delta T = 25$ K shows a sharp transition between the liquid and solid phase.



Figure 4: The fraction of liquid phase through the radius for all values of ΔT . For smaller values of ΔT , the transition is sharper.



Figure 5: The fraction of liquid phase along the centerline for all values of ΔT . For smaller values of ΔT , the transition is sharper.

Application Library path: Heat_Transfer_Module/Thermal_Processing/ cooling solidification metal

Modeling Instructions

From the File menu, choose New.

NEW

I In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 2D Axisymmetric.
- 2 In the Select physics tree, select Heat Transfer>Heat Transfer in Fluids (ht).
- 3 Click Add.
- 4 Click Study.

- 5 In the Select study tree, select Preset Studies>Stationary.
- 6 Click Done.

GLOBAL DEFINITIONS

First, set up parameters and variables used in the continuous casting process model analysis.

Parameters

- I On the Home toolbar, click Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** Click Load from File.
- **4** Browse to the application's Application Library folder and double-click the file cooling_solidification_metal_parameters.txt.

GEOMETRY I

Create two rectangles representing the strand within the mold, and spray cooled region outside of the mold.

Rectangle 1 (r1)

- I On the Geometry toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size section.
- **3** In the **Width** text field, type **0.1**.
- 4 In the **Height** text field, type 0.6.

Rectangle 2 (r2)

- I On the Geometry toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size section.
- **3** In the **Width** text field, type **0.1**.
- 4 In the **Height** text field, type 0.2.
- **5** Locate the **Position** section. In the **z** text field, type **0.6**.
- 6 Click the Build All Objects button.



7 Click the Zoom Extents button on the Graphics toolbar.

MATERIALS

Material I (mat1)

- I In the Model Builder window, under Component I (compl) right-click Materials and choose Blank Material.
- 2 In the Settings window for Material, type Solid Metal Alloy in the Label text field.
- 3 Locate the Material Contents section. In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	300	W/(m·K)	Basic
Density	rho	8500	kg/m³	Basic
Heat capacity at constant pressure	Ср	Cp_s	J/(kg·K)	Basic
Ratio of specific heats	gamma	1	I	Basic

Material 2 (mat2)

- I In the Model Builder window, right-click Materials and choose Blank Material.
- 2 In the **Settings** window for Material, type Liquid Metal Alloy in the **Label** text field.
- **3** Select Domains 1 and 2 only.

Property	Name	Value	Unit	Property group
Thermal conductivity	k	150	W/(m·K)	Basic
Density	rho	8500	kg/m³	Basic
Heat capacity at constant pressure	Ср	Cp_1	J/(kg·K)	Basic
Ratio of specific heats	gamma	1	1	Basic

4 Locate the Material Contents section. In the table, enter the following settings:

Set up the physics.

HEAT TRANSFER IN FLUIDS (HT)

Initial Values 1

- I In the Model Builder window, under Component I (compl)>Heat Transfer in Fluids (ht) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- 3 In the *T* text field, type T_in.

Heat Transfer with Phase Change I

- I On the Physics toolbar, click Domains and choose Heat Transfer with Phase Change.
- **2** Select Domains 1 and 2 only.
- **3** In the **Settings** window for Heat Transfer with Phase Change, locate the **Model Inputs** section.
- 4 Specify the **u** vector as

0	r
-v_cast	z

- **5** Locate the **Phase Change** section. In the $T_{\text{pc},1 \rightarrow 2}$ text field, type T_m.
- **6** In the $\Delta T_{1 \rightarrow 2}$ text field, type dT.
- 7 In the $L_{1 \rightarrow 2}$ text field, type dH.
- 8 Locate the Phase I section. From the Material, phase I list, choose Solid Metal Alloy (mat1).
- 9 Locate the Phase 2 section. From the Material, phase 2 list, choose Liquid Metal Alloy (mat2).

Temperature 1

I On the Physics toolbar, click Boundaries and choose Temperature.



2 Select Boundary 5 only.

- 3 In the Settings window for Temperature, locate the Temperature section.
- **4** In the T_0 text field, type T_in.

Heat Flux 1

I On the Physics toolbar, click Boundaries and choose Heat Flux.



2 Select Boundary 7 only.

- 3 In the Settings window for Heat Flux, locate the Heat Flux section.
- **4** Click the **Convective heat flux** button.
- **5** In the *h* text field, type h_mold.
- **6** In the T_{ext} text field, type T0.

Heat Flux 2

I On the Physics toolbar, click Boundaries and choose Heat Flux.



2 Select Boundary 6 only.

- 3 In the Settings window for Heat Flux, locate the Heat Flux section.
- 4 Click the **Convective heat flux** button.
- 5 In the *h* text field, type h_spray.
- **6** In the $T_{\rm ext}$ text field, type T0.

Diffuse Surface I

- I On the Physics toolbar, click Boundaries and choose Diffuse Surface.
- **2** Select Boundary 6 only.
- 3 In the Settings window for Diffuse Surface, locate the Surface Emissivity section.
- **4** From the ε list, choose **User defined**. In the associated text field, type eps_s.
- **5** Locate the **Ambient** section. In the T_{amb} text field, type T0.

Outflow I

I On the Physics toolbar, click Boundaries and choose Outflow.



2 Select Boundary 2 only.

MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Mesh Settings section.
- 3 From the Element size list, choose Extremely fine.

STUDY I

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, locate the Study Settings section.
- **3** Clear the **Generate default plots** check box.

Step 1: Stationary

Set up an auxiliary continuation sweep for the dT parameter.

- I In the Model Builder window, under Study I click Step I: Stationary.
- 2 In the Settings window for Stationary, click to expand the Study extensions section.
- **3** Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 4 Click Add.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Ъ	300 200 150 100 75	

6 Select the Adaptive mesh refinement check box.

Solution 1

- I On the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution I node.
- 3 In the Model Builder window, expand the Study I>Solver Configurations>Solution I>Stationary Solver I node, then click Adaptive Mesh Refinement.
- **4** In the **Settings** window for Adaptive Mesh Refinement, locate the **Mesh Refinement** section.
- 5 From the Refinement method list, choose Mesh initialization.
- 6 In the Model Builder window, under Study I>Solver Configurations>Solution I>Stationary Solver I click Fully Coupled I.
- 7 In the Settings window for Fully Coupled, click to expand the Method and termination section.
- 8 Locate the Method and Termination section. From the Nonlinear method list, choose Double dogleg.
- 9 On the Study toolbar, click Compute.

RESULTS

2D Plot Group 1

- I On the Home toolbar, click Add Plot Group and choose 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, type Solid and Liquid Phases (Adaptive Mesh) in the Label text field.

Solid and Liquid Phases (Adaptive Mesh)

- I Right-click Results>Solid and Liquid Phases (Adaptive Mesh) and choose Surface.
- 2 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Heat Transfer in Fluids>Phase change>ht.thetal Phase indicator, phase 1.
- 3 On the Solid and Liquid Phases (Adaptive Mesh) toolbar, click Plot.

The reproduced figure describes the fraction of liquid phase for $\Delta T = 75$ K.

ADD STUDY

- I On the Home toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select study tree, select Preset Studies.
- 4 In the Select study tree, select Preset Studies>Stationary.
- 5 Click Add Study in the window toolbar.

STUDY 2

Step 1: Stationary

- I On the Home toolbar, click Add Study to close the Add Study window.
- 2 In the Model Builder window, click Study 2.
- 3 In the Settings window for Study, locate the Study Settings section.
- 4 Clear the Generate default plots check box.
- 5 In the Model Builder window, click Step 1: Stationary.
- 6 In the Settings window for Stationary, click to expand the Values of dependent variables section.
- 7 Locate the Values of Dependent Variables section. Select the Initial values of variables solved for check box.
- 8 From the Method list, choose Solution.
- 9 From the Study list, choose Study I, Stationary.
- 10 From the Solution list, choose Adaptive Mesh Refinement 1.
- II From the Parameter value (dT) list, choose 75.
- 12 Click to expand the Mesh selection section. Locate the Study Extensions section. Select the Auxiliary sweep check box.
- I3 Click Add.

I4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
dT	50 25	

Solution 3

- I On the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution 3 node.

- 3 In the Model Builder window, expand the Study 2>Solver Configurations>Solution
 3>Stationary Solver I node, then click Fully Coupled I.
- **4** In the **Settings** window for Fully Coupled, locate the **Method and Termination** section.
- 5 From the Nonlinear method list, choose Double dogleg.
- 6 On the Study toolbar, click Compute.

RESULTS

2D Plot Group 2

- I On the Home toolbar, click Add Plot Group and choose 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, type Solid and Liquid Phases in the Label text field.
- 3 Locate the Data section. From the Data set list, choose Study 2/Solution 3.

Solid and Liquid Phases

- I Right-click Results>Solid and Liquid Phases and choose Surface.
- In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Heat Transfer in Fluids>Phase change>ht.thetal Phase indicator, phase I.
- **3** On the Solid and Liquid Phases toolbar, click Plot.

This shows the fraction of liquid phase for $\Delta T = 25$ K.

ID Plot Group 3

- I On the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for 1D Plot Group, type Phase Indicator at Symmetry Axis in the Label text field.

Phase Indicator at Symmetry Axis

- I On the Phase Indicator at Symmetry Axis toolbar, click Line Graph.
- 2 Select Boundaries 1 and 3 only.
- 3 In the Settings window for Line Graph, locate the y-axis data section.
- 4 Click ht.thetal Phase indicator, phase I in the upper-right corner of the section. Locate the x-Axis Data section. From the Parameter list, choose Expression.
- **5** In the **Expression** text field, type **z**.
- 6 Click to expand the Legends section. Select the Show legends check box.

- 7 Right-click Results>Phase Indicator at Symmetry Axis>Line Graph I and choose Duplicate.
- 8 In the Settings window for Line Graph, locate the Data section.
- 9 From the Data set list, choose Study 2/Solution 3.
- 10 On the Phase Indicator at Symmetry Axis toolbar, click Plot.

Compare the resulting plot with Figure 5 showing the fraction of liquid phase through the centerline for all values of ΔT .

Phase Indicator at Symmetry Axis I

- I In the Model Builder window, right-click Phase Indicator at Symmetry Axis and choose Duplicate.
- 2 In the Settings window for 1D Plot Group, type Phase Indicator through Radius in the Label text field.

Phase Indicator through Radius

- I In the Model Builder window, expand the Results>Phase Indicator through Radius node, then click Line Graph I.
- 2 In the Settings window for Line Graph, locate the Selection section.
- 3 Click Clear Selection.
- **4** Select Boundary 4 only.
- 5 Locate the x-Axis Data section. In the Expression text field, type r.
- 6 On the Phase Indicator through Radius toolbar, click Plot.
- 7 In the Model Builder window, under Results>Phase Indicator through Radius click Line Graph 2.
- 8 In the Settings window for Line Graph, locate the Selection section.
- 9 Click Clear Selection.
- **IO** Select Boundary 4 only.
- II Locate the x-Axis Data section. In the Expression text field, type r.
- 12 In the Model Builder window, click Phase Indicator through Radius.
- 13 In the Settings window for 1D Plot Group, click to expand the Legend section.
- **I4** From the **Position** list, choose **Upper left**.
- **I5** On the **Phase Indicator through Radius** toolbar, click **Plot**.

Compare the resulting plot with Figure 4 showing the fraction of liquid phase through the radius for all values of ΔT .

Laser Heating of a Silicon Wafer

Introduction

A silicon wafer is heated up by a laser that moves radially in and out over time while the wafer itself rotates on its stage. Modeling the incident heat flux from the laser as a spatially distributed heat source on the surface, the transient thermal response of the wafer is obtained. The peak, average, and minimum temperatures during the heating process are computed, as well as the temperature variations across the wafer.



Figure 1: A silicon wafer is heated with a laser that moves back and forth. The wafer is also being rotated about its axis.

Model Definition

A 2-inch silicon wafer, as shown in Figure 1, is heated for one minute by a 10 W laser that moves radially inwards and outwards, while the wafer rotates on its stage. Assuming good thermal isolation from the environment, the only source of heat loss is from the top surface via radiation to the processing chamber walls, which are assumed to be at a fixed temperature of 20 °C.

The laser beam is modeled as a heat source in the plane with Gaussian profile. To set up the heating profile the model uses the built-in Gaussian Pulse functions, which enforce that the integral under the curve equals unity. The focal point is moved by using a triangular waveform to define its position along the x-axis over time. The wafer is assigned a bulk rotational velocity in the governing heat transfer equation.

The emissivity of the surface of the wafer is approximately 0.8. At the operating wavelength of the laser, it is assumed that absorptivity equals emissivity. The heat load due to the laser is thus multiplied by the emissivity. Assuming also that the laser is operating at a wavelength at which the wafer is opaque, no light is passing through the wafer. Therefore, all of the laser heat is deposited at the surface.

The wafer is meshed using a triangular swept mesh. Swept meshing allows for only a single thin element through the thickness, and still maintains reasonable element size in the plane. A finer mesh would give slightly more accurate predictions of the peak temperature, but predictions of average and minimum temperature would not be greatly affected.

Results and Discussion

Figure 2 plots the maximum, minimum, and average temperatures of the wafer, while Figure 3 shows the difference between the maximum and minimum temperature. The temperature distribution across the wafer is plotted in Figure 4.

The heating profile does introduce some significant temperature variations, because the laser deposits the same amount of heat over a larger total swept area when it is focused at the outside of the wafer. An interesting modification to this example would be to investigate alternative heating profiles for smoother heating.



Figure 2: Maximum, minimum, and average temperatures of the wafer as functions of time.



Figure 3: Difference between maximum and minimum temperatures on the wafer.

Time=60 s Surface: Temperature (K)



Figure 4: Temperature variation across the wafer. The arrow plot describes the velocity of the wafer.

Application Library path: COMSOL_Multiphysics/Heat_Transfer/ laser_heating_wafer

Modeling Instructions

From the File menu, choose New.

NEW

I In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 3D.
- 2 In the Select physics tree, select Heat Transfer>Heat Transfer in Solids (ht).
- 3 Click Add.

- 4 Click Study.
- 5 In the Select study tree, select Preset Studies>Time Dependent.
- 6 Click Done.

GLOBAL DEFINITIONS

Start by defining parameters for use in the geometry, functions, and physics settings.

Parameters

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

Name	Expression	Value	Description
r_wafer	1[in]	0.0254 m	Wafer radius
thickness	275[um]	2.75E-4 m	Wafer thickness
v_rotation	60[rpm]	l Hz	Rotational speed
angular_v	2*pi*v_rotation	6.283 Hz	Angular velocity
period	10[s]	10 s	Time for laser to move back and forth
r_spot	2.5[mm]	0.0025 m	Radius of laser spot size
emissivity	0.8	0.8	Surface emissivity of wafer
p_laser	10[W]	10 W	Laser power

Here, the unit 'rpm' is revolution per minute.

GEOMETRY I

Create a cylinder for the silicon wafer.

Cylinder I (cyl1)

- I On the Geometry toolbar, click Cylinder.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r_wafer.
- 4 In the **Height** text field, type thickness.

5 Click the Build All Objects button.



y Z x

DEFINITIONS

Define functions for use before setting up the physics.

Gaussian Pulse I (gpl)

- I On the Home toolbar, click Functions and choose Local>Gaussian Pulse.
- 2 In the Settings window for Gaussian Pulse, locate the Parameters section.
- 3 In the Standard deviation text field, type r_spot/3.

The laser beam radius is equal to three standard deviations of the Gaussian pulse. These three standard deviations account for 99.7% of the total laser energy.



4 Click the **Plot** button.

Waveform 1 (wv1)

- I On the Home toolbar, click Functions and choose Local>Waveform.
- 2 In the Settings window for Waveform, locate the Parameters section.
- **3** From the **Type** list, choose **Triangle**.
- **4** Clear the **Smoothing** check box.
- 5 In the Angular frequency text field, type 2*pi/period.
- 6 In the **Phase** text field, type pi/2.
- 7 In the Amplitude text field, type r_wafer.



8 Click the **Plot** button.

Analytic I (an I)

- I On the Home toolbar, click Functions and choose Local>Analytic.
- 2 In the Settings window for Analytic, type hf in the Function name text field.
- 3 Locate the Definition section. In the Expression text field, type
 p_laser*gp1(x-wv1(t))*gp1(y).
- 4 In the Arguments text field, type x, y, t.
- **5** Locate the **Units** section. In the **Arguments** text field, type m, m, s.
- **6** In the **Function** text field, type W/m².
- 7 Locate the Plot Parameters section. In the table, enter the following settings:

Argument	Lower limit	Upper limit
x	-r_spot	r_spot
у	-r_spot	r_spot
t	period/4	period/4



8 Click the **Plot** button.

Next, add coupling operators for the result analysis.

Average 1 (aveop1)

- I On the Definitions toolbar, click Component Couplings and choose Average.
- **2** Select Domain 1 only.

Maximum I (maxopI)

- I On the Definitions toolbar, click Component Couplings and choose Maximum.
- **2** Select Domain 1 only.

Minimum I (minop I)

- I On the Definitions toolbar, click Component Couplings and choose Minimum.
- **2** Select Domain 1 only.

HEAT TRANSFER IN SOLIDS (HT)

Set up the physics. First, include the wafer's rotational velocity in the governing heat transfer equation.

Heat Transfer in Solids 1

In the Model Builder window, under Heat Transfer in Solids (ht), click Heat Transfer in Solids 1.

Translational Motion I

- I On the Physics toolbar, click Attributes and choose Translational Motion.
- **2** In the **Settings** window for Translational Motion, locate the **Translational Motion** section.
- **3** Specify the \mathbf{u}_{trans} vector as

-y*angular_v	x
x*angular_v	у
0	z

Next, add heat flux and surface-to-ambient radiation on the wafer's top surface.

Heat Flux 1

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



y Z x

- 3 In the Settings window for Heat Flux, locate the Heat Flux section.
- **4** In the q_0 text field, type emissivity*hf(x,y,t).

Diffuse Surface I

- I On the Physics toolbar, click Boundaries and choose Diffuse Surface.
- **2** Select Boundary 4 only.
- 3 In the Settings window for Diffuse Surface, locate the Surface Emissivity section.

4 From the ε list, choose User defined. In the associated text field, type emissivity.

ADD MATERIAL

- I On the Home toolbar, click Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select **Built-In>Silicon**.
- 4 Click Add to Component in the window toolbar.
- 5 On the Home toolbar, click Add Material to close the Add Material window.

MESH I

Use a fine triangular swept mesh.

Swept I

- I In the Model Builder window, under Component I (compl) right-click Mesh I and choose Swept.
- 2 In the Settings window for Swept, click to expand the Sweep method section.
- **3** Locate the Sweep Method section. From the Face meshing method list, choose Triangular (Generate prisms).

Distribution I

- I Right-click Component I (compl)>Mesh I>Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Distribution section.
- **3** In the Number of elements text field, type **1**.

Size

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

4 Click the Build All button.



y Z x

STUDY I

Step 1: Time Dependent

- I In the Model Builder window, under Study I click Step I: Time Dependent.
- 2 In the Settings window for Time Dependent, locate the Study Settings section.
- 3 In the **Times** text field, type range(0,0.1,60).
- **4** On the **Home** toolbar, click **Compute**.

RESULTS

Temperature (ht)

The first default plot shows the temperature on the wafer surface. Add an arrow plot for the velocity field describing the wafer rotation.

- I In the Model Builder window, under Results right-click Temperature (ht) and choose Arrow Surface.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Heat Transfer in Solids>ht.ux,ht.uy,ht.uz Velocity field.

- 3 Locate the Coloring and Style section. Select the Scale factor check box.
- 4 In the associated text field, type 0.036.
- 5 From the Color list, choose Green.

Compare the temperature variation with that shown in Figure 4.

Isothermal Contours (ht)

The second default plot shows the isosurface temperature. Time=60 s Isosurface: Temperature (K)



ID Plot Group 3

- I On the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for 1D Plot Group, click to expand the Legend section.
- **3** From the **Position** list, choose **Lower right**.
- 4 On the ID Plot Group 3 toolbar, click Global.
- 5 In the Settings window for Global, locate the y-Axis Data section.
- 6 In the table, enter the following settings:

Expression	Unit	Description
maxop1(T)	degC	Maximum temperature
minop1(T)	degC	Minimum temperature
aveop1(T)	degC	Average temperature

7 On the ID Plot Group 3 toolbar, click Plot.

Compare the plot showing the maximum, minimum and average temperature with Figure 2.

ID Plot Group 4

- I On the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 On the ID Plot Group 4 toolbar, click Global.
- 3 In the Settings window for Global, locate the y-Axis Data section.
- **4** In the table, enter the following settings:

Expression	Unit	Description
<pre>maxop1(T)-minop1(T)</pre>	К	Temperature difference

5 On the ID Plot Group 4 toolbar, click Plot.

Finish the result analysis by comparing the generated plot with Figure 3.



Figure 1: A smiley face.