

# Case Study VII

## VII Radioimmunotherapy of metastatic melanoma

Metastatic melanoma is the most dangerous form of skin cancer and causes 77% of all skin cancer-related deaths. New methods for its treatment are, therefore, urgently needed. The feasibility of radioimmunotherapy (RIT) in mice, which involves the binding of the antibody to a tumor-associated antigen to deliver a lethal dose of radiation to tumor cells, was established in a study by Dadachova *et al.* (2004). Another study (Schweitzer *et al.*, 2007) looked at the process of radioimmunotherapy in detail with the use of a computer model. In this particular example, we will follow this paper to develop a mathematical model of the process.

### Problem formulation

Figure 6.11 shows the process of radioimmunotherapy. The process involves intravenous administration of a radio-labeled antibody in the patient's body which circulates in the plasma and is transported across capillary walls into the normal tissue. The shape of the tumor is assumed to be a sphere. The antibody then diffuses through normal tissue to the tumor to reach the antigen present inside the tumor and binds with it to form an antibody-antigen complex. Also, the antibody-antigen complex that is formed dissociates into free antibody and antigen. Some amount of the antibody in the normal tissue is removed by the lymphatic vessels and there is no significant binding of the antibody in the normal tissue.

### Governing equations

The governing equations that describe the set of processes are given by:

(I) Antibody uptake from blood:

$$c_{Abp}(t) = c_{Abo}e^{-\lambda t} \quad (6.12)$$

where  $c_{Abo}$  is the initial plasma antibody concentration after intravenous administration,  $\lambda$  is the plasma kinetics constant and  $c_{Abp}$  is the antibody concentration in the plasma as a function of time.

(II) Transport, uptake and clearance of antibody in normal tissue:

$$\frac{\partial c_{Abt}}{\partial t} = D_{tis} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{Abt}}{\partial r} \right) + k^{bl} c_{Abp} - k^{ly} c_{Abt} \quad (6.13)$$

where  $c_{Abt}$  is the antibody concentration in the normal tissue,  $D_{tis}$  is the diffusivity of antibody in the tissue,  $r$  is the radial distance from the tumor center, and  $k^{bl}$  and  $k^{ly}$  are the rate constants for uptake into and removal from tissue, respectively.

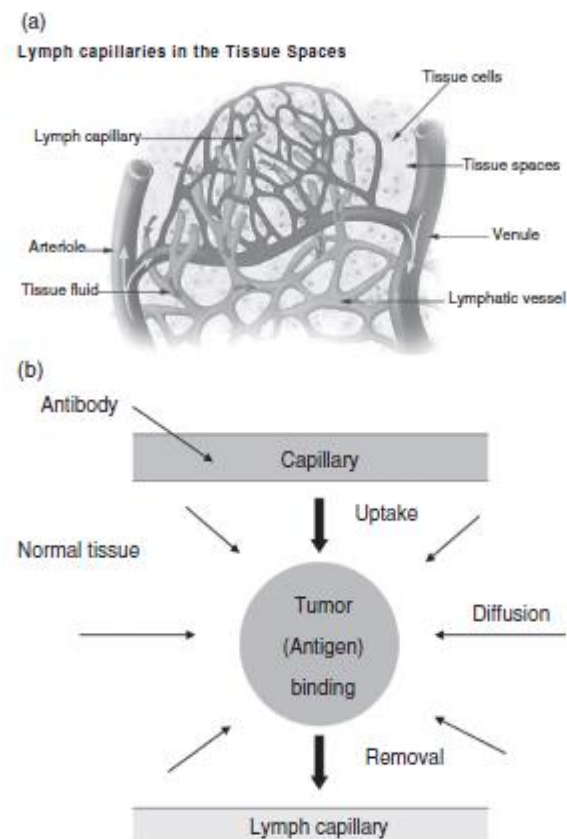


Figure 6.11

(a) The blood and lymph capillary system in the tissue. Figure from [http://upload.wikimedia.org/wikipedia/commons/1/19/llu\\_lymph\\_capillary.png](http://upload.wikimedia.org/wikipedia/commons/1/19/llu_lymph_capillary.png); (b) physical description of radioimmunotherapy.

(III) Transport, complex formation and dissociation in tumor:

$$\frac{\partial c_{Ab}}{\partial t} = D_{tum} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{Ab}}{\partial r} \right) - k_{+1} c_{Ab} c_{Ag} + k_{-1} c_{Ab-Ag} \quad (6.14)$$

where  $c_{Ab}$  is the concentration of free antibody in the tumor,  $D_{tum}$  is the diffusivity of antibody in the tumor and  $k_{+1}$  and  $k_{-1}$  are the rates of the forward and backward reactions, respectively.

(IV) Antigen concentration due to complex formation and dissociation:

$$\frac{\partial c_{Ag}}{\partial t} = n (-k_{+1} c_{Ab} c_{Ag} + k_{-1} c_{Ab-Ag}) \quad (6.15)$$

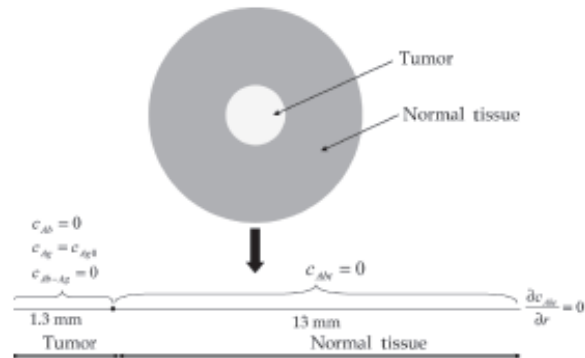


Figure 6.12

Schematic, boundary and initial conditions for the problem. The computations are done in 1D considering spherical symmetry (as discussed in the text).

Table 6.5 Input parameters (all values taken from Schweitzer *et al.*, 2007).

Input parameter	Value
Radius of tumor, $r_{\text{tum}}$	1.3 mm
Radius of tissue, $r_{\text{tis}}$	14.3 mm
Initial antibody concentration, $c_{\text{Ab}0}$	4.94 nM
Antigen concentration, $c_{\text{Ag}0}$	76 000 nM
Diffusivity of antibody in tumor, $D_{\text{tum}}$	$4.16 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$
Diffusivity of antibody in tissue, $D_{\text{tis}}$	$2.0 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$
Rate constant, $\lambda$	$2.96 \times 10^{-5} \text{ s}^{-1}$
Rate constant for transcapillary transport, $k^{\text{bl}}$	$4.6 \times 10^{-5} \text{ mL}/(\text{s}^+\text{mL ECF})$
Rate constant for lymphatic clearance, $k^{\text{ly}}$	$1.78 \times 10^{-5} \text{ mL}/(\text{s}^+\text{mL ECF})$
Forward binding rate constant, $k_{+1}$	$5.0 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$
Dissociation rate constant, $k_{-1}$	$1.0 \times 10^{-5} \text{ s}^{-1}$
Valence of antibody/antigen binding, $n$	5

where  $c_{\text{Ag}}$  is the antigen concentration and  $n$  is the valence of 6D2/melanin binding.  
(V) Complex concentration due to formation and dissociation:

$$\frac{\partial c_{\text{Ab-Ag}}}{\partial t} = k_{+1} c_{\text{Ab}} c_{\text{Ag}} - k_{-1} c_{\text{Ab-Ag}} \quad (6.16)$$

where  $c_{\text{Ab-Ag}}$  is the complex concentration.

**Boundary conditions** The boundary conditions are shown in Figure 6.12. On the left tumor boundary, species flux for all species is zero due to symmetry. On the right normal tissue boundary, species flux is zero as the boundary is considered to be at a large distance. Initially, there is no antibody and complex in the domain. The tumor has an initial antigen concentration of 76 000 nM (Table 6.5).

**Input parameters** Input parameters are shown in Table 6.5.

## References

- Dadachova, E., Nosanchuk, J. D., Shi, L., *et al.* (2004). Dead cells in melanoma tumors provide abundant antigen for targeted delivery of ionizing radiation by a monoclonal antibody to melanin. *Proc Natl Acad Sci USA* 2004;101:14865–14870.
- Schweitzer A. D., Rakesh V., Revskaya E., Datta A., Casadevall A., Dadachova E. (2007). Computational model predicts effective delivery of 188-Re-labeled melanin-binding antibody to the metastatic melanoma tumors with wide range of melanin concentrations. *Melanoma Research*, 17(5):291–303.

## Implementation in COMSOL

As discussed earlier, the shape of the tumor is a sphere. All the computations can, therefore, be done in the spherical coordinate system. Since the concentrations are dependent only on the radial distances, as can be seen in Equations 6.13 and 6.14, a simplified geometry consisting of a line can be used for the model (Figure 6.12). This reduces the amount of computational resources that would be required if we modeled the complete sphere. However, the governing equations need to be solved in the spherical coordinate system. COMSOL solves all the governing equations in the Cartesian system and hence, we need to modify the equations in COMSOL to implement the spherical coordinate system. We take the species transfer equation in the Cartesian (1D) and spherical (with radial dependence only) systems:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D_{\text{cart}} \frac{\partial c}{\partial x} \right) + R_{\text{cart}} \quad (6.17)$$

$$\frac{\partial c}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D \frac{\partial c}{\partial r} \right) + R \quad (6.18)$$

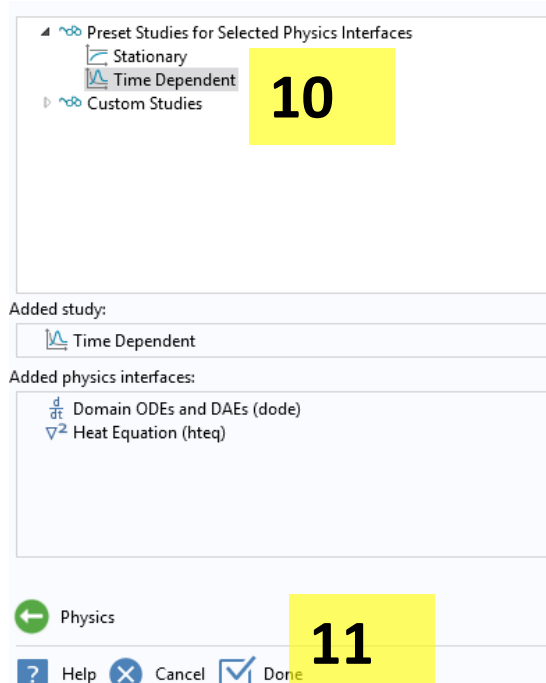
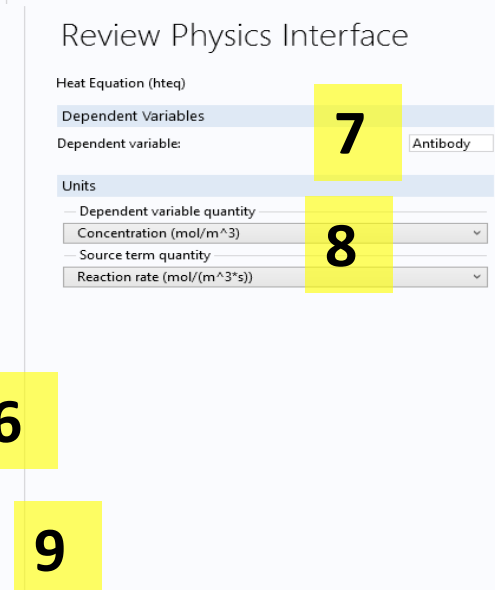
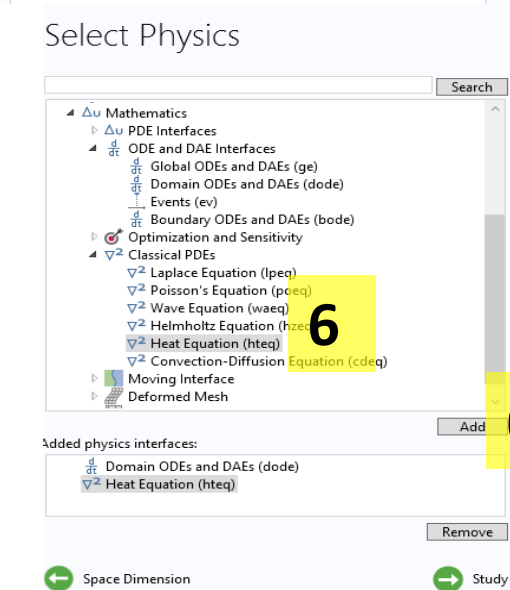
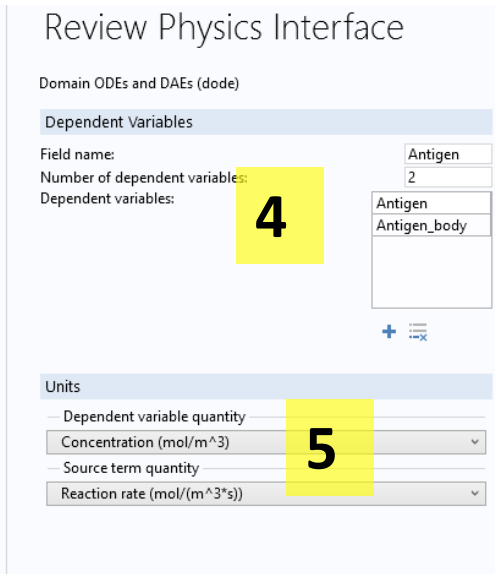
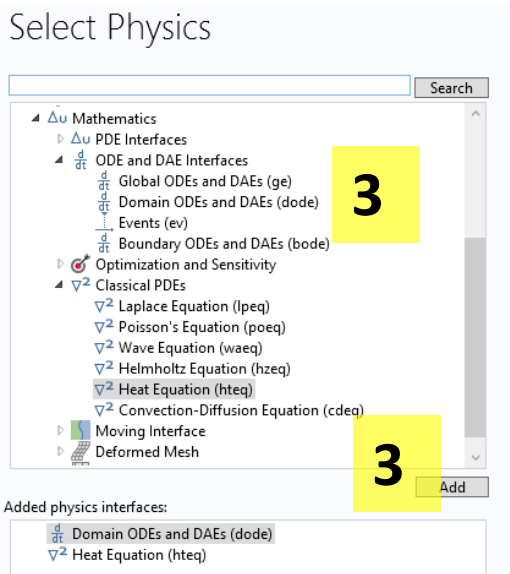
Equation 6.18 can be multiplied by  $r^2$  on both sides giving:

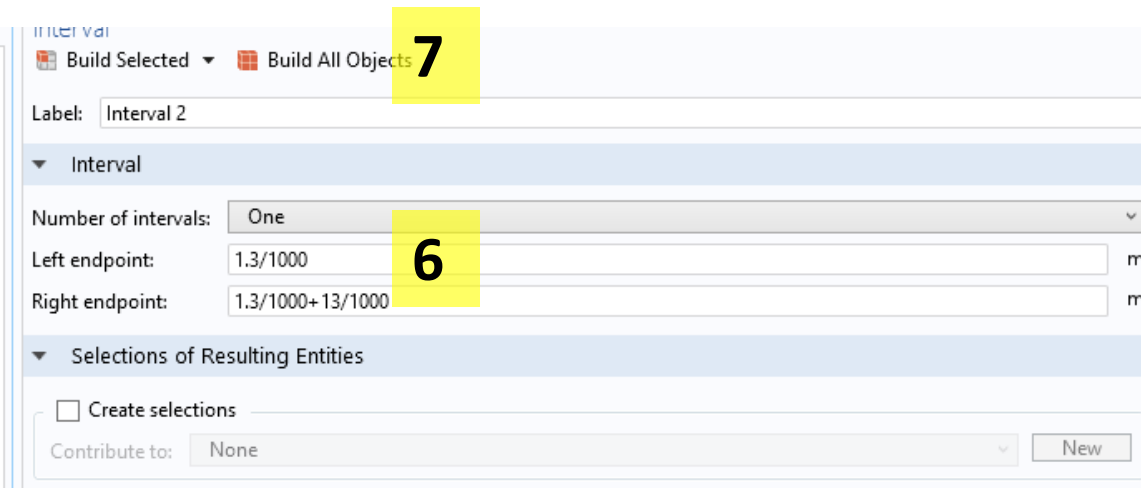
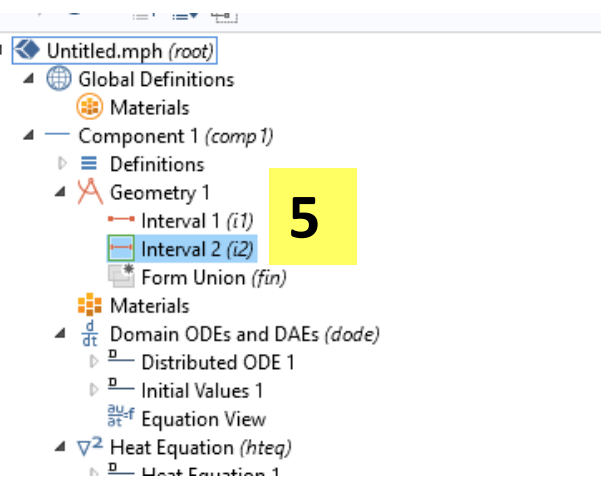
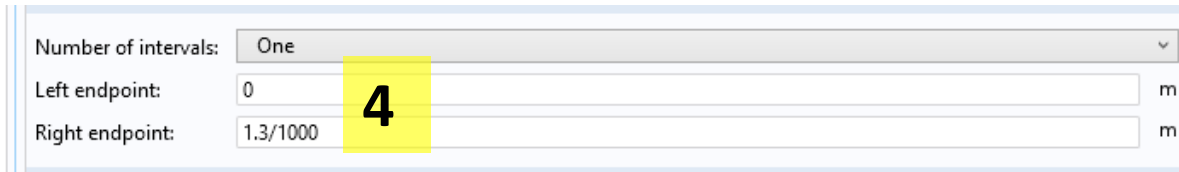
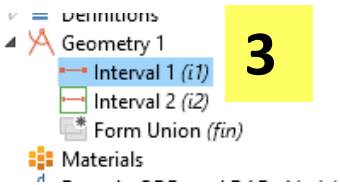
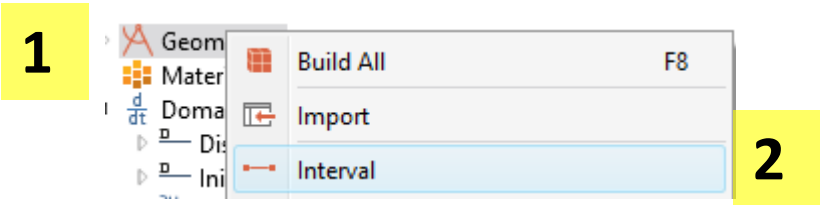
$$r^2 \frac{\partial c}{\partial t} = \frac{\partial}{\partial r} \left( r^2 D \frac{\partial c}{\partial r} \right) + r^2 R \quad (6.19)$$

Equation 6.19 can be implemented in COMSOL as Equation 6.17 using the coefficient of  $\partial c / \partial t$  as  $r^2$ ,  $D_{\text{cart}} = r^2 D$  and  $R_{\text{cart}} = r^2 R$ . The problem has been solved using this method for conversion to the spherical coordinate system in this example.

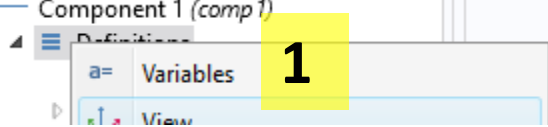


- 1) Select model wizard
- 2) Select 1D
- 3) Under mathematics>>ODE and DAE Interfaces, add 'Domain ODEs and DAEs'
- 4) Rename the field name, number, and variable names as shown
- 5) Change quantity and source term
- 6) Under mathematics>>Classical PDEs, add 'Heat equation'
- 7) Rename the variable names as shown
- 8) Change quantity and source term
- 9) Click study
- 10) Select time dependent
- 11) Click done

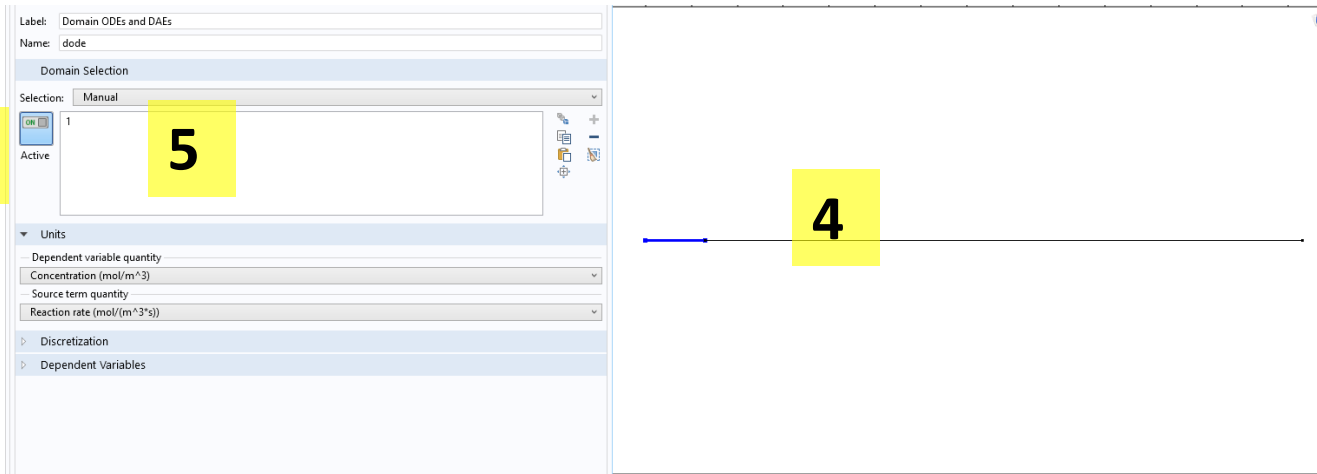




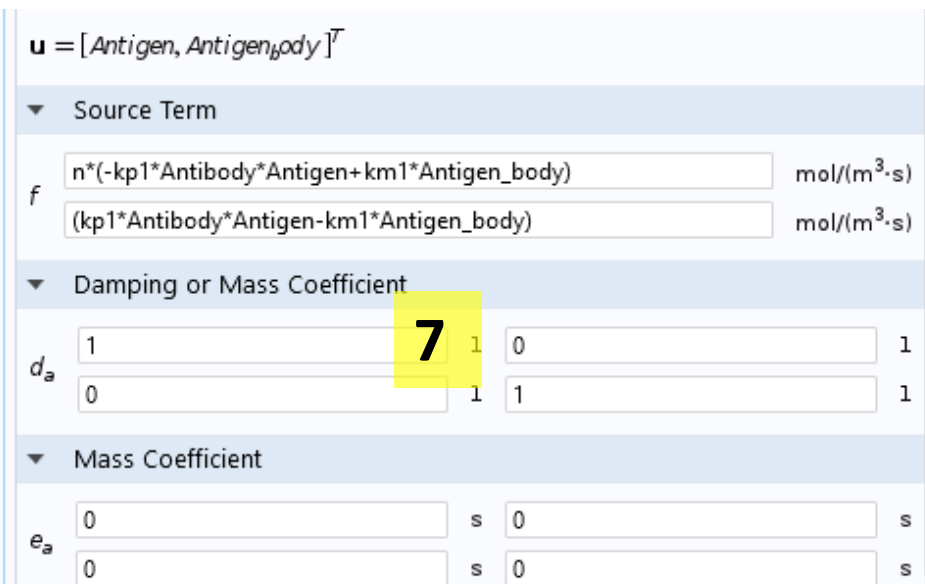
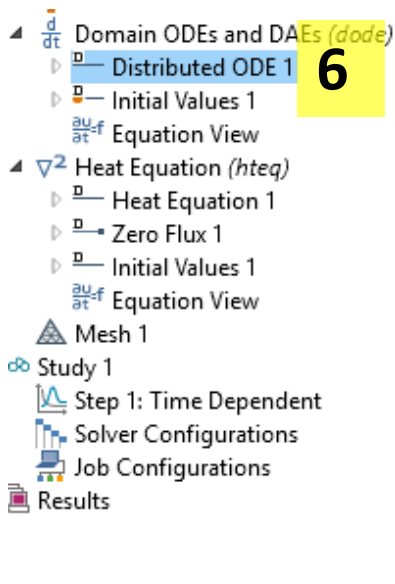
- 1) Right click geometry and select interval
- 2) Repeat step 1
- 3) Left click interval 1
- 4) Enter the dimensions
- 5) Left click interval 2
- 6) Enter the dimensions
- 7) Click Build all

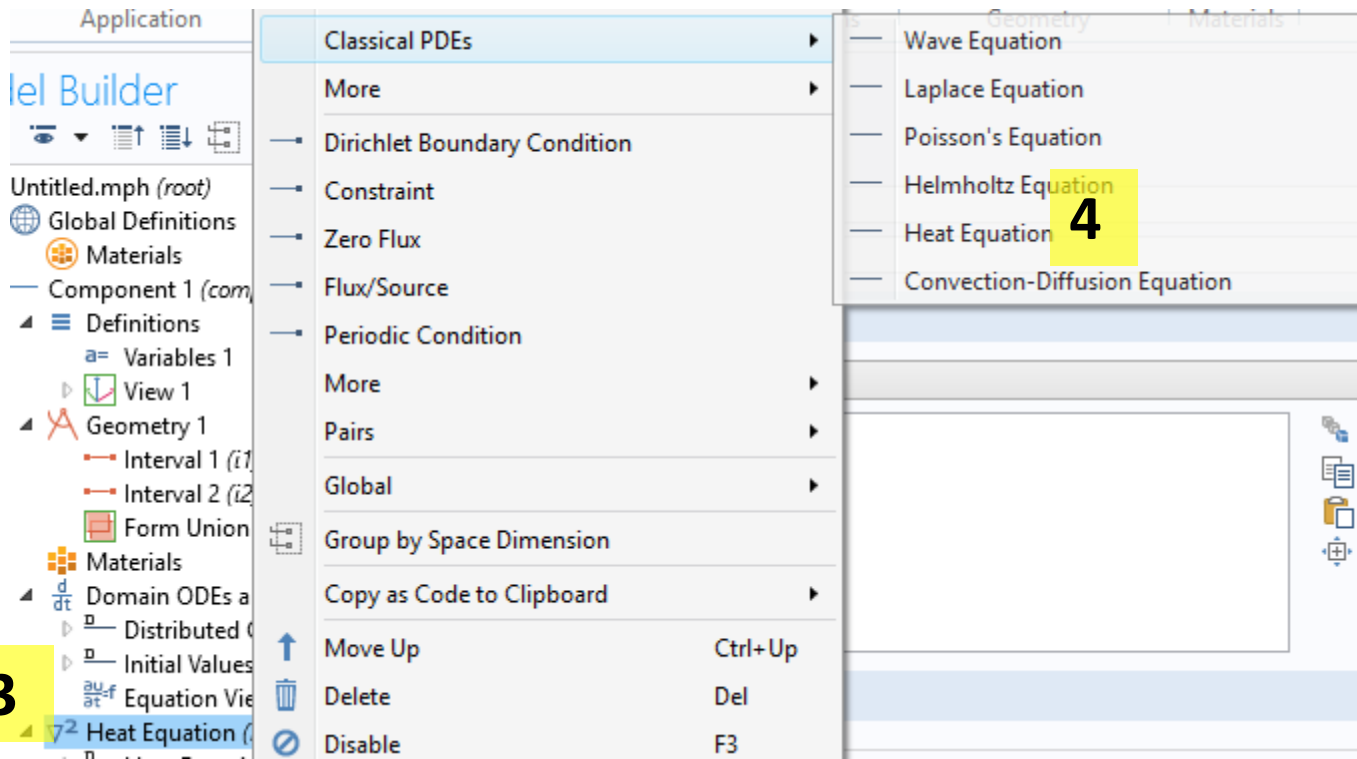
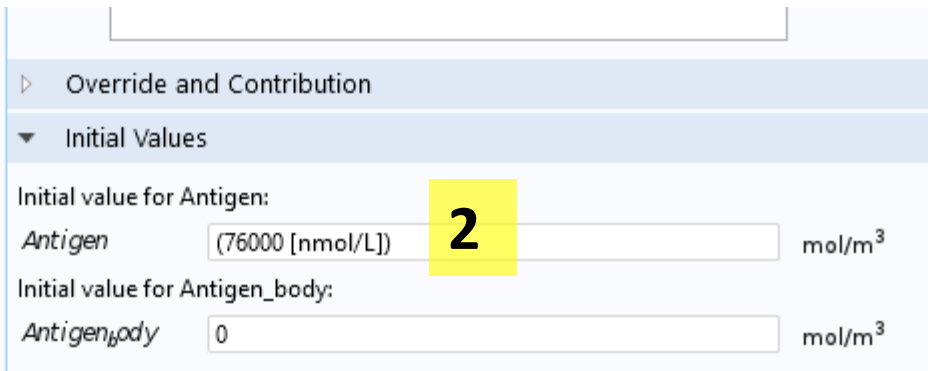
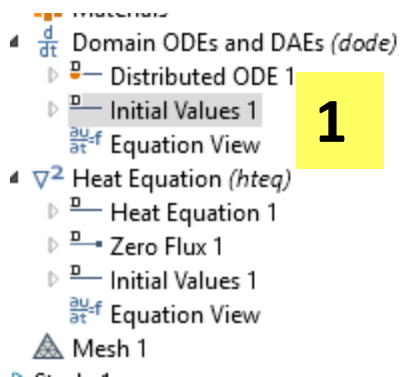


Name	Expression	Unit	Description
n	5		
kp1	(5e4) [L/(mol*s)]	m <sup>3</sup> /(s.m...	
km1	1e-5 [1/s]	1/s	
kbl	4.6e-5 [1/s]	1/s	
kly	1.78e-5 [1/s]	1/s	
lambda	2.96e-5 [1/s]	1/s	
D_tum	4.16e-7 [cm^2/s]	m <sup>2</sup> /s	
D_tis	2e-7 [cm^2/s]	m <sup>2</sup> /s	

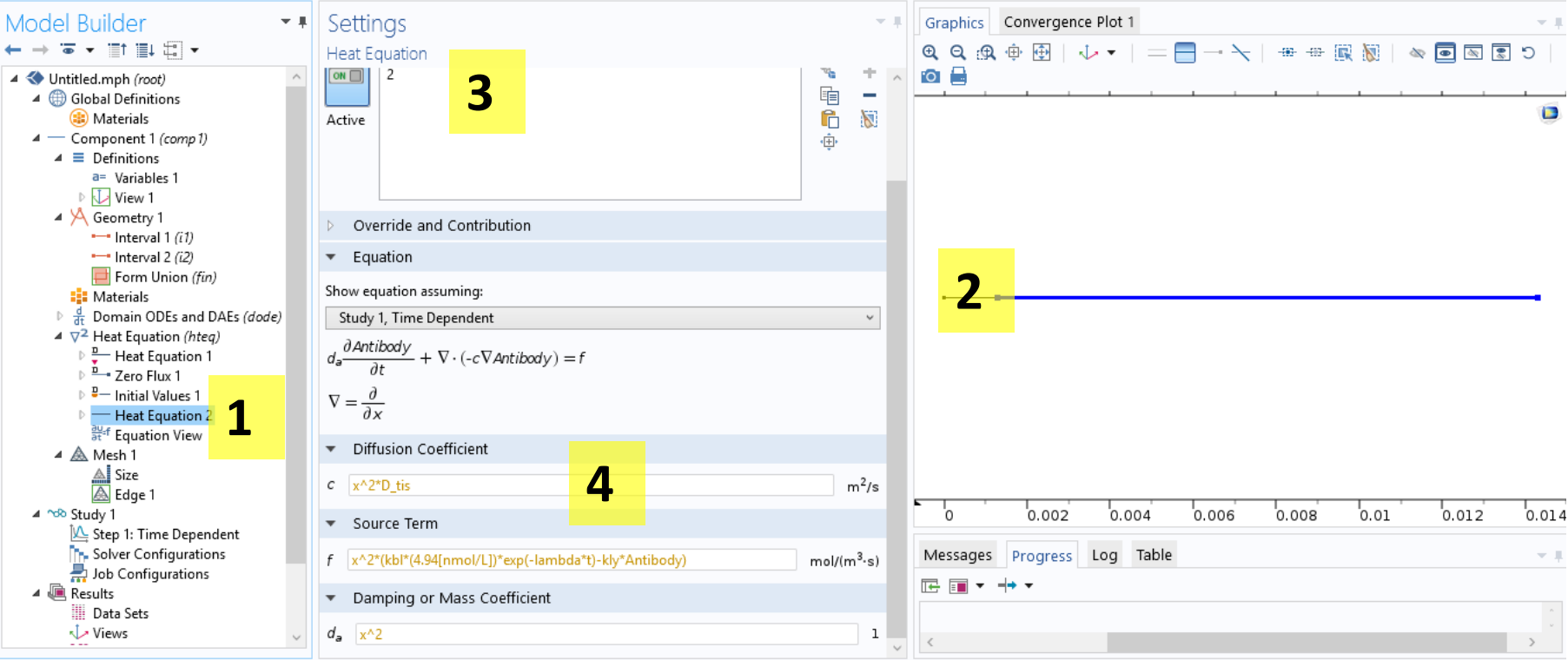


- 1) Click definitions and select variables
- 2) Enter the table
- 3) Click 'Domain ODEs and DAEs'
- 4) Left click domain 2
- 5) You should only see domain 1
- 6) Left click 'Distributed ODE 1'
- 7) Enter the following values

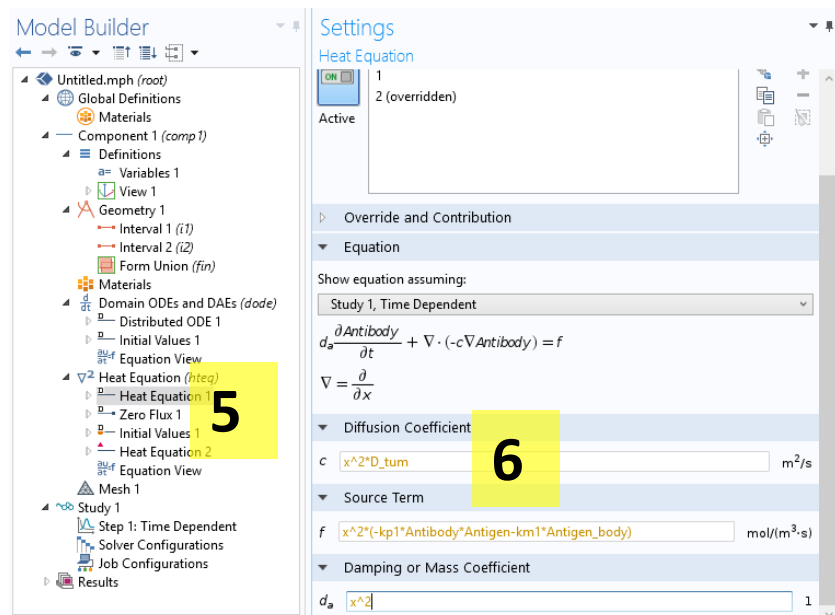




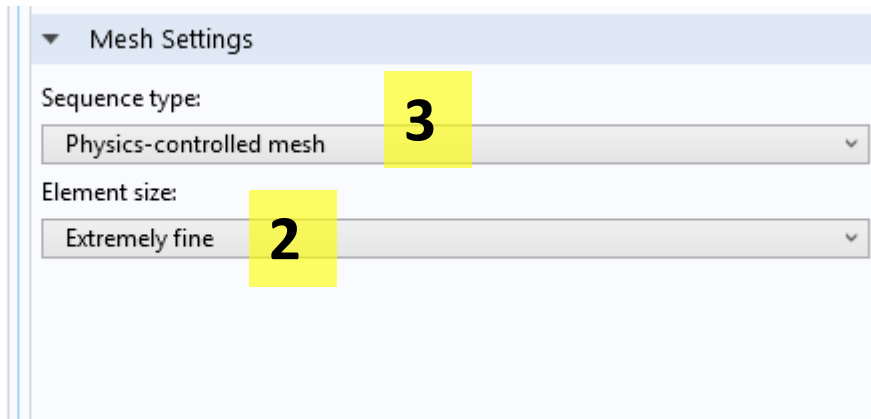
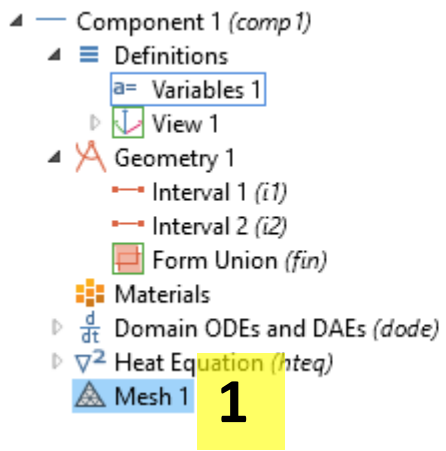
- 1) Left click 'Initial Values 1' under Domain ODEs
- 2) Enter the antigen concentration
- 3) Right click the Heat equation physics
- 4) Add another 'Heat equation'



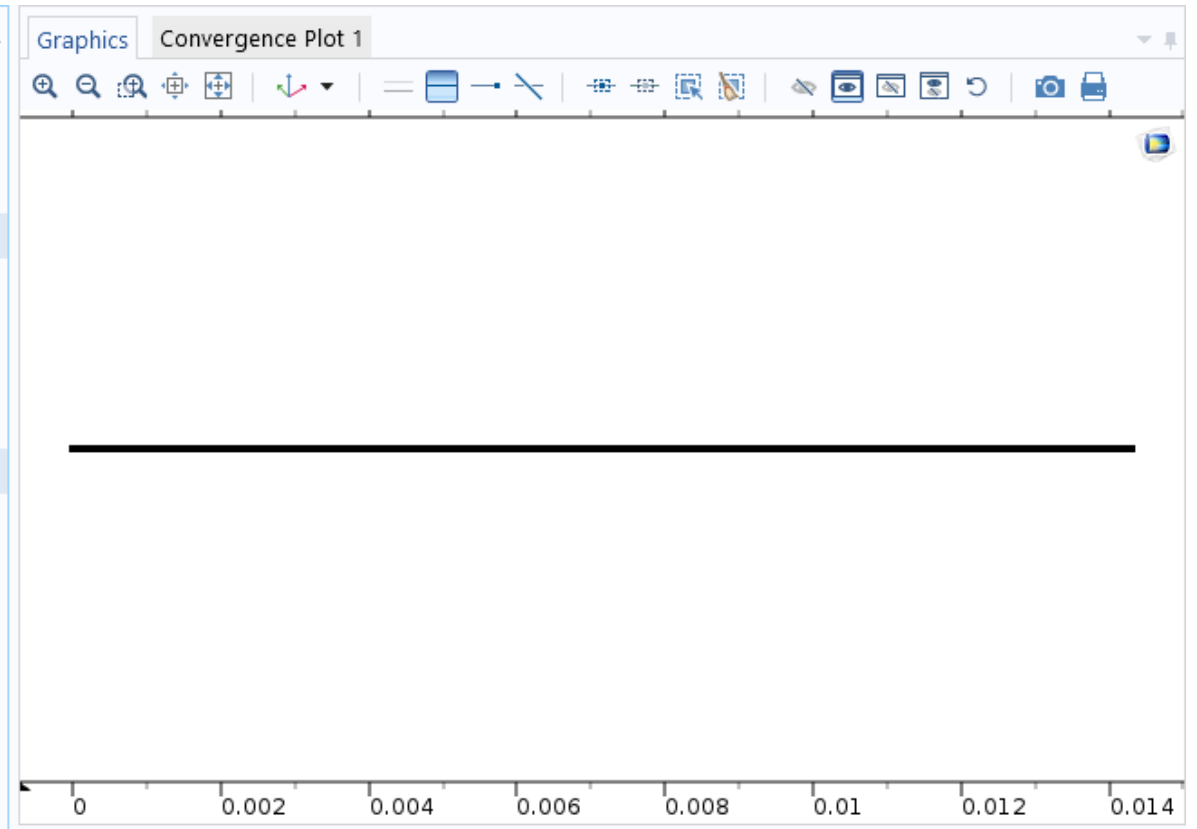
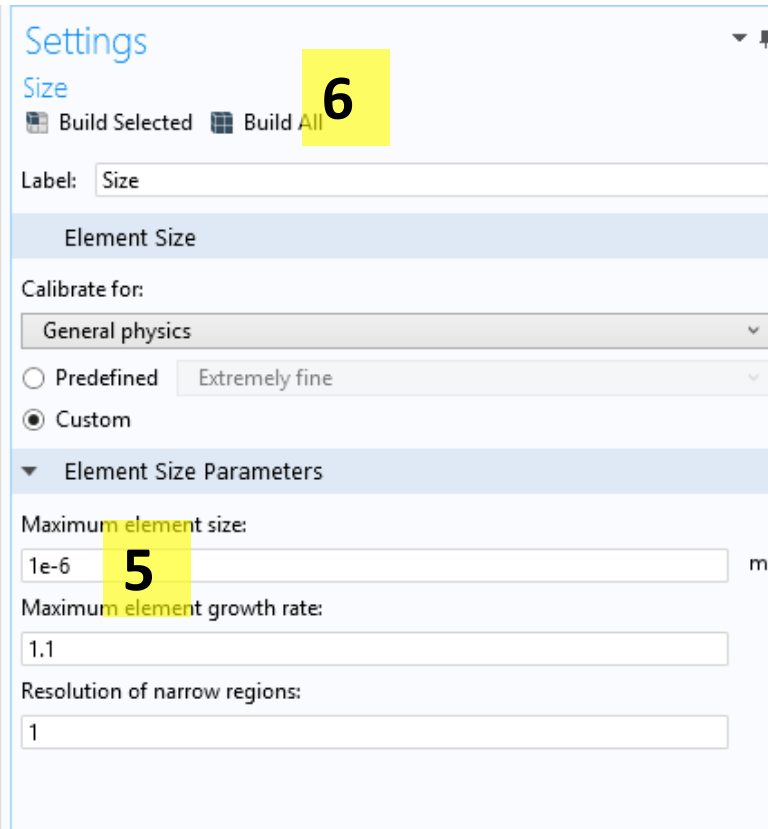
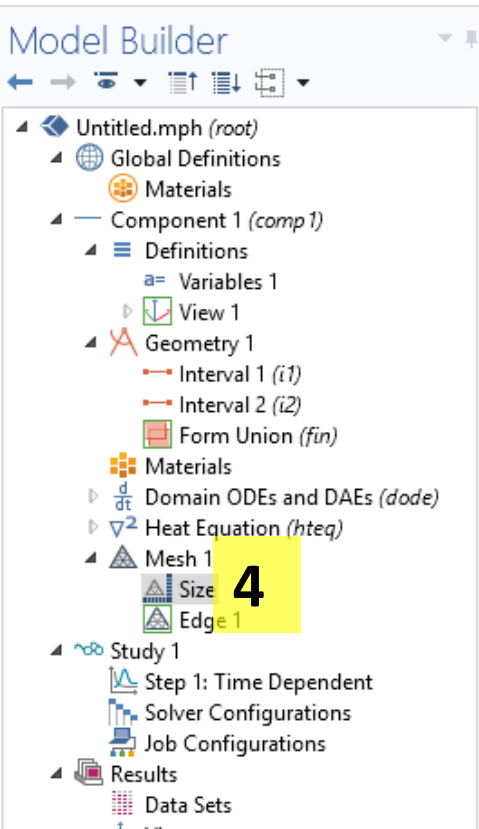
- 1) Left click 'Heat equation 2'
- 2) Left click the tumor domain (domain 1) deselecting it
- 3) You should only see domain 2
- 4) Enter the diffusivity and reaction rate
- 5) Left click 'Heat equation 1'
- 6) Enter the diffusivity and reaction rate







- 1) Left click mesh 1
- 2) Select extremely fine
- 3) Select 'User defined' from the dropdown
- 4) Left click size
- 5) Enter 1e-6
- 6) Click build all



- 1) Left click "Step 1: Time dependent"
- 2) Change time unit to hours
- 3) Enter range(0,1,72)
- 4) Click compute

The image shows a software interface with two main panels: "Model Builder" on the left and "Settings" on the right.

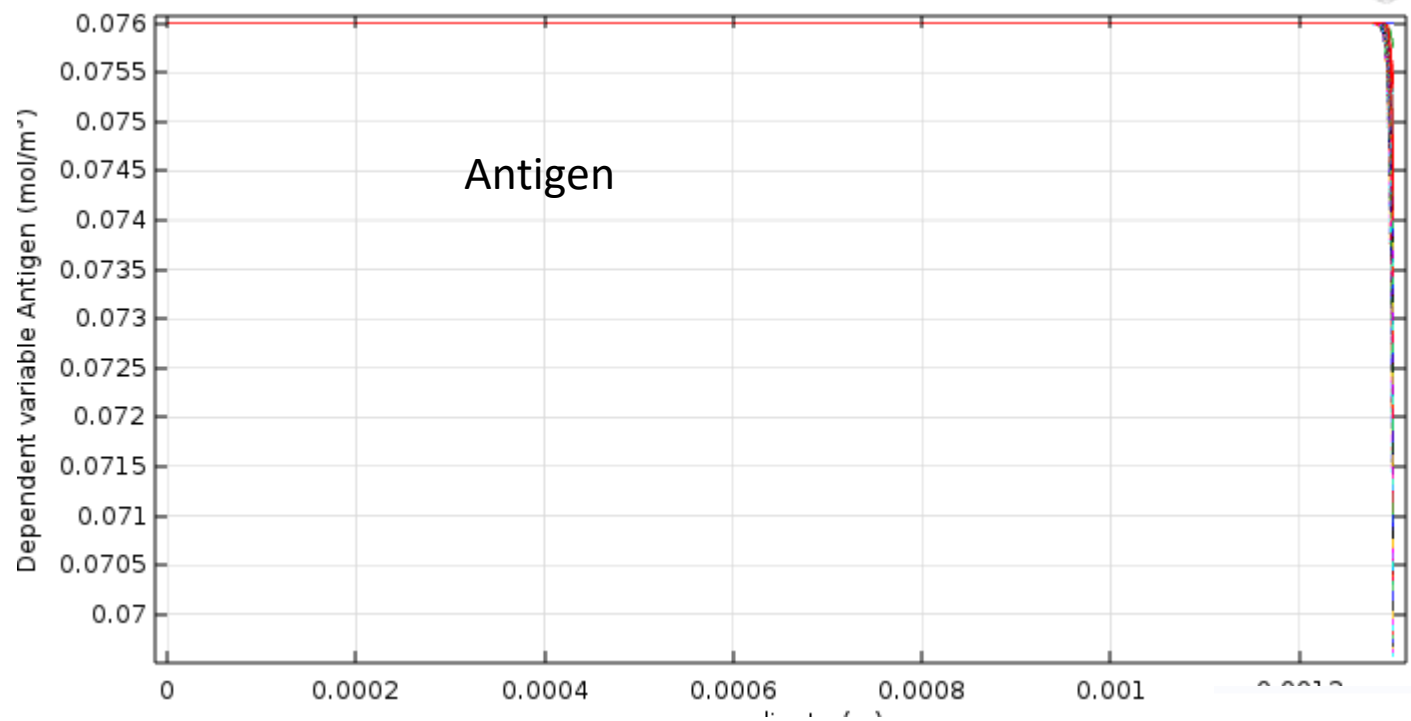
**Model Builder Panel:**

- Tree view structure:
  - Untitled.mph (root)
    - Global Definitions
      - Materials
    - Component 1 (comp 1)
      - Study 1
        - Step 1: Time Dependent** (highlighted with a yellow box labeled **1**)
        - Solver Configurations
        - Job Configurations
      - Results

**Settings Panel:**

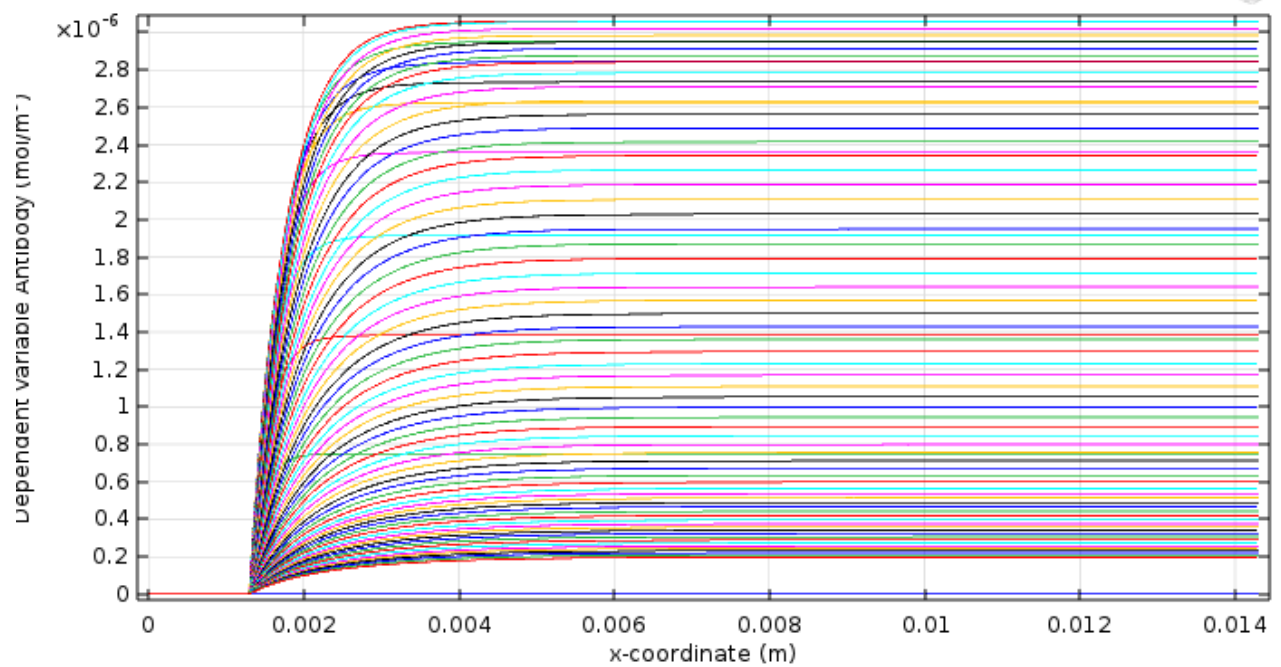
- Section: Time Dependent
- Buttons: Compute (highlighted with a yellow box labeled **4**)
- Label: Time Dependent
- Section: Study Settings
  - Time unit: h (highlighted with a yellow box labeled **2**)
  - Times: range(0,1,72) (highlighted with a yellow box labeled **3**)
  - Relative tolerance:  0.01

Line Graph: Dependent variable Antigen (mol/m<sup>3</sup>)



### Antibody

Line Graph: Dependent variable Antibody (mol/m<sup>3</sup>)



# Case Study IX

## IX Radiofrequency cardiac ablation

Arrhythmia is irregular beating of the heart which causes decreased blood flow and oxygen supply to the brain and body. Radiofrequency (RF) ablation (see Section 8.5) is the standard procedure for treating arrhythmias. In this example, we look at radiofrequency heating in a tissue using a partly modified and simplified version of this process modeled by Tungjitkusolmun *et al.* (2000).

### Problem formulation

A cylindrical electrode is introduced into the middle of the tissue where RF ablation is needed. The problem is therefore axisymmetric and the schematic is shown in Figure 6.14. The properties of the tissue are homogenous. The tissue is heated by resistive heating due to Joule heat generation as there is a potential difference between the electrode tip and the outer edge of the tissue. The optimal goal of RF ablation is to increase the temperature of the tissue from 37 °C to more than 50 °C, when the desired myocardial injury takes place (Tungjitkusolmun *et al.*, 2000). However, the temperatures in the tissue should be kept below 100 °C to avoid unwanted phenomena such as boiling, charring etc.

### Governing equations

The heat transfer in the tissue is governed by the bioheat equation:

$$\rho C_p \frac{\partial T}{\partial t} = \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \right] + \rho_b C_{p,b} \dot{V}_b (T_a - T) + Q \quad (6.22)$$

where  $\rho_b C_{p,b} \dot{V}_b (T_a - T)$  is the blood perfusion term and  $Q$  is the heat generated during RF ablation.

The electric potential is given by:

$$\nabla \cdot (\sigma \nabla V) = 0 \quad (6.23)$$

The heat generated,  $Q$ , due to Joule heating is given by:

$$Q = \sigma |\nabla V|^2 \quad (6.24)$$

where  $V$  is the electric potential and  $\sigma$  is the electrical conductivity.

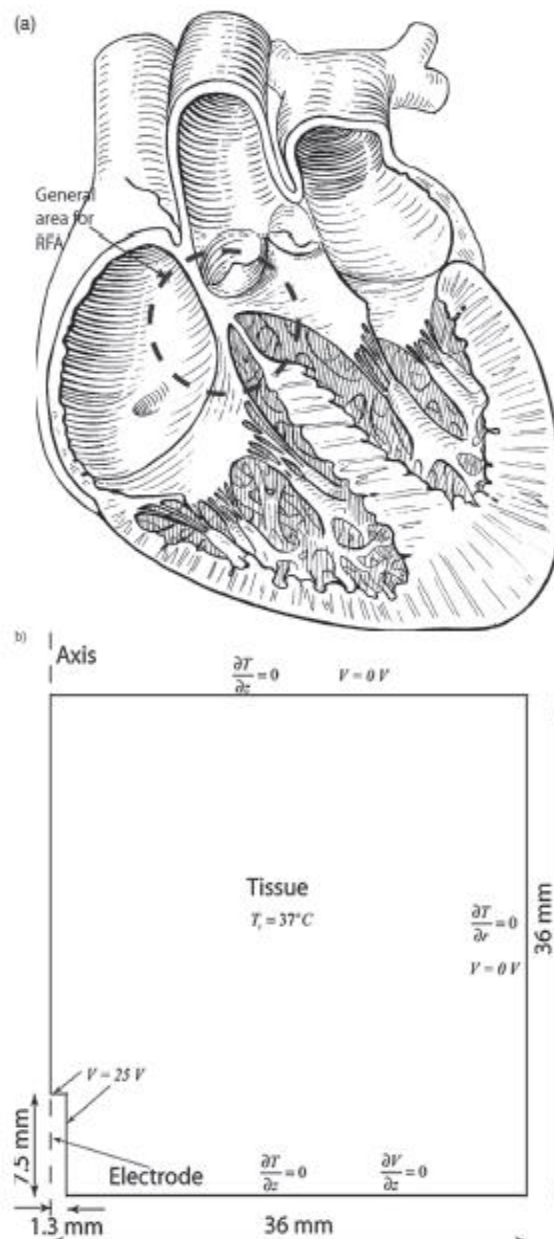


Figure 6.14

(a) Placement of the electrode for RF ablation in the heart; (b) the computational domain and initial conditions for the problem.

Table 6.7 Input parameters (all values taken from Tungjitkusolmun *et al.*, 2000).

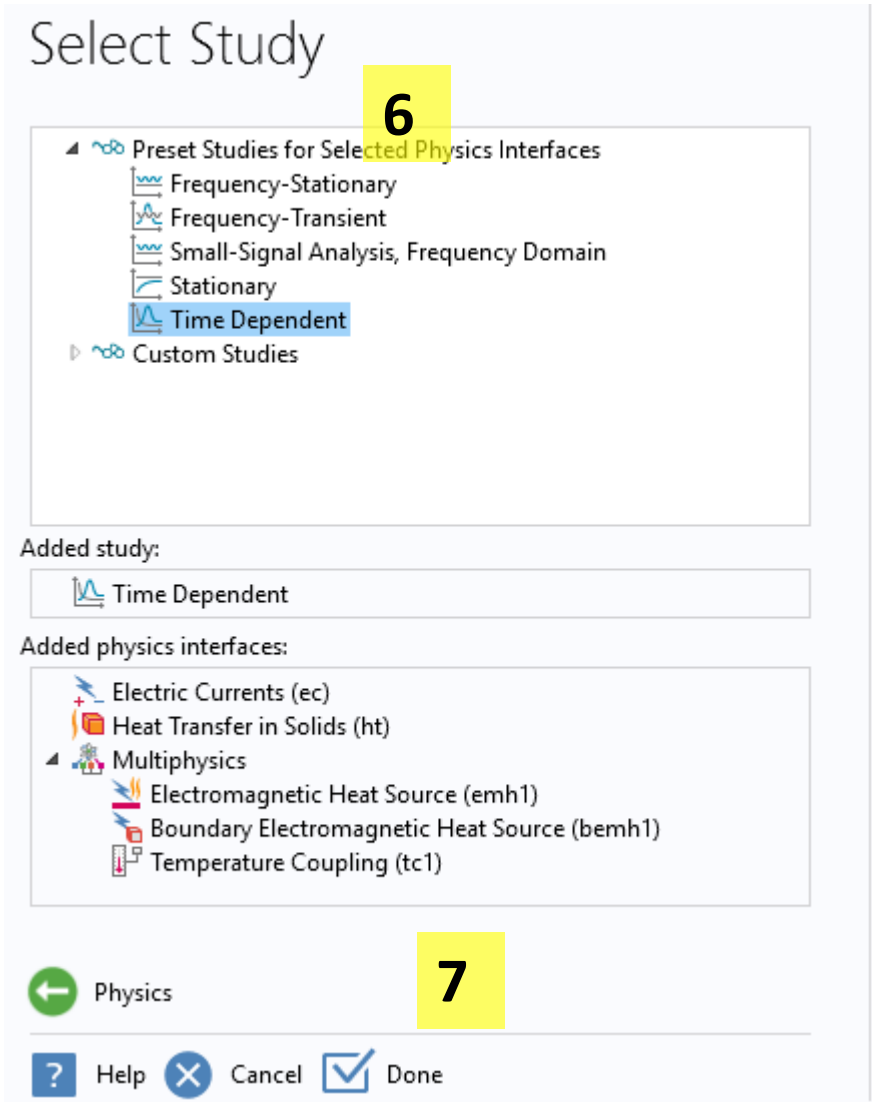
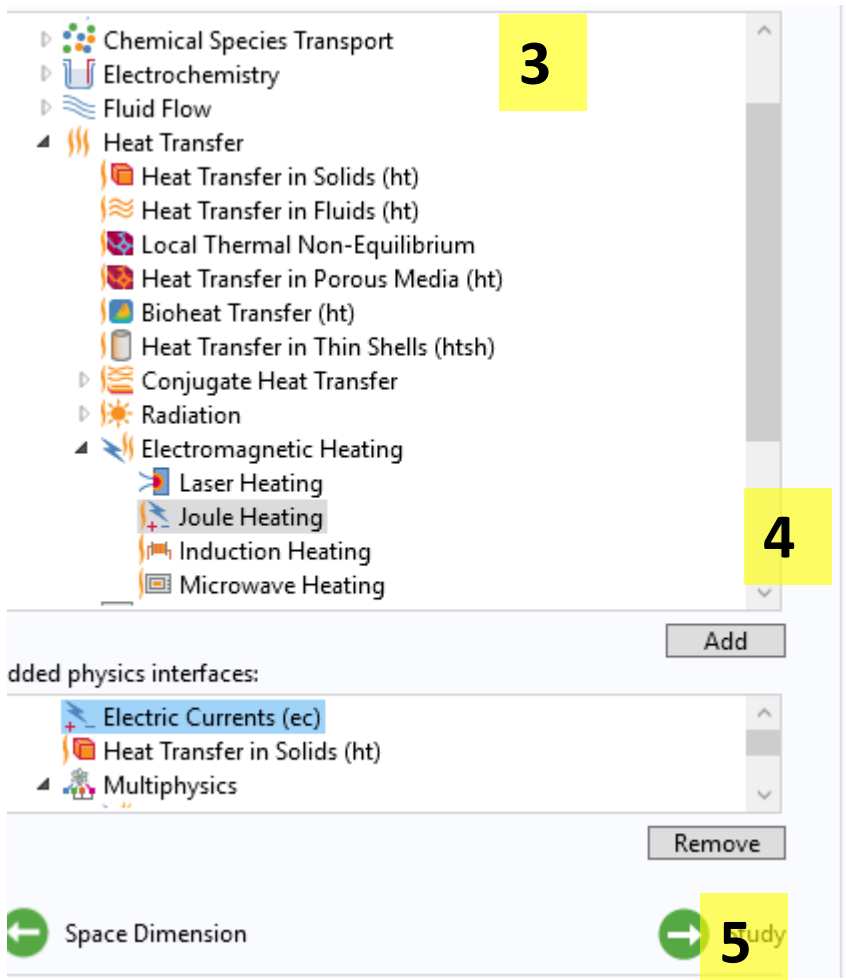
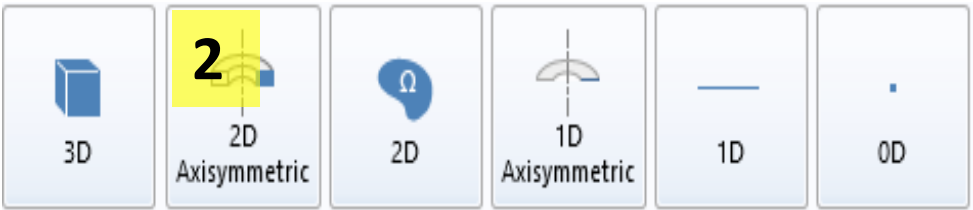
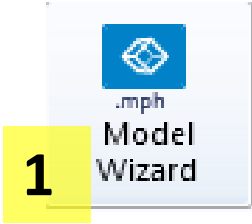
Parameter	Value
Thermal conductivity of the tissue, $k$	$0.4925 + 0.001195T \text{ Wm}^{-1}\text{K}^{-1}$
Specific heat of the tissue, $C_p$	$3200 \text{ Jkg}^{-1}\text{K}^{-1}$
Density of the tissue, $\rho$	$1200 \text{ kgm}^{-3}$
Duration of heating, $t$	60 s
Blood perfusion coefficient, $\rho_b C_{p,b} \dot{V}_b$	$2000 \text{ Wm}^{-3}\text{K}^{-1}$
Electrical conductivity, $\sigma$	$0.222 \text{ S m}^{-1}$
Arterial blood temperature, $T_a$	37 °C
Initial tissue temperature, $T_i$	37 °C
Electric potential at the electrode surface, $V$	25 V

**Boundary conditions** The boundary conditions and the schematic used for the model in COMSOL are shown in Figure 6.14. The geometry is modeled as axisymmetric as discussed earlier. The tissue is at a constant initial temperature of 37 °C. The electrode is not included in the geometry for simplicity and the electric potential to the surface of the electrode is implemented as a boundary condition. The heat fluxes at all surfaces are zero as the left surface is the axis and the other surfaces are assumed to be at a very far distance.

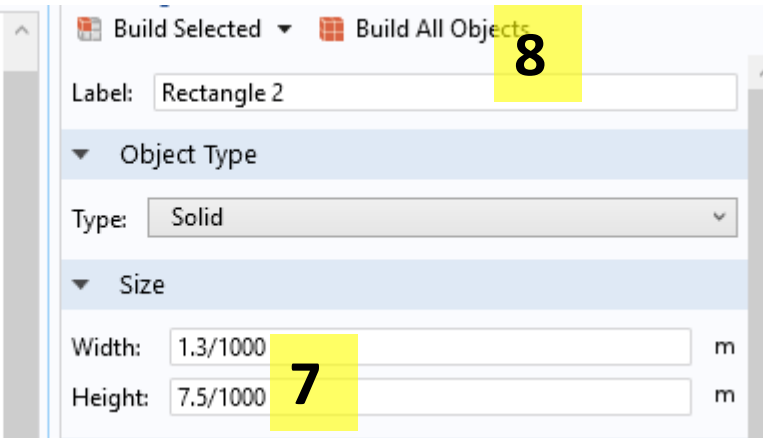
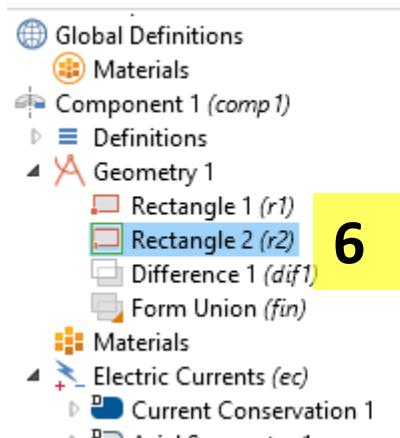
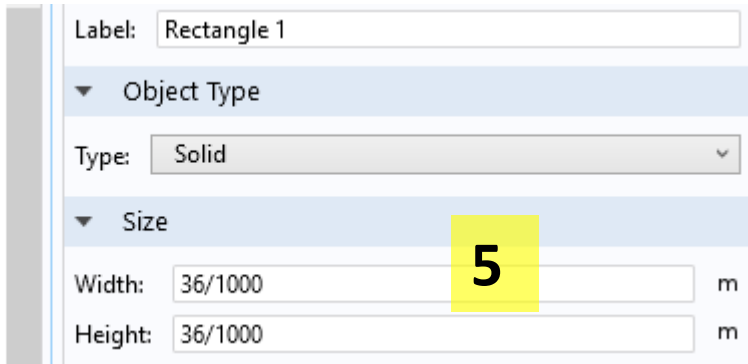
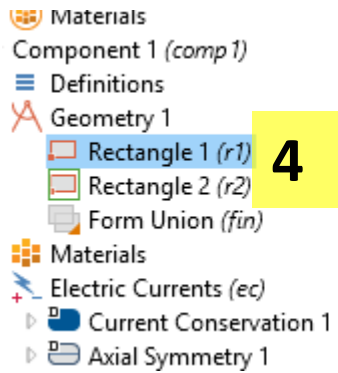
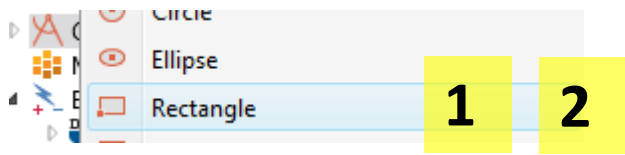
**Input parameters** Input parameters for the problem are listed in Table 6.7.

### Reference

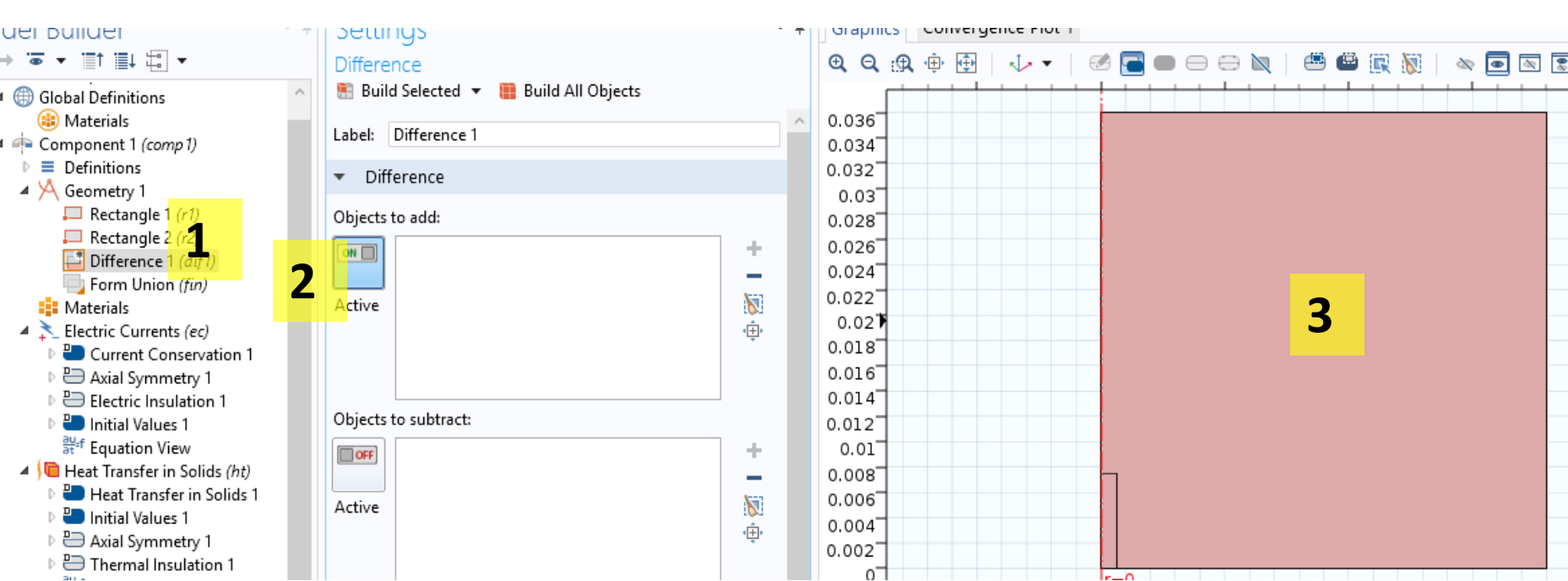
Tungjitkusolmun, S., Woo, E. J., Cao, H., Tsai, J. Z., Vorperian, V. R. and Webster, J. G. (2000). Finite element analyses of uniform current density electrodes for radio-frequency cardiac ablation. *IEEE Transactions on Biomedical Engineering*, **47**, pp. 32–40.



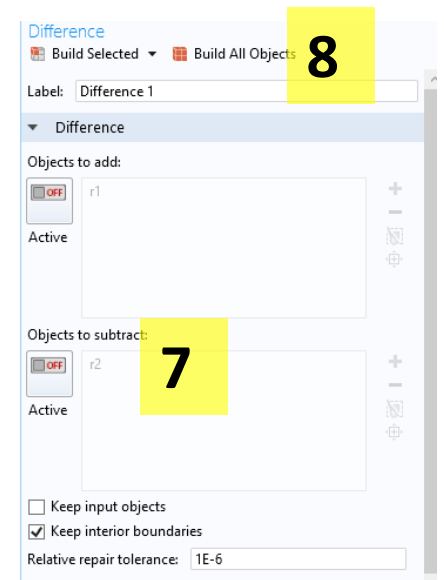
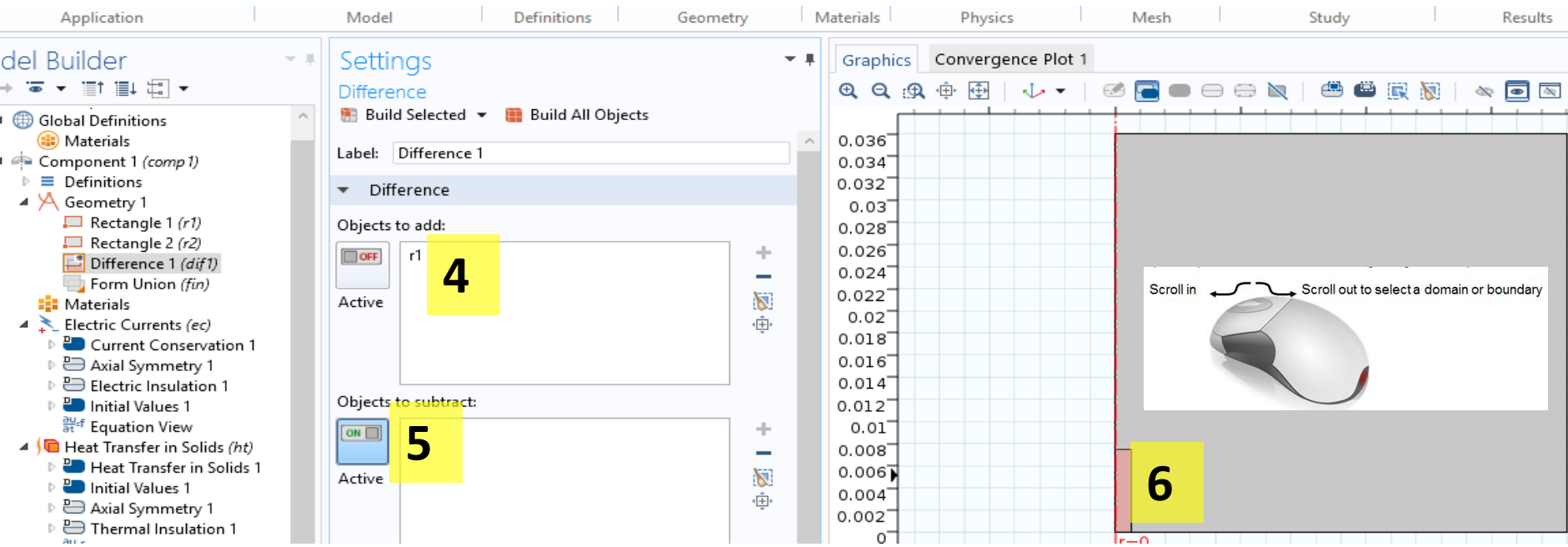
- 1) Select model wizard
- 2) Select 2D Axisymmetric
- 3) Select 'Joule Heating' under 'Electromagnetic heating'
- 4) Click 'Add'
- 5) Click 'Study'
- 6) Click 'Time Dependent'
- 7) Click 'Done'



- 1) Right click geometry, select rectangle
- 2) Repeat 1
- 3) Right click geometry and add 'Difference'
- 4) Left click rectangle
- 5) Input dimensions
- 6) Left click rectangle 2
- 7) Input dimensions
- 8) Build all



- 1) Left click difference 1
- 2) Make 'add' 'on'
- 3) Hover over the big domain, left click
- 4) R1 should appear
- 5) Make 'subtract' 'on'
- 6) Hover over the electrode domain, scroll with your mouse forward, and only the electrode domain should be red. Left click
- 7) R2 should appear
- 8) Build all





# 1 Heat Transfer in Solids (ht)

- ▶ Heat Transfer in Solids 1
- ▶ Initial Values 1
- ▶ Axial Symmetry 1
- ▶ Thermal Insulation 1
- Equation View

- 1) Go to 'Heat transfer in solids' >> 'Heat transfer in solids 1'
- 2) In the middle panel, scroll down to k, ρ, and Cp
- 3) Select 'user defined' for all 3 properties
- 4) Input heat transfer properties as shown

Settings  
Heat Transfer in Solids

Label: Heat Transfer in Solids 1

Domain Selection

Selection: All domains

1  
2

Active

Override and Contribution

Equation

Show equation assuming:  
Study 1, Time Dependent

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q + Q_{\text{rad}}$$
$$\mathbf{q} = -k \nabla T$$

Model Inputs

Coordinate System Selection

Coordinate system: Global coordinate system

Heat Conduction, Solid

Thermal conductivity:  
k From material

Thermodynamics, Solid

Density:  
ρ From material

Heat capacity at constant pressure:  
C<sub>p</sub> From material

User defined

From material

User defined

Isotropic

Heat Conduction, Solid

Thermal conductivity:

k User defined

(.4925+.001195\*(T[1/K])) [W/(m\*K)] W/(m\*K)

Isotropic

Thermodynamics, Solid

Density:

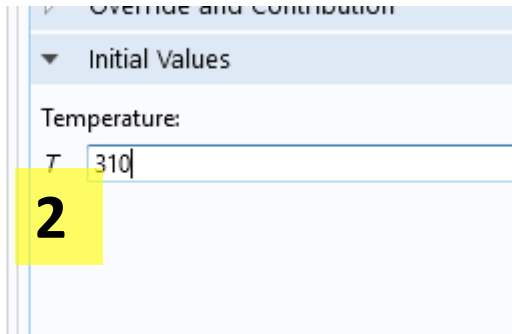
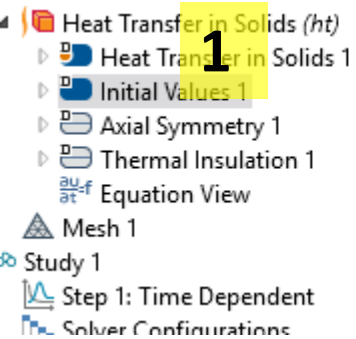
ρ User defined

1200 kg/m<sup>3</sup>

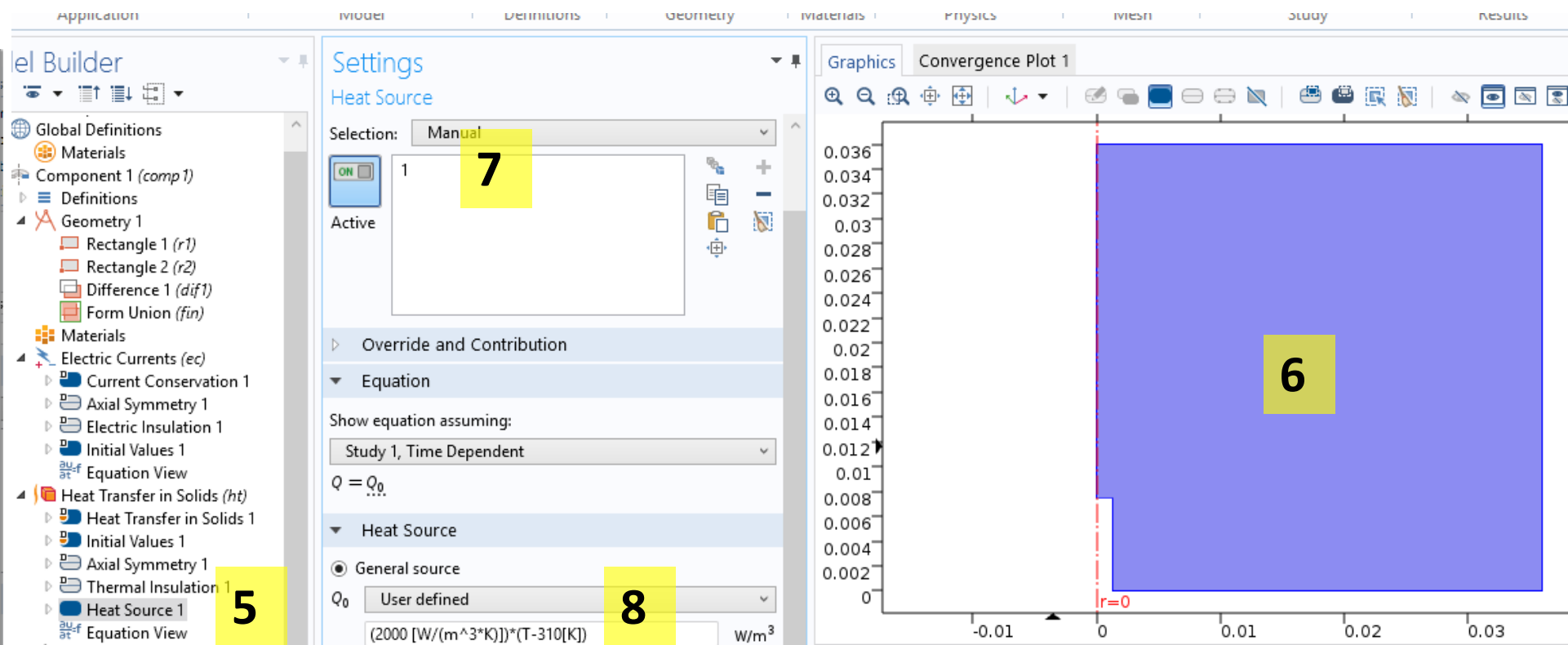
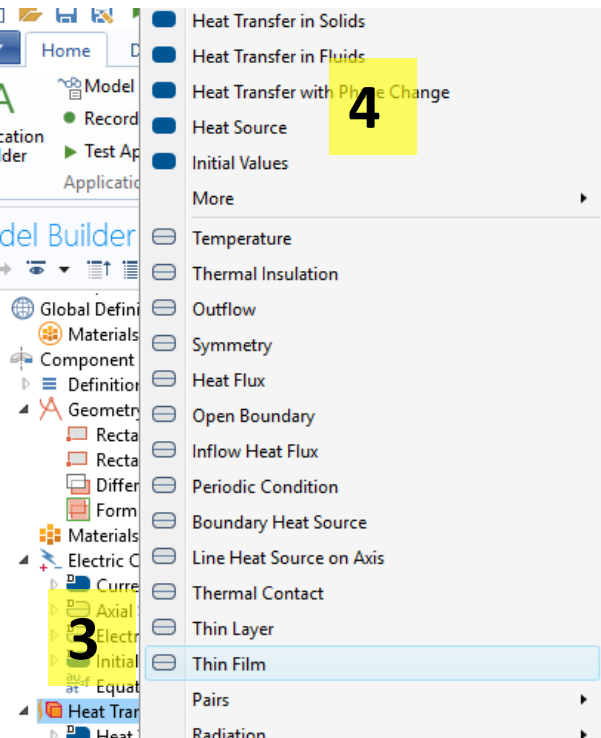
Heat capacity at constant pressure:

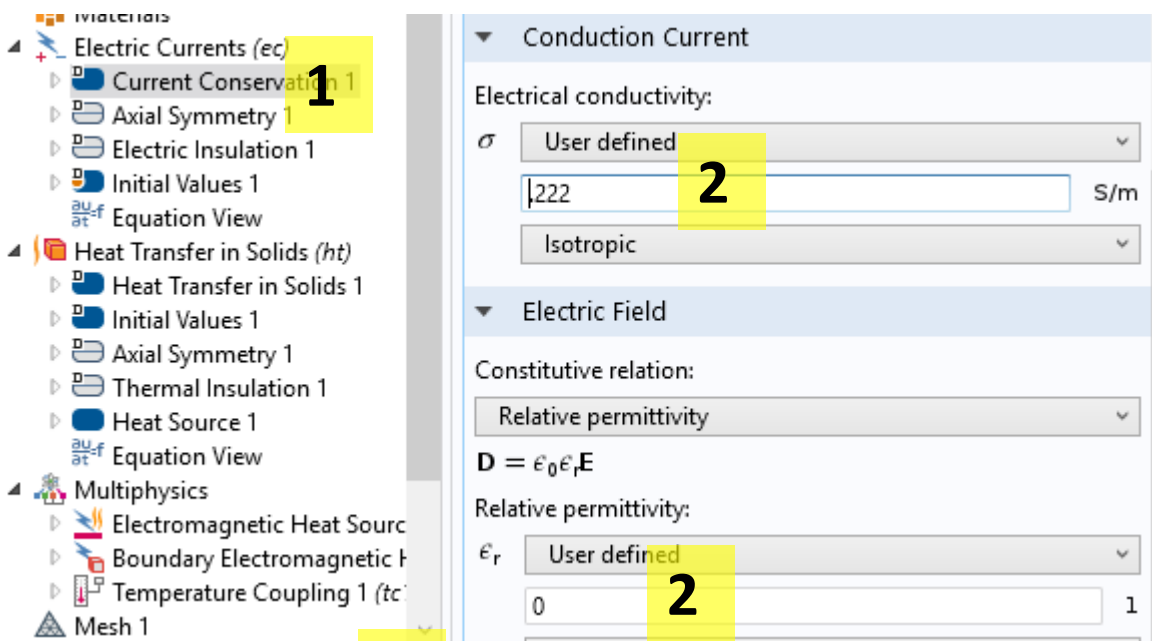
C<sub>p</sub> User defined

3200 J/(kg\*K)

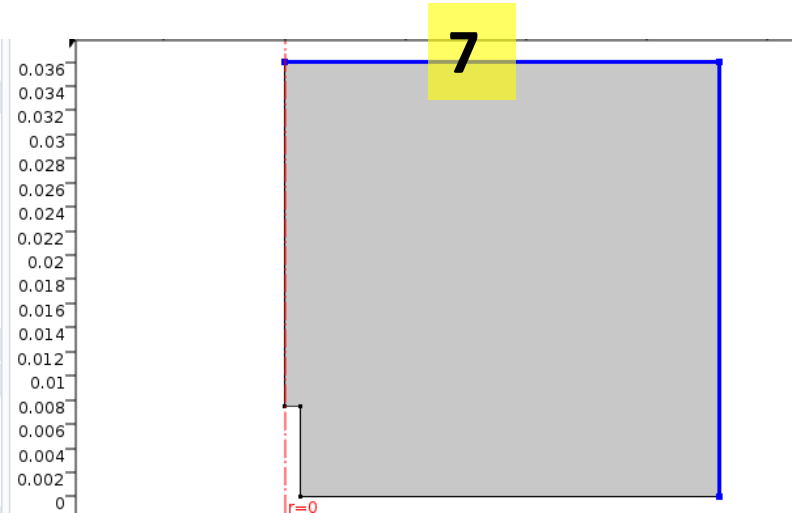
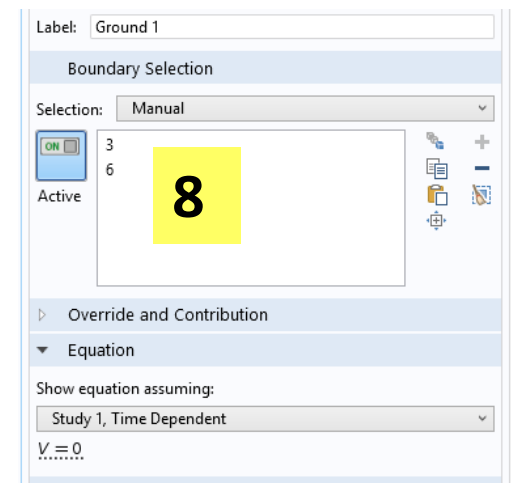
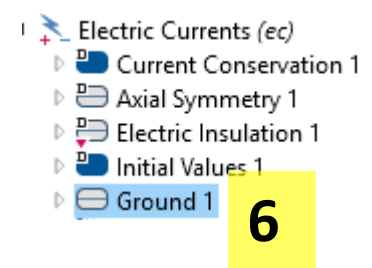
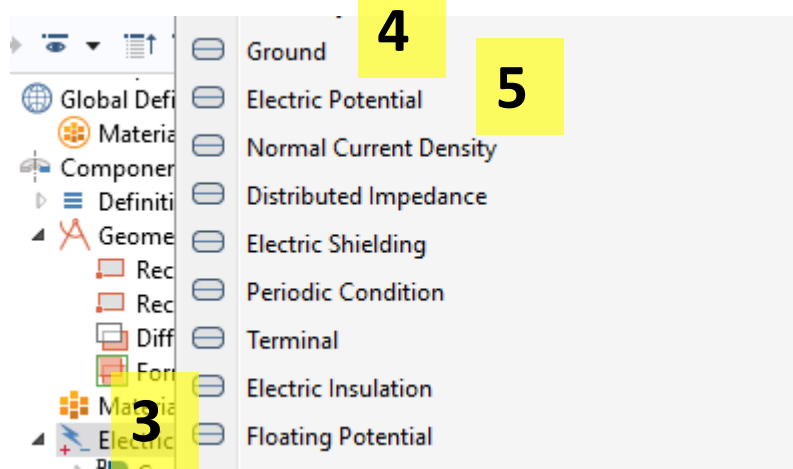


- 1) Left click 'Initial values 1'
- 2) Enter 310 K
- 3) Right click 'Heat transfer in solids'
- 4) Select heat source'
- 5) Left click on 'heat source 1'
- 6) Left click domain
- 7) 1 should appear
- 8) Enter heat source value shown





- 1) Left click Current conservation 1
- 2) Enter electrical conductivity and relative permittivity
- 3) Right click 'Electric currents'
- 4) Select 'Ground'
- 5) Repeat 3 and select electric potential
- 6) Left click on 'ground 1'
- 7) Select 2 boundaries in below
- 8) 3 and 6 should appear



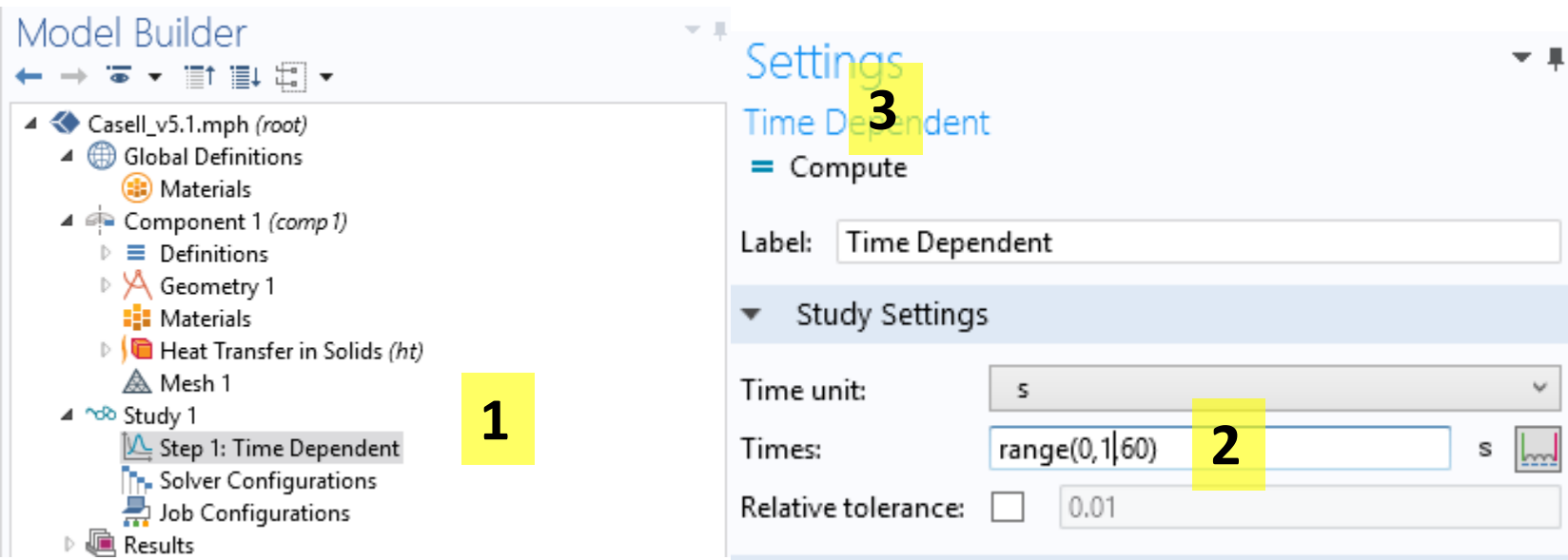
- 1) Select electric potential 1
- 2) Enter 25
- 3) Select 2 boundaries in blue
- 4) 2 and 4 should appear

The screenshot displays the COMSOL Multiphysics software interface. On the left, the 'Model Builder' tree shows the hierarchy: Global Definitions, Materials, Component 1 (comp 1), Definitions, Geometry 1, Materials, Electric Currents (ec), and Heat Transfer in Solids (ht). The 'Electric Potential 1' node is highlighted with a yellow box labeled '1'. In the center, the 'Settings' panel for 'Electric Potential' is shown. The 'Label' is 'Electric Potential 1'. Under 'Boundary Selection', the 'Selection' is set to 'Manual', and the list contains '2' and '4', with '4' highlighted by a yellow box labeled '4'. The 'Equation' section shows 'Show equation assuming: Study 1, Time Dependent' and the equation  $V = V_0$ . The 'Electric Potential' section has 'Electric potential:  $V_0$ ' set to '25', with '25' highlighted by a yellow box labeled '2'. On the right, the 'Graphics' window shows a 'Convergence Plot 1' with a plot area. A vertical red dashed line is at  $r=0$ . Two blue brackets on the plot indicate selected boundaries, with the right one highlighted by a yellow box labeled '3'. The plot axes range from -0.01 to 0.03 on the x-axis and 0 to 0.036 on the y-axis.

- 1) Left click mesh 1
- 2) Select 'normal'
- 3) Click build all

The screenshot displays the COMSOL Multiphysics interface. On the left, the 'Model Builder' tree shows a hierarchy of objects, with 'Mesh 1' highlighted at the bottom and a yellow '1' next to it. The central 'Settings' pane is open to the 'Mesh' section, where the 'Build All' button is highlighted with a yellow '3'. Below it, the 'Mesh Settings' section shows 'Sequence type' set to 'Physics-controlled mesh' and 'Element size' set to 'Normal', with a yellow '2' next to the 'Normal' dropdown. On the right, the 'Graphics' window shows a 'Convergence Plot 1' with a triangular mesh. A vertical red dashed line at  $r=0$  is visible on the left side of the mesh.

- 1) Left click "Step 1: Time dependent"
- 2) Enter range(0,1,60)
- 3) Click compute



1

Materials  
Component 1 (comp 1)  
Definitions  
Geometry 1  
Materials  
Heat Transfer in Solids (ht)  
Mesh 1  
Study 1  
Step 1: Time Dependent  
Solver Configurations  
Job Configurations  
Results  
Data Sets

Particle  
Ray  
Array 3D  
Mirror 3D  
Sector 3D  
Isosurface  
Parameterized Surface  
Parameterized Curve 3D  
Grid 3D  
Array 2D  
Mirror 2D  
Sector 2D  
Contour  
Parametric Extrusion 2D  
Parameterized Curve 2D  
Grid 2D  
Parametric Extrusion 1D  
Grid 1D  
Average  
Integral  
Maximum  
Minimum  
Time Average  
Time Integral

2

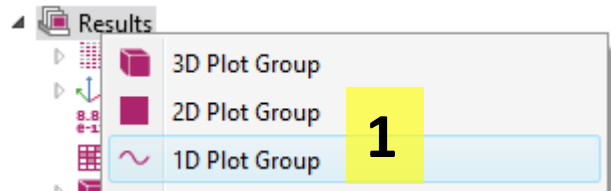
- 1) Right click data sets
- 2) Select 'cut point 2d'
- 3) Do step 1 again and select 'Average'
- 4) Left click 'cut point 2D 1'
- 5) Enter r=0.0013 and z = 0.0075

Equation View  
Heat Transfer in Solids (ht)  
Heat Transfer in Solids 1  
Initial Values 1  
Axial Symmetry 1  
Thermal Insulation 1  
Heat Source 1  
Equation View  
Multiphysics  
Electromagnetic Heat Source  
Boundary Electromagnetic He  
Temperature Coupling 1 (tc1)  
Mesh 1  
Study 1  
Step 1: Time Dependent  
Solver Configurations  
Job Configurations  
Results  
Data Sets  
Study 1/Solution 1  
Revolution 2D 1  
Revolution 2D 2  
Cut Point 2D 1

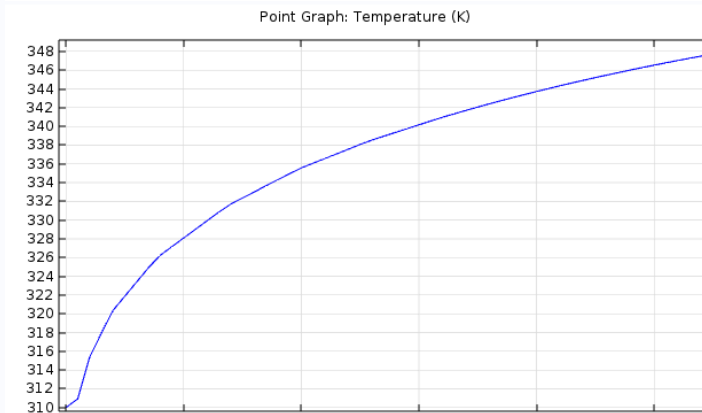
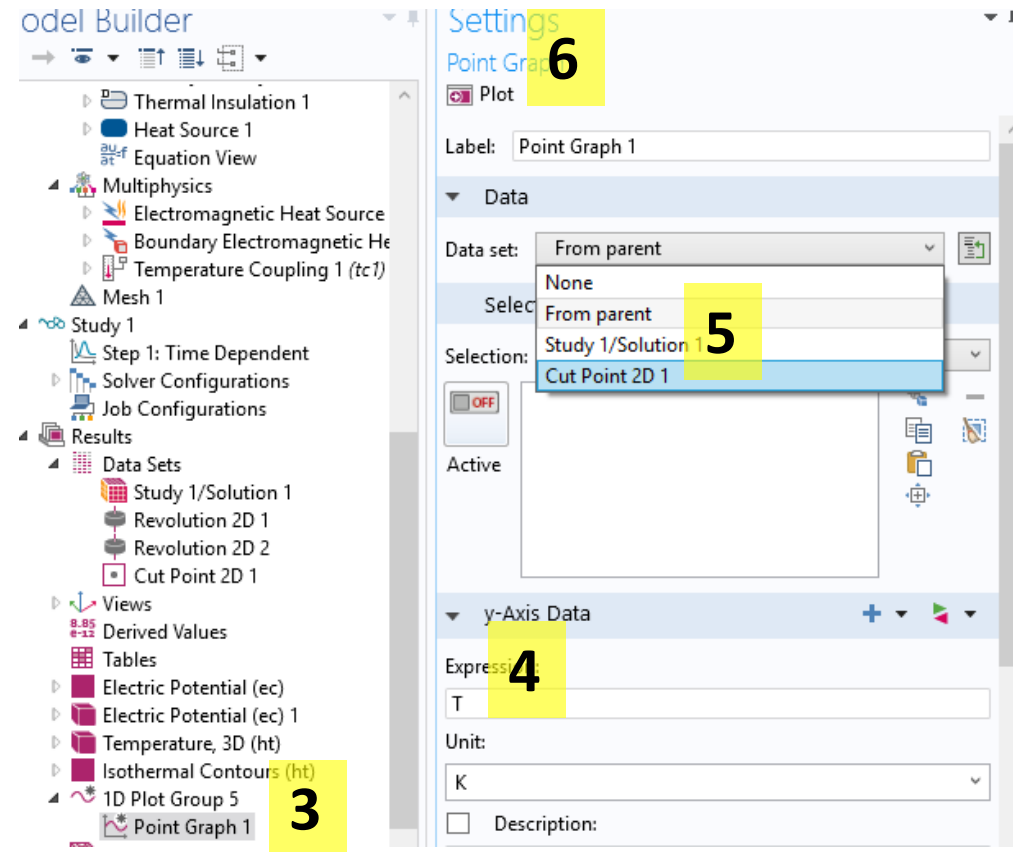
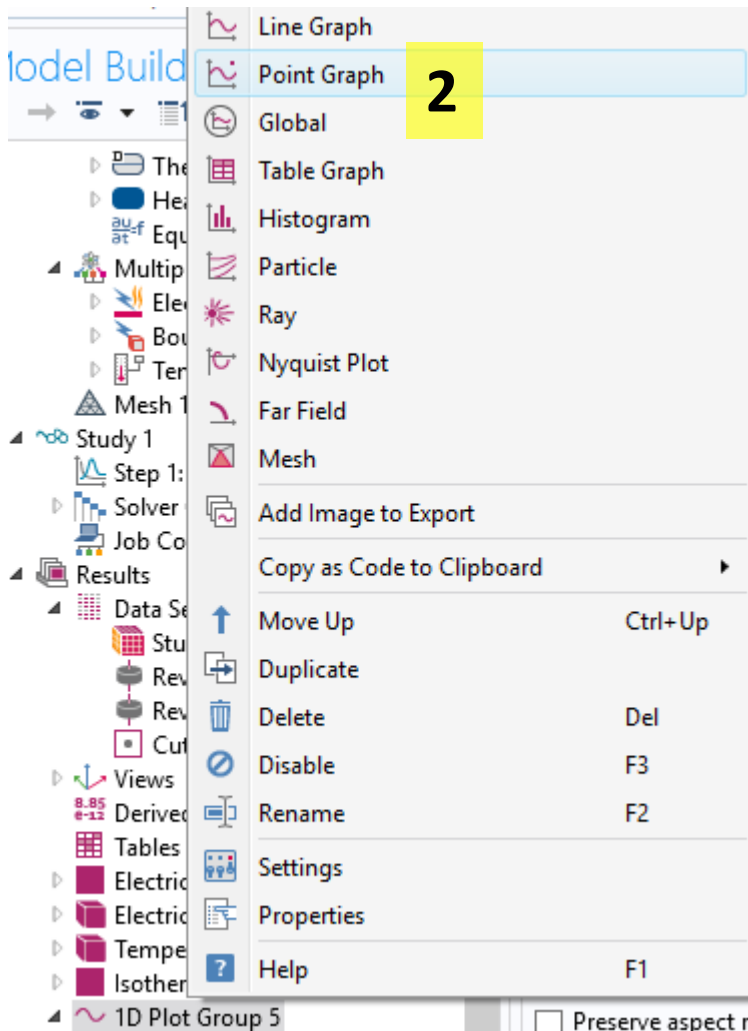
4

CUT POINT 2D  
Plot  
Label: Cut Point 2D 1  
Data  
Data set: Study 1/Solution 1  
Point Data  
Entry method: Coordinates  
r: 0.0013 m  
z: 0.0075 m  
 Snap to closest boundary

5



- 1) Right click 'results', Select '1D plot group'
- 2) Right click '1D plot group 5' and add 'point graph'
- 3) Left click 'point graph 1'
- 4) Enter T
- 5) Select 'Cut point 2D 1'
- 6) Click plot





Tooth



This homework assignment will teach the basics of doing simulations and actual geometries. The example here will be the heating of a tooth. The tooth was acquired from a full body MRI scan in the website listed herein. We will download the data from the scan just for the tooth. Clean the geometry by smoothing it, filling gaps in the surface, and decreasing the number of faces. Then, we will convert it to a solid object to simulate in COMSOL. Finally, we will solve a heat conduction problem.

The one major step we are not covering here is the geometry segregation step. This step involves taking raw MRI images and extracting the tooth geometry using imaging algorithms. Fortunately, the website here has done that step for us. We will focus on cleaning up the geometry such that it is capable of having a simulation run on it.

BodyParts3D/Anatomography : Select parts and Make Embeddable Model of Your Own. See What You can get See How to

Data Version 4.3

1 Parts of FMA (3.0) content  
 2 IS-A Tree (14)  
 HAS PART Tree (0)

3 obj2FMA Information

View Sort by Models for concepts in "IS-A Tree of FMA3.0"  
 Front Volume ELEMENT/PRIMARY: COMPOUND/SECONDARY: Good -- poor  
 Show only Unique models

4

5

Representation: BP23278

Representation: BP23278  
 Model component: FJ1261, FJ1263, FJ1275, FJ1276

download obj files

Representation method: COMPOUND

Share comments on BP23278 (0)

Model / Concept density: 66.66%  
 Represented / missing component

BP19601: FMA55697 Right upper second secondary molar tooth

BP20230: FMA55698 Right upper first secondary molar tooth

BP20252: FMA55699 Left upper first secondary molar tooth

BP21638: FMA55700 Left upper second secondary molar tooth

NONE: FMA55696 Right upper third secondary molar tooth

NONE: FMA55701 Left upper third secondary molar tooth

92 Objs

Name	Represented	Volume(cm3)
Upper secondary	FMA55720	4.9044
Upper secondary	FMA55716	3.1473
Upper first secor	FMA55811	2.7949
Upper second se	FMA55812	2.1095
Upper first secor	FMA55801	1.6079
Upper second se	FMA55802	1.5395
Left upper first se	FMA55699	1.3979
Right upper first :	FMA55698	1.3969
Right upper seco	FMA55697	1.0551
Left upper secon	FMA55700	1.0544
Right upper first :	FMA55689	0.8043
Left upper first se	FMA55690	0.8036
Left upper secon	FMA55691	0.7698
Right upper seco	FMA55688	0.7697
Cement of upper	FMA55874	
Alveolar compart	FMA269926	
Socket for right u	FMA269646	
Alveolar compart	FMA269920	
Socket for left up	FMA269686	

- 1) Go to: <http://lifesciencedb.jp/bp3d/?lng=en>
- 2) Select 4.3
- 3) Search for 'Upper secondary molar tooth'
- 4) Click 'Upper secondary molar tooth'
- 5) Click 'download obj'
- 6) Select the first one 'FJ1261'
- 7) Click download

BP23278 - Google Chrome

lifesciencedb.jp/bp3d/download-art\_file-list.cgi?type=html&rep\_id=BP23278&lng=en

check all uncheck all

	del comp	represented	english name	model	compatibility	timestamp	volume
1	<input checked="" type="checkbox"/>	FJ1261	Left upper first secondary molar tooth	BodyParts3D	4.0	2011/05/18	1.4100
2	<input type="checkbox"/>	FJ1263	Left upper second secondary molar tooth	BodyParts3D	4.0	2011/05/18	1.0660
3	<input type="checkbox"/>	FJ1275	Right upper second secondary molar tooth	BodyParts3D	4.0	2011/05/18	1.0660
4	<input type="checkbox"/>	FJ1276	Right upper first secondary premolar tooth	BodyParts3D	4.0	2011/05/18	1.4089

6

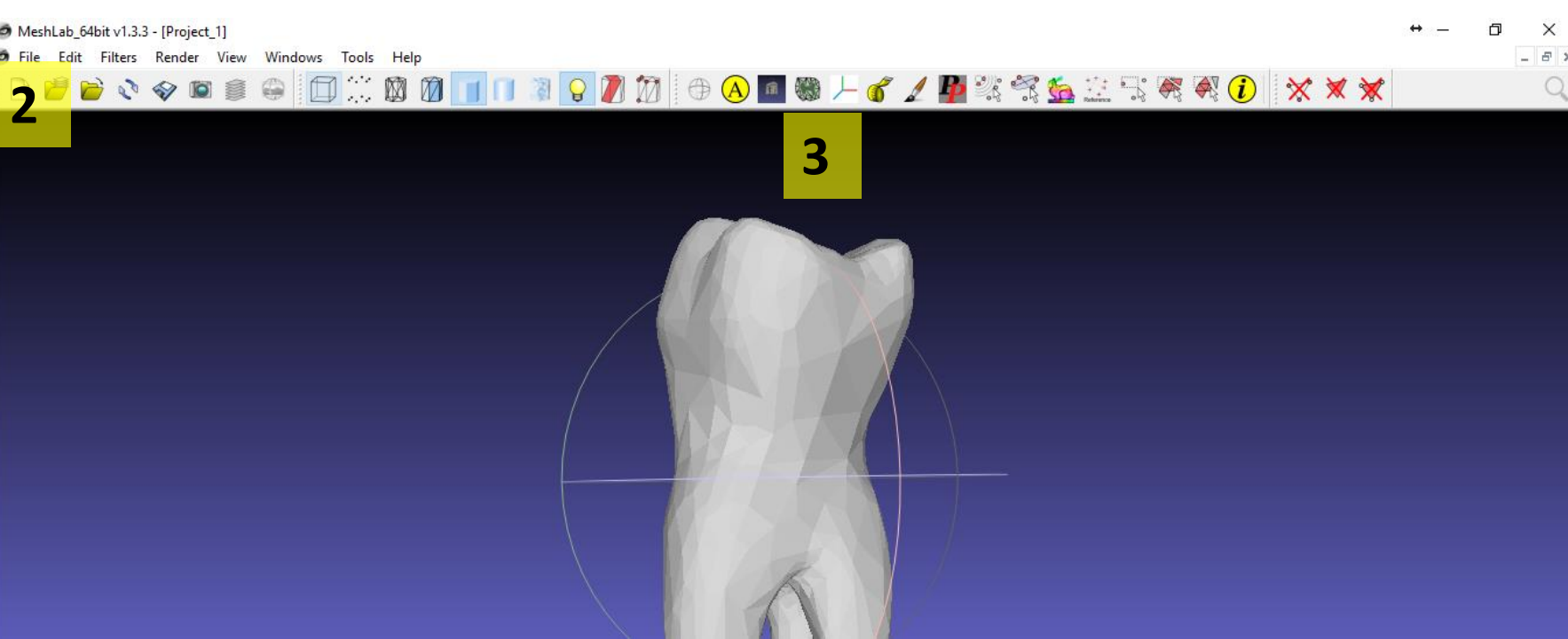
7

Page 1 of 1 1 - 4 / 4

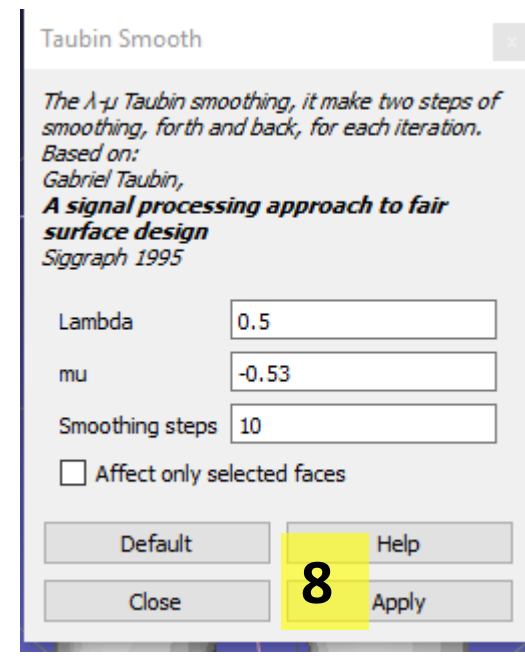
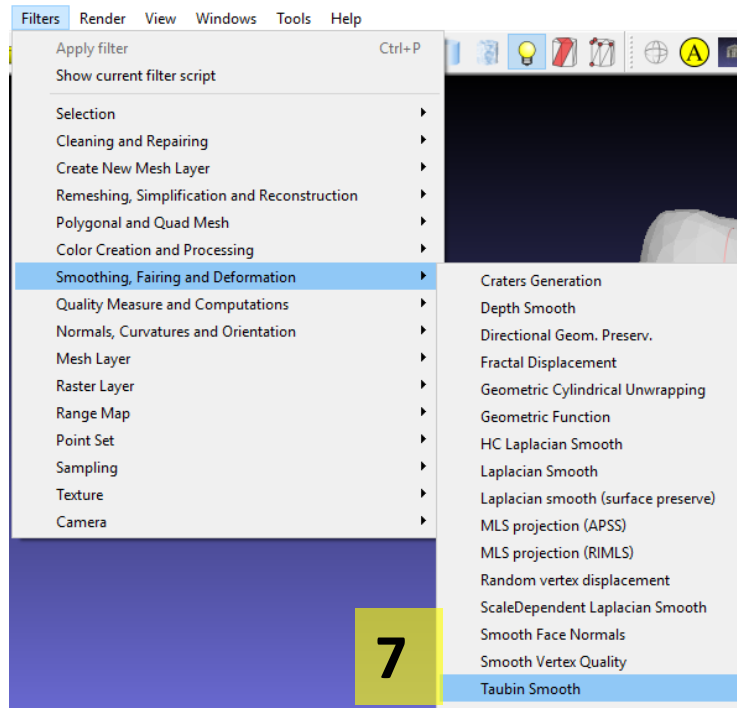
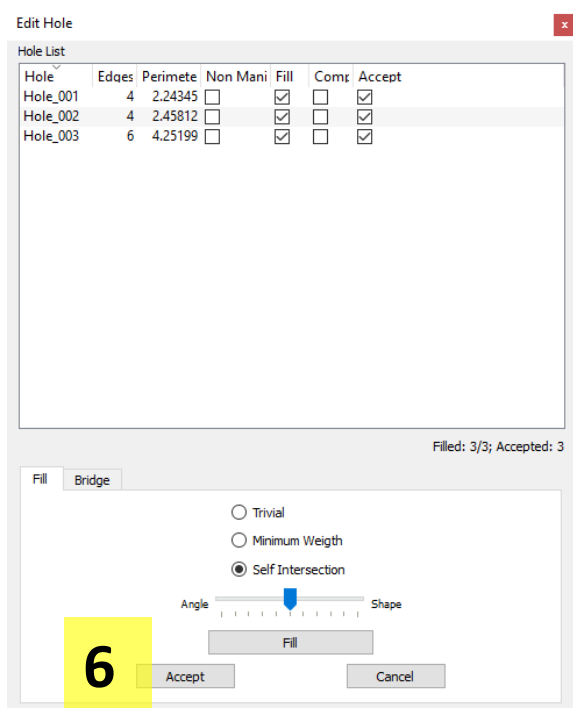
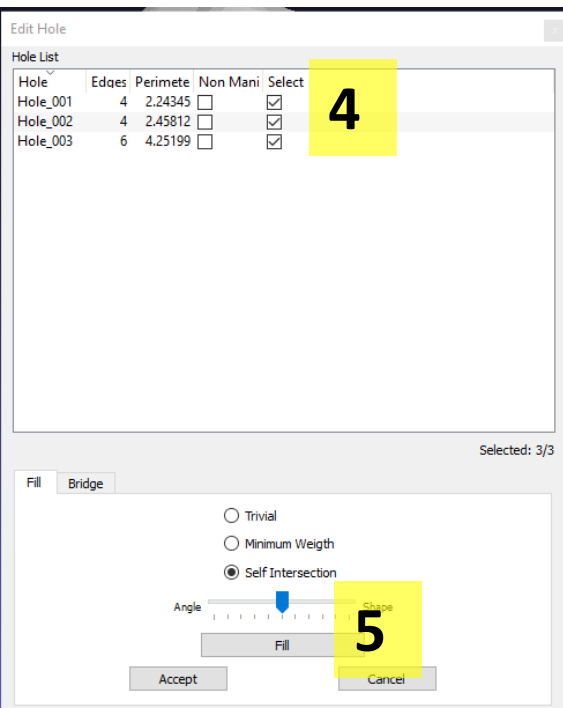
Download License terms

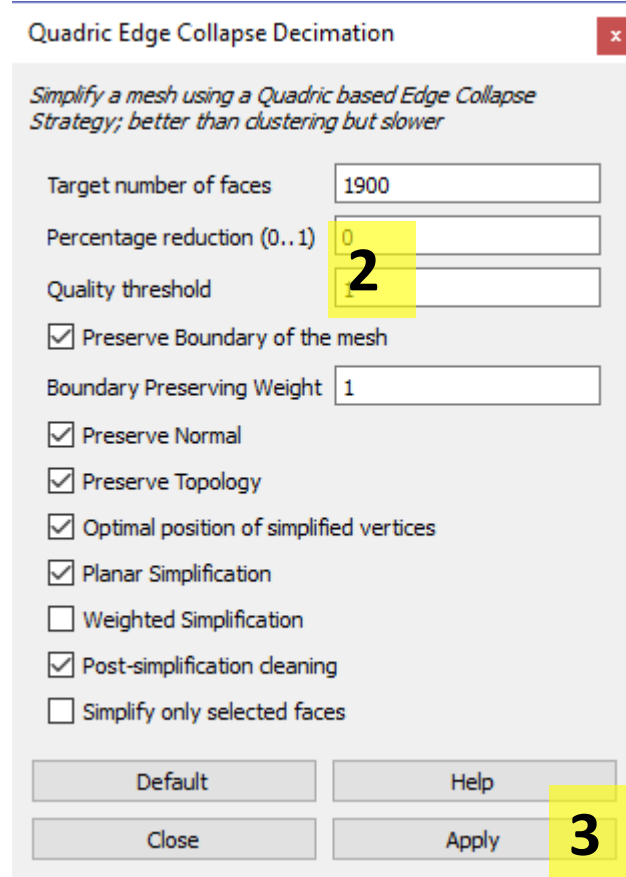
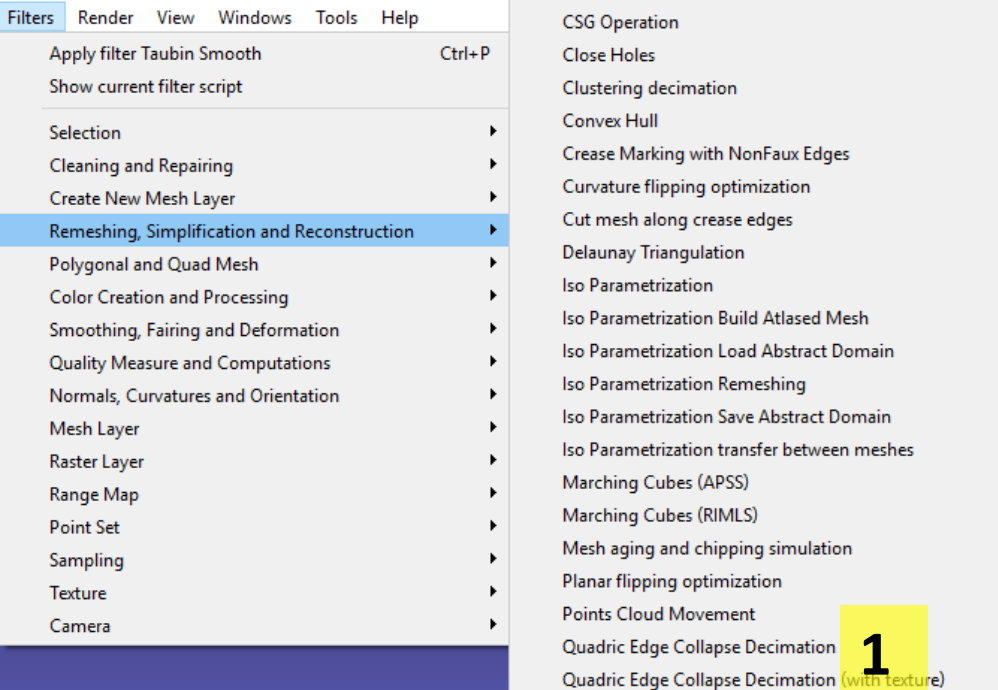
BP23278\_FMA3\_0\_isa...zip

Show all downloads...

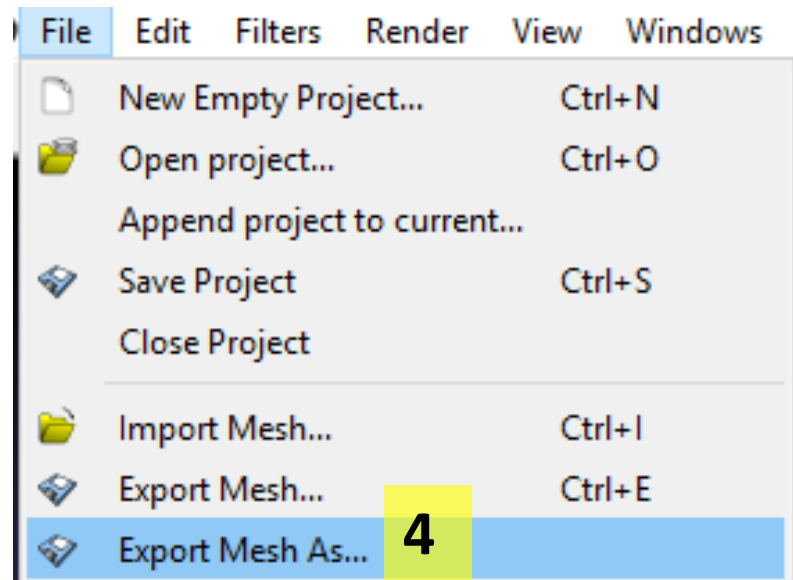


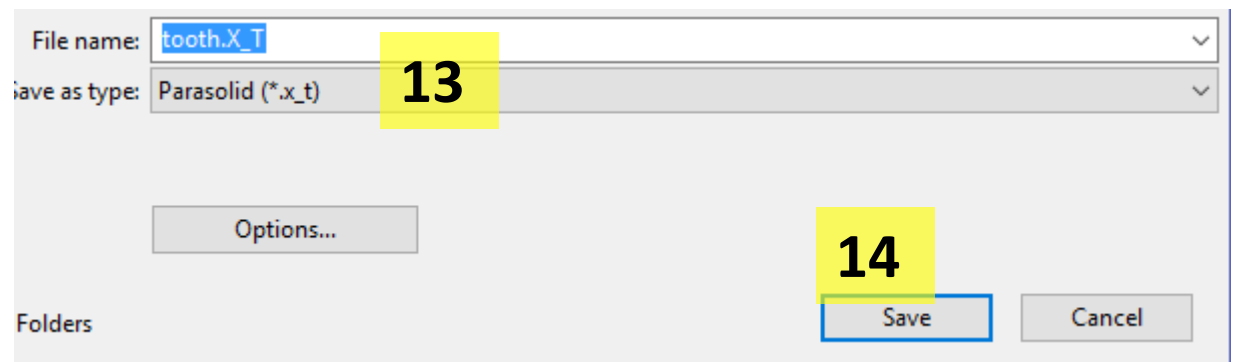
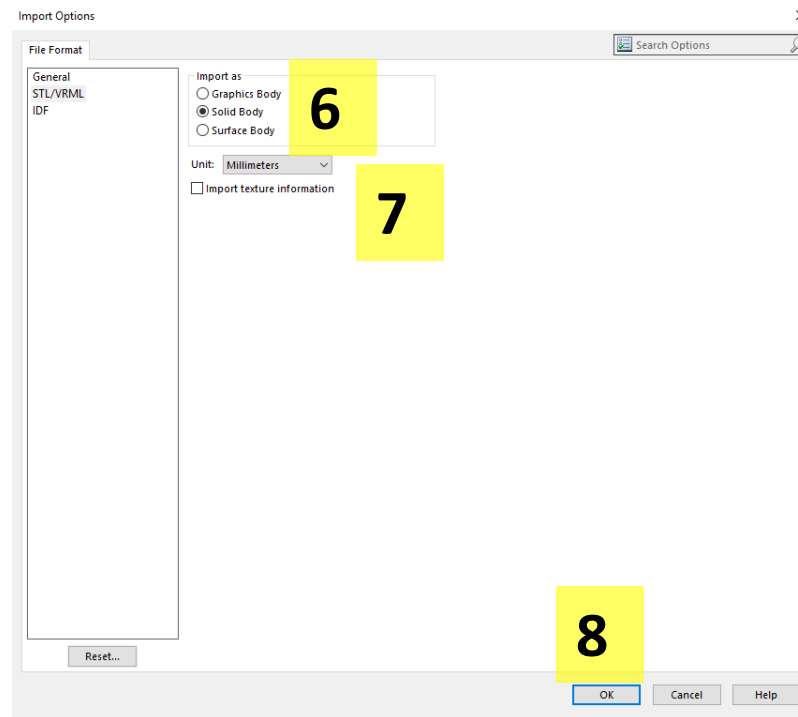
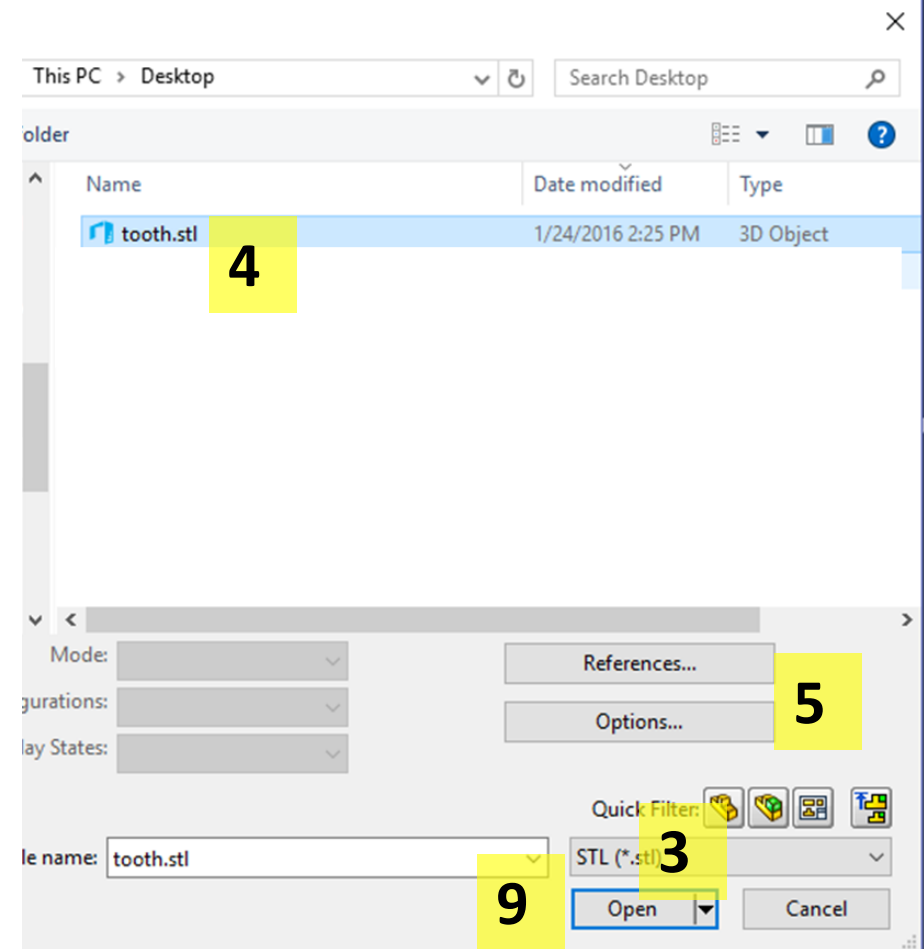
- 1) Open Meshlab or download from: <http://meshlab.sourceforge.net/>
- 2) In Meshlab, File>>import Mesh and select the obj file you downloaded
- 3) Click the 'fill hole' icon (you can hover over with the cursor to make sure which one it is)
- 4) Select all
- 5) Click 'Fill'
- 6) Click accept
- 7) Go to filters>>Smoothing, Fairing, and deformation>>Taubin smooth
- 8) Click apply
- 9) **Repeat 3-6 again**



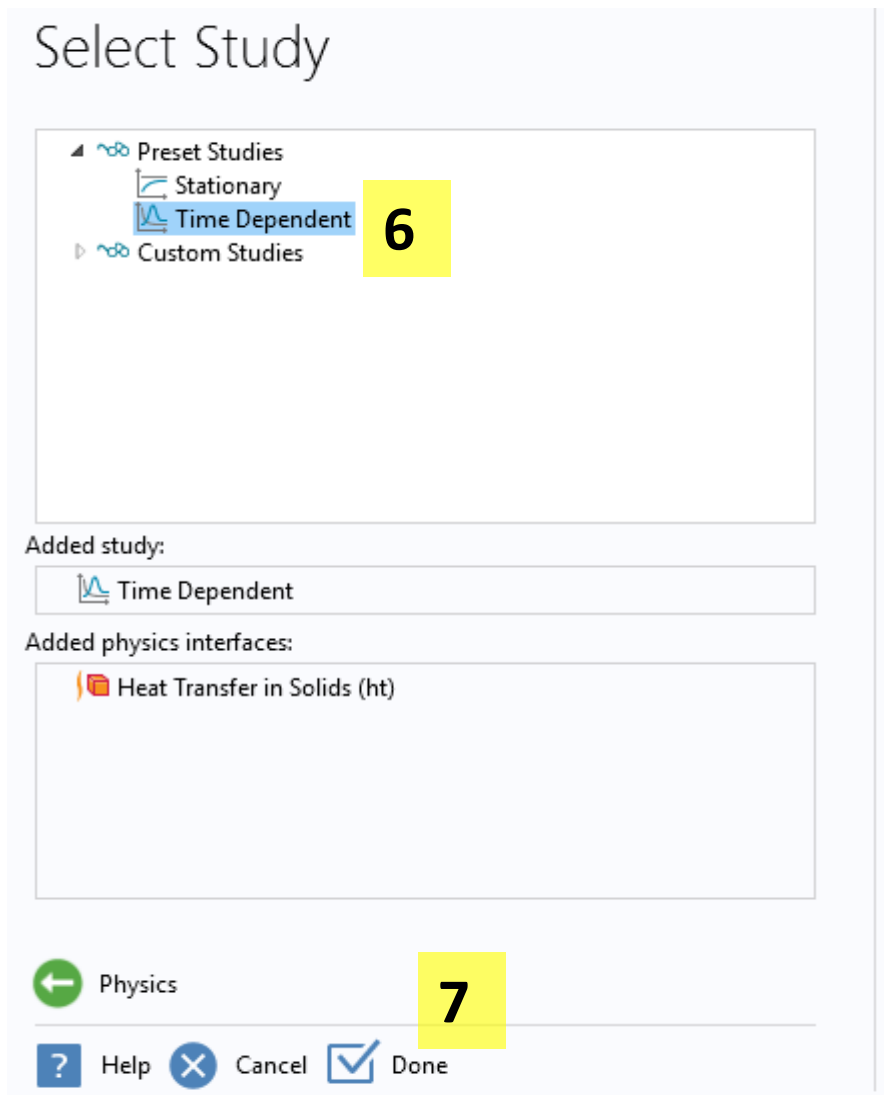
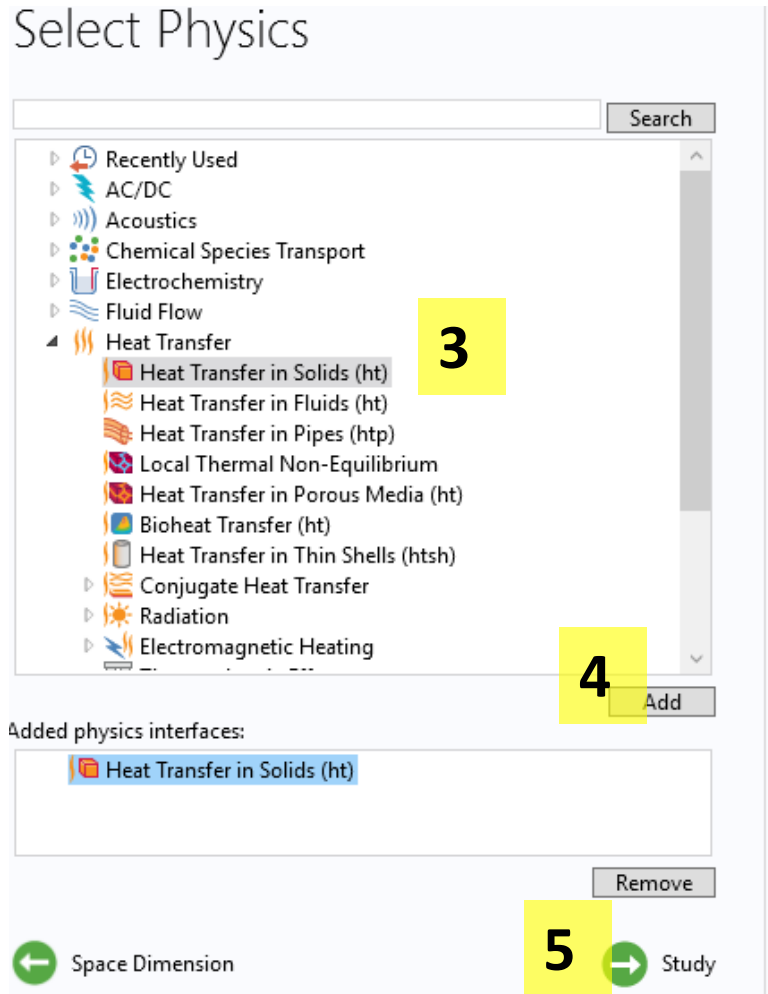
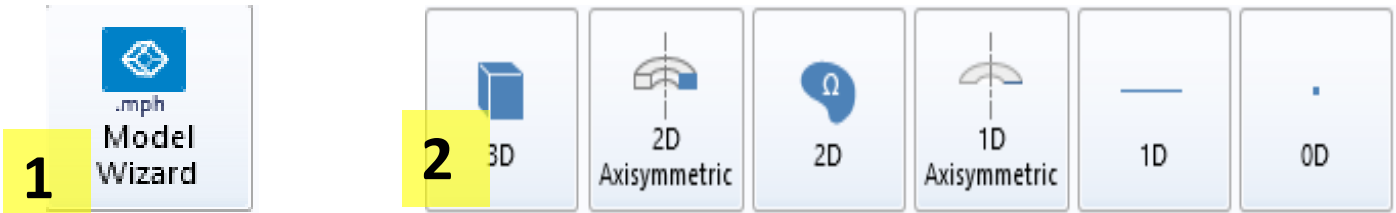


- 1) Go to filters>>Remeshing, simplifications, and reconstruction>>Quadratic edge collapse decimation
- 2) Enter the settings shown
- 3) Click apply
- 4) Go to file>>export mesh as...
- 5) **Save the file as \*.stl format and click ok to whatever boxes appear.**

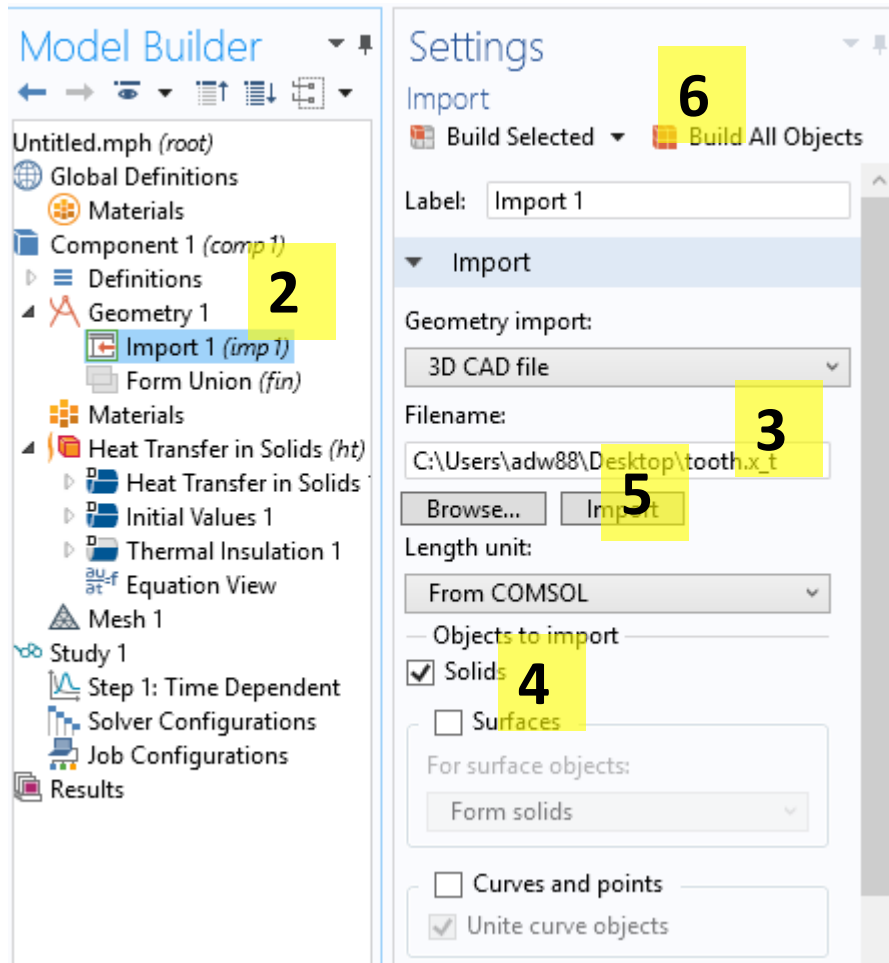
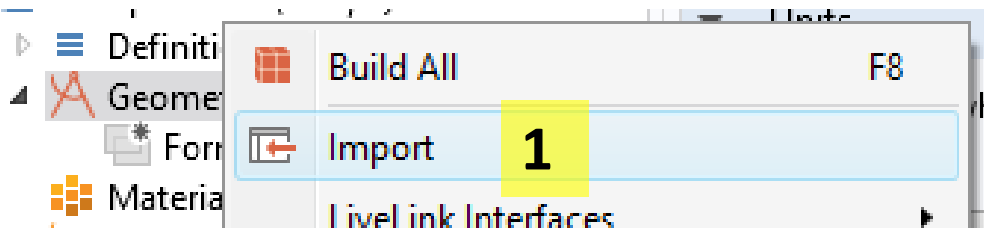




- 1) Open solidworks
- 2) Click the 'open' folder in the top left
- 3) Choose \*.stl file
- 4) Click your file
- 5) Select 'options'
- 6) Select solid body
- 7) Select millimeters
- 8) Click ok
- 9) Click open
- 10) Click ok to a message box about units
- 11) You do not need to run the diagnostics
- 12) Click save icon in top left
- 13) Save as a parasolid \*.x\_t
- 14) Click save



- 1) Select model wizard
- 2) Select 2D Axisymmetric
- 3) Select 'Heat transfer in solids'
- 4) Click 'Add'
- 5) Click 'Study'
- 6) Click 'Time Dependent'
- 7) Click 'Done'



- 1) Right click geometry, select import
- 2) Left click import 1
- 3) Select your .x\_t file
- 4) Only select solids
- 5) Click import
- 6) Build all



- Heat Transfer in Solids (ht)
  - Heat Transfer in Solids 1 **1**
  - Initial Values 1
  - Thermal Insulation 1 **5**
  - Equation View

- 1) Go to 'Heat transfer in solids' >> 'Heat transfer in solids 1'
- 2) In the middle panel, scroll down to k, ρ, and Cp
- 3) Select 'user defined' for all 3 properties
- 4) Input heat transfer properties as shown
- 5) Click initial values 1
- 6) Enter 310 K

Settings  
Heat Transfer in Solids

Label: Heat Transfer in Solids 1

Domain Selection

Selection: All domains

1  
Active

Override and Contribution

Equation

Show equation assuming:  
Study 1, Time Dependent

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q + Q_{\text{ext}}$$

$$\mathbf{q} = -k \nabla T$$

Model Inputs

Coordinate System Selection

Coordinate system: Global coordinate system **2**

Heat Conduction, Solid

Thermal conductivity:

k From material

Thermodynamics, Solid

Density:

ρ From material

Heat capacity at constant pressure:

C<sub>p</sub> From material

**3** User defined

From material

User defined

Isotropic

Coordinate System Selection

Coordinate system: Global coordinate system

Heat Conduction, Solid

Thermal conductivity:

k User defined

0.93 W/(m·K)

Isotropic

Thermodynamics, Solid

Density:

ρ User defined **4**

2800 kg/m<sup>3</sup>

Heat capacity at constant pressure:

C<sub>p</sub> User defined

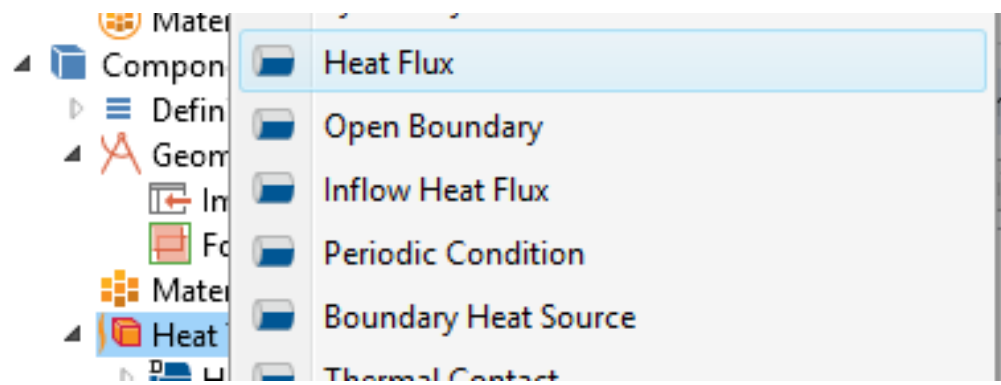
780 J/(kg·K)

Override and Contribution

Initial Values

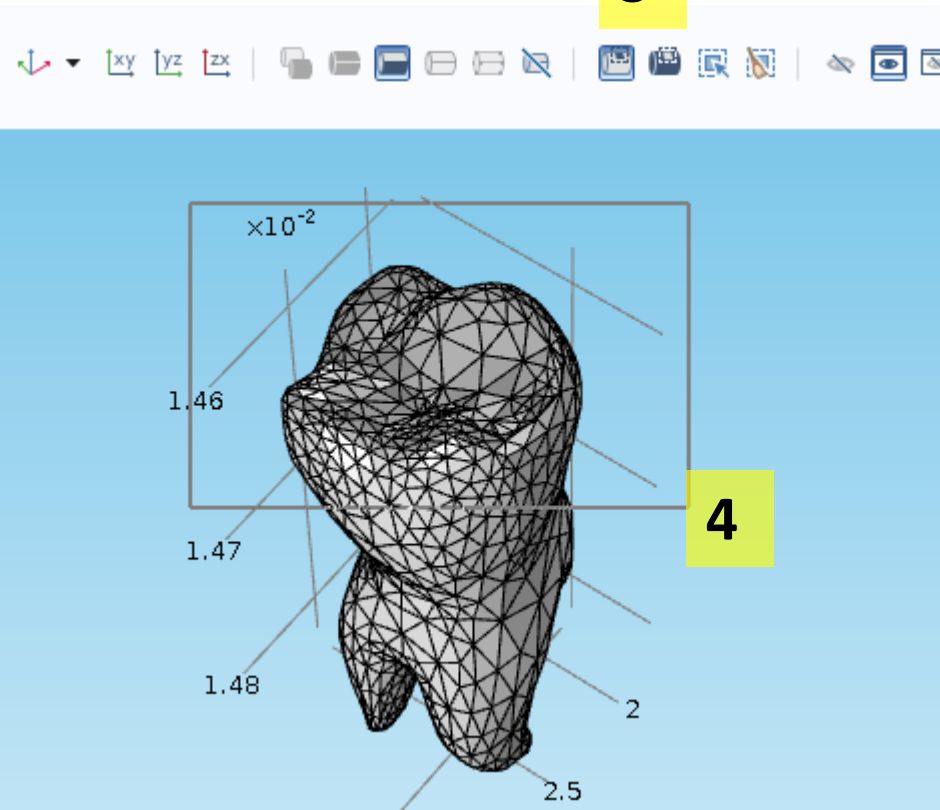
Temperature:

T 310 **6**

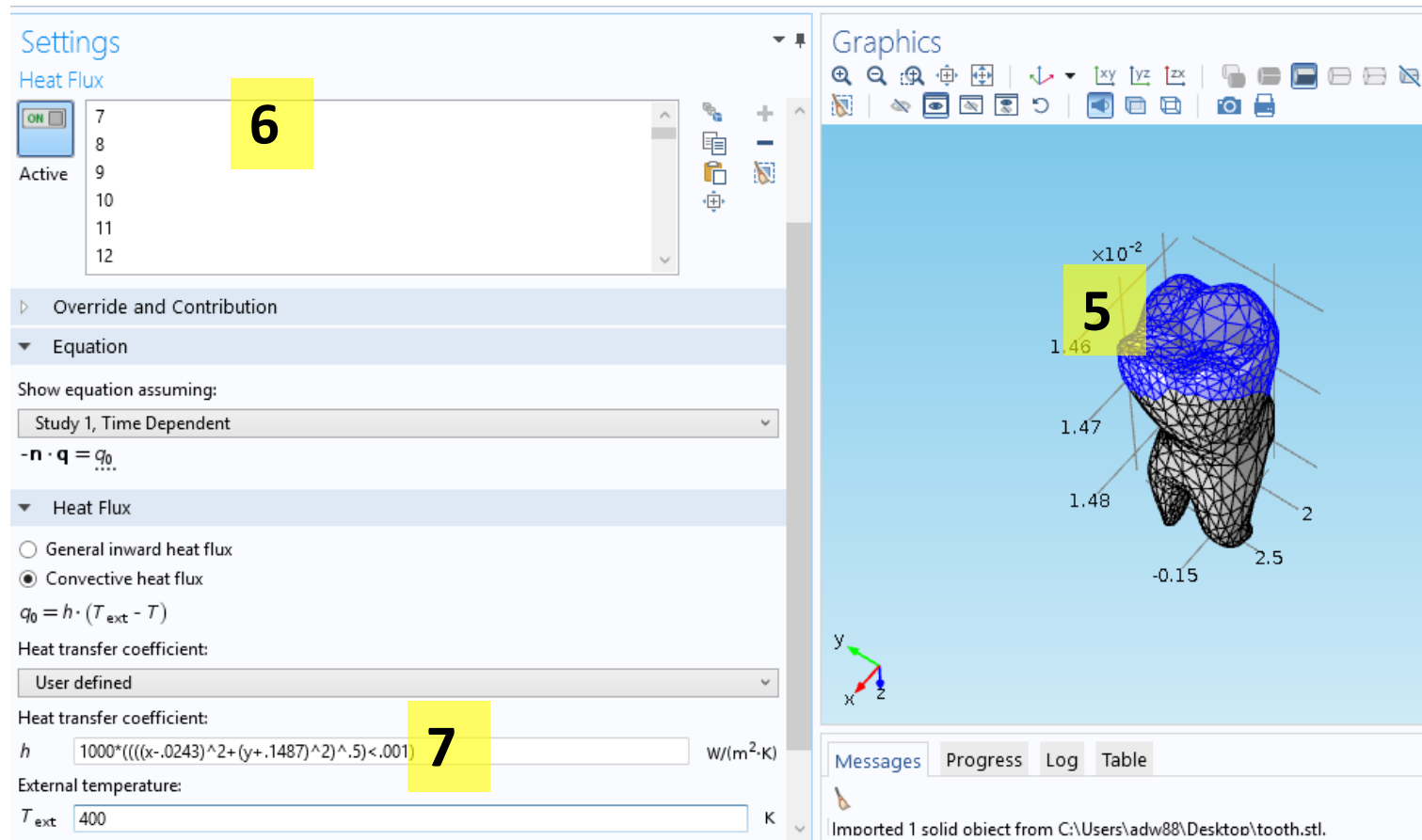


- 1) Right click 'Heat transfer in solids'
- 2) Select 'heat flux'
- 3) Select 'select box'
- 4) Draw a box as shown and let go
- 5) You should see the top turn blue
- 6) And boundaries appear
- 7) Enter the heat flux as shown

3



4

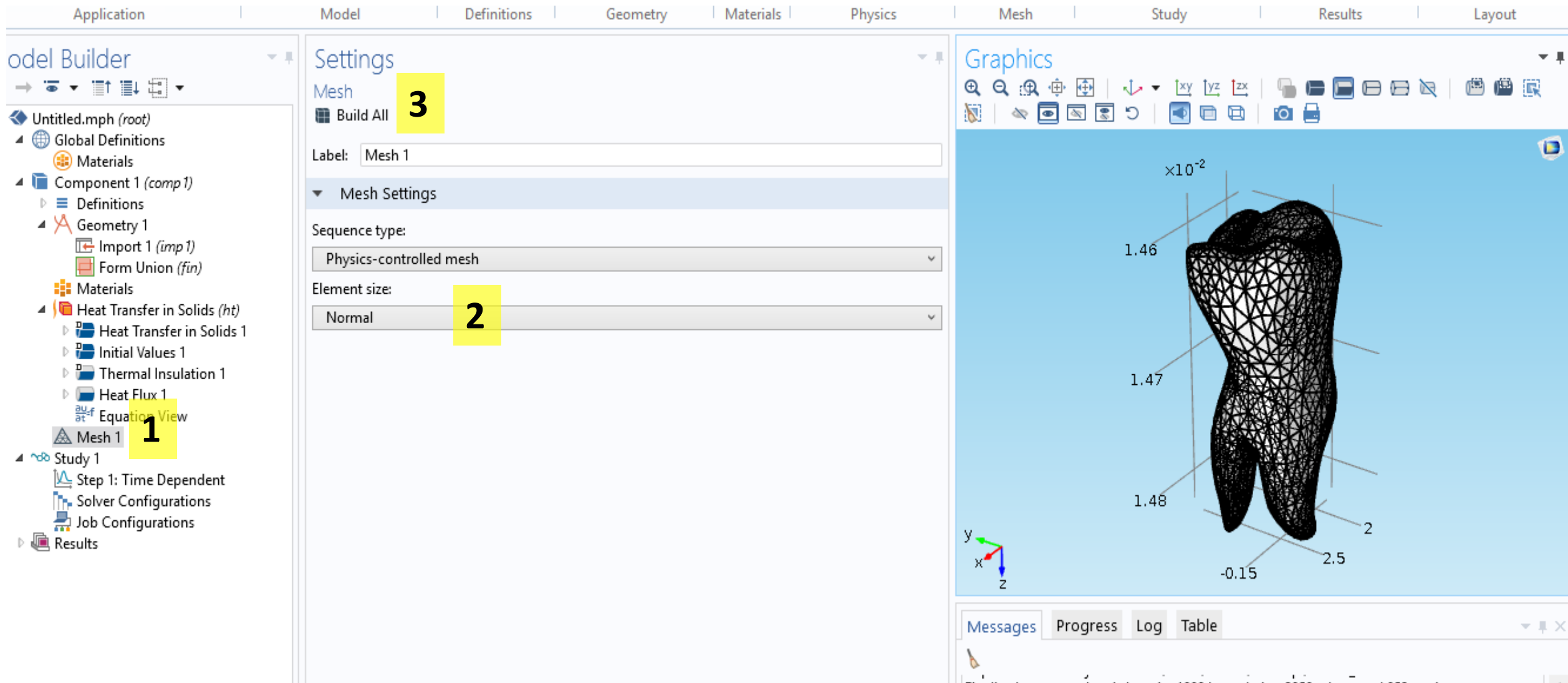


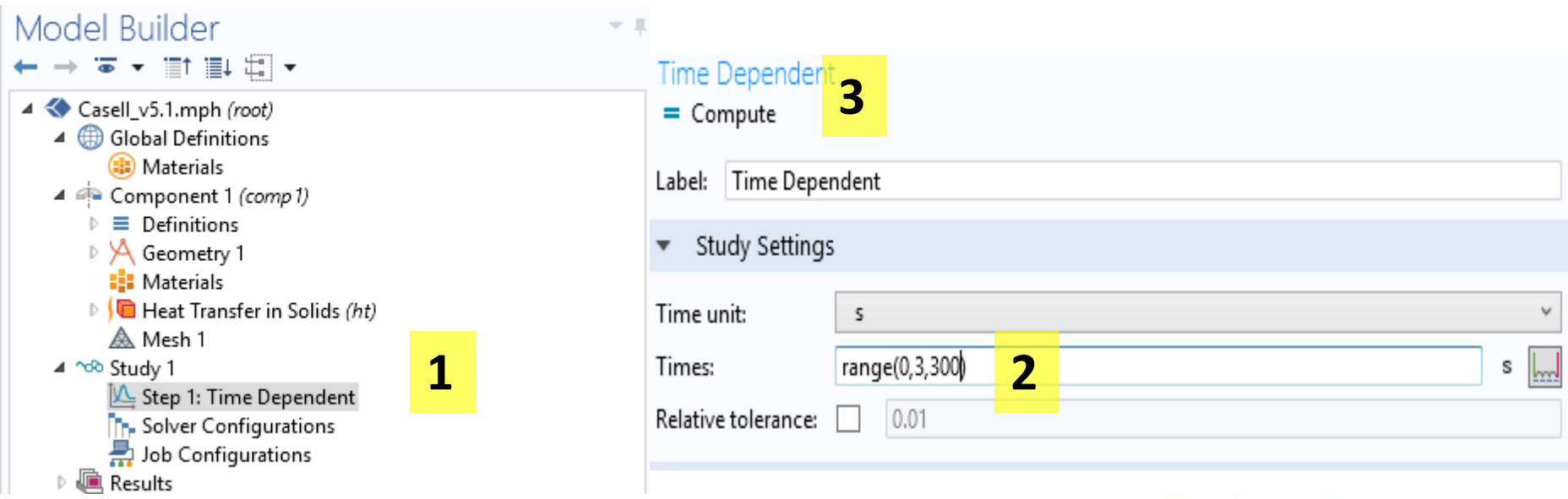
6

5

7

- 1) Left click mesh 1
- 2) Select 'normal'
- 3) Click build all





- 1) Left click "Step 1: Time dependent"
- 2) Enter range(0,3,300)
- 3) Click compute



**Homework (Case studies VII and IX in text): Due Feb. 26, 2016 in class**

Go through the case studies and submit materials asked for. Each student needs to submit this individually. **All plots must be properly labeled (title and axis names).** There are tutorials on the course website to help you use the software, please check "Tutorials" before asking.

**What to submit for Case study VII:**

- 1) How many governing equations are you solving and for what variables?
- 2) What are the boundary conditions at the distance far away from the tumor and what is the reason for this? Can another boundary condition be used here?
- 3) When inputting the diffusivity and source variables, they are each multiplied by a factor of  $x^2$ . What is the reason for this?
- 4) Plot and describe the antigen concentration from  $r=0$  to  $r=0.13$  (tumor region only) after 3 days. Based on this, do you think that the antibody treatment worked? Why or why not?
- 5) Re-run the problem but this time use an antibody concentration of 3,000 nM instead of 4.94 nM. Submit the new plot of antigen concentration vs,  $r$ -position and compare with that obtained in 4.

**What to submit for Case study IX:**

- 1) Is there another way to solve the voltage equation (Eq. 6.23) using a different physics interface?
- 2) Why do you think that the domain size chosen is appropriate, i.e., large enough?
- 3) Obtain the Contour plot of temperature (in °C) for the entire geometry with user-specified labels after 60 s. The isotherms should be 38 40 45 50 55 60 70°C
- 4) Plot in EXCEL temperature vs. time for the point (.0013, .0075)
- 5) Run the same problem but with different blood perfusion terms (set  $Q_{\text{blood}} = 4000*(310.15-T), 2000*(310.15-T), 1000*(310.15-T), 500*(310.15-T), \dots, 0$ ). As before, you can use a parametric sweep for the coefficient term. Plot temperature vs. time for the point (.0013, .0075) on a different graph than part 4 (For this problem, you might want to consider doing a parametric sweep to run it quickly)
- 6) Discuss part 5

**What to submit for the tooth assignment:**

- 1) Turn in a multislice plot of temperature at 300s
- 2) On one plot, turn in a plot of the mean, maximum, minimum and standard deviation of temperature in the tooth versus time