

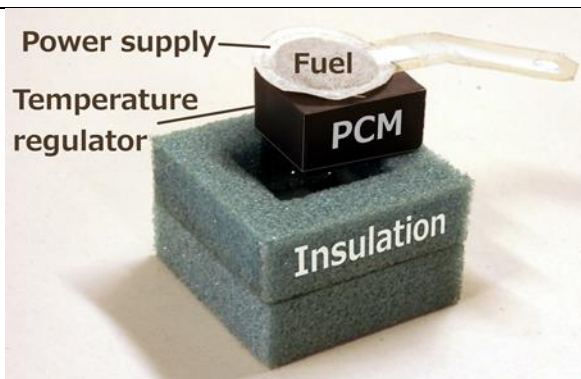
## Laboratory 7b: Thermal PDE: Phase Change Temperature Control

### Part 1: Introductory material

Despite their demonstrated utility, many diagnostic technologies can only be used in laboratories with significant infrastructure. The required supplies, electrical power, and trained users are often unavailable in low-resource settings. Decoupling diagnostics from these requirements could enable a new level of effective diagnosis and treatment at the point of care in low-resource settings.

Temperature control is an especially important aspect of diagnostic assays such as nucleic acid amplification tests (NAATs)

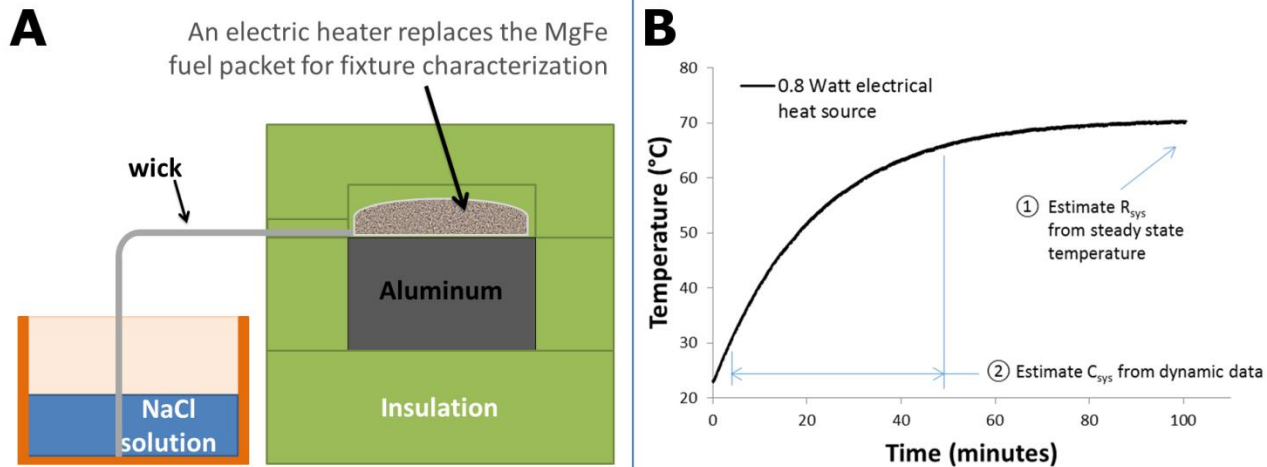
Chemical heater designed and built for use with isothermal NAATs, exploded view. The heated diagnostic assay would sit beneath the temperature regulator (PCM block) within an appropriate cut-out in the insulation. Top insulation omitted for clarity, saline reservoir not shown.



For this exercise, assume a fuel packet has already been chosen. Here, we first need to calculate the power output of the fuel pack over time, which will later be used in a PDE model to optimize device geometry. For this purpose a test fixture was designed, described below.

#### 1. Model and characterize the fuel pack test fixture

To determine the power output over time of the fuel packet, it is first necessary to quantify the thermal characteristics of the test fixture. The plotted line in the figure below represents the temperature recorded beneath an aluminum cylinder for a 0.8 W electrical heater power input. The electrical heater sits in the location of the fuel pack in panel A below, affixed to the top of the aluminum cylinder with heat transfer tape.



In order to use the chemical power source test fixture to determine the power profile produced by a given fuel pack, a simplified model can be devised. This system can be approximated by a thermal mass conducting heat through an insulating shell to an ambient temperature. A power input is applied to this thermal mass. The heat loss to ambient can then be written as:

$$P = \frac{T_{sys} - T_{amb}}{R_{sys}} \quad [1]$$

where  $R_{sys}$  is the system insulation value. Changing the temperature of the thermal mass requires

$$P = \frac{dT_{sys}}{dt} C_{sys} \quad [2]$$

where  $C_{sys}$  is the system thermal mass. The total power in to the system is then:

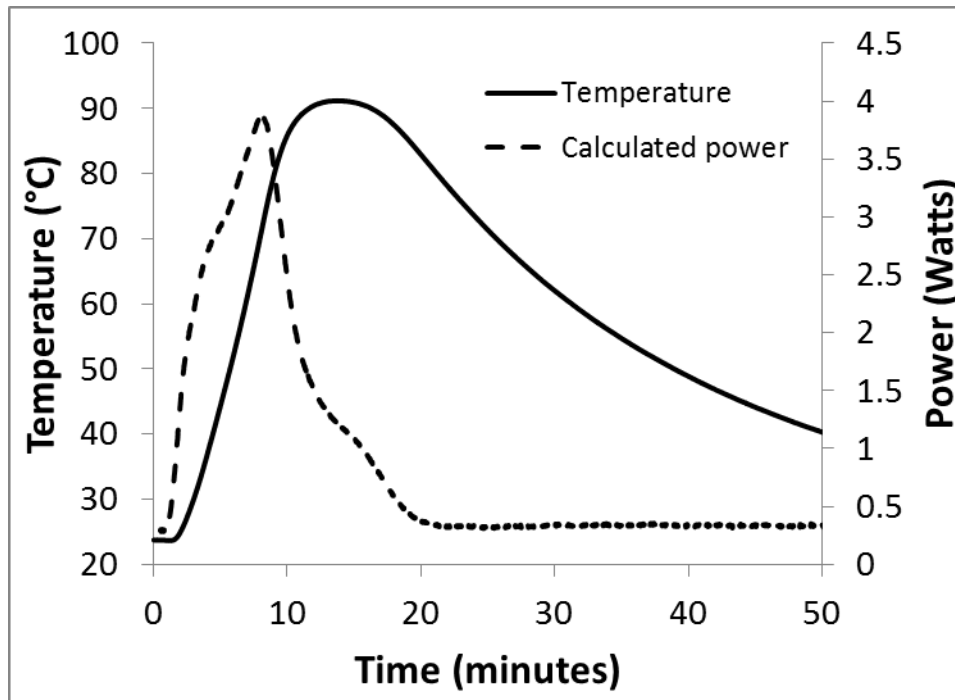
$$P = \frac{T_{sys} - T_{amb}}{R_{sys}} + \frac{dT_{sys}}{dt} C_{sys} \quad [3]$$

The  $R_{sys}$  term can be found by holding the power input constant and waiting for the system to reach a steady state where  $dT/dt = 0$ .  $C_{sys}$  can be fit using the dynamic data before  $dT/dt$  gets too small.

Note: this model assumes the temperature distribution in aluminum is not important. Can you think of a way to use the thermal properties of the system components (aluminum thermal conductivity and geometry, along with  $R_{sys}$ ) to test whether this is a good assumption?

## 2. Now the test fixture can be loaded with a fuel pack, and the temperature data can be converted to a power profile using the ODE model from part 1.

After characterization of the test fixture, the fixture can be used with a fuel pack, and temperature data can be converted to a power profile which can be used in a PDE heat transfer model. Figure X below shows temperature data obtained with a fuel pack in the test fixture. Use the ODE model shown above was used to convert this temperature profile to a power profile.



This power profile can now be used in a finite element model of a system including a fuel pack.

### 3. Create a 2D axisymmetric heat transfer model in COMSOL.

**First, a simplified model without phase change is created**

Use the model wizard to set up a 2D axisymmetric time-dependent model, using the “Heat transfer in solids” physics. It’s important to note that this will model the system as a solid, and not allow for convection. This may or may not be safe to assume for the reaction solution, which is a liquid in which convection may be important in a realistic system. For now, though, we will proceed with a solid model for a simplicity, we can interpret the results later to predict what effect convection would have if we allowed it.

To start, draw a polygon which will represent the sample tube in which we'd like to regulate temperature. The assay reagents will go in this tube in the device.

**Polygon**

☐ Build Selected ☒ Build All Objects

Label:

Object Type

Type:

Coordinates

Data source:

r:  m

z:  m

Selections of Resulting Entities



Fillet the lower right and middle right vertices to look more like an Eppendorf tube.

**Settings**

**Fillet**

☐ Build Selected ☒ Build All Objects

Label:

Points

Vertices to fillet:

☐ OFF ☒ Active

pol1

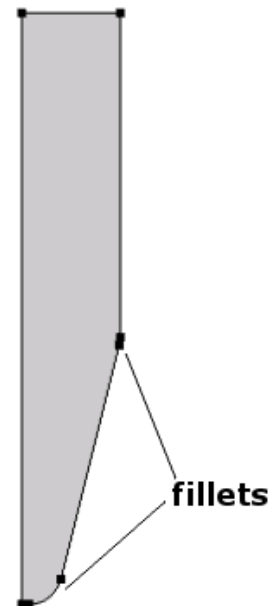
3

4

Radius

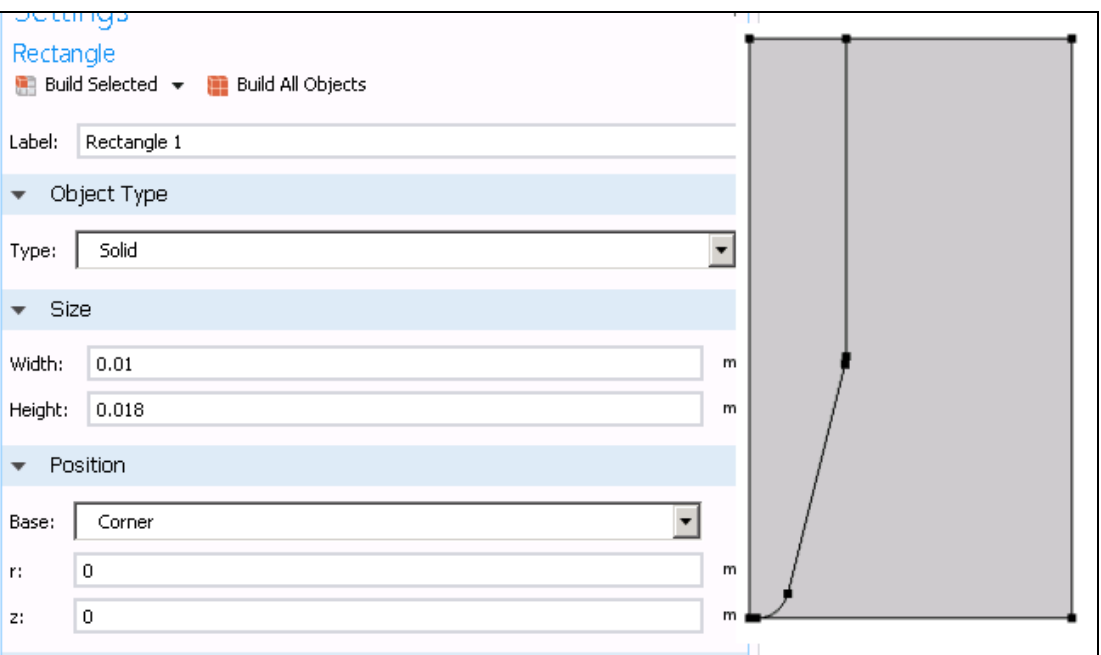
Radius:  m

Selections of Resulting Entities

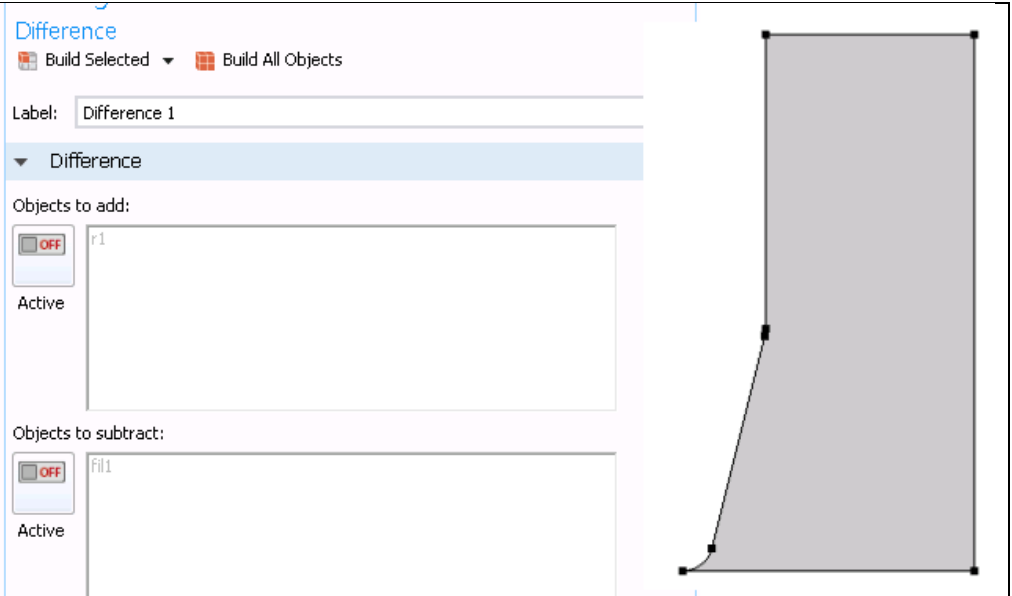


Draw the PCM:  
First we will draw  
an overlapping  
rectangle, then  
subtract off the  
tube area with a  
Boolean operation.

Draw overlapping  
rectangle

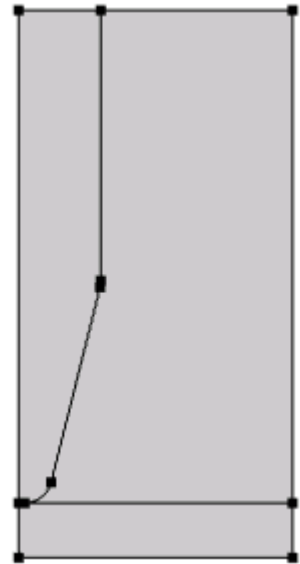


2: Subtract off the tube  
area to leave just the  
PCM. Right click  
“Geometry 1” and select  
Booleans and partitions  
→ Difference. The object  
to add is the overlapping  
rectangle, and the object  
to subtract is the tube  
area.



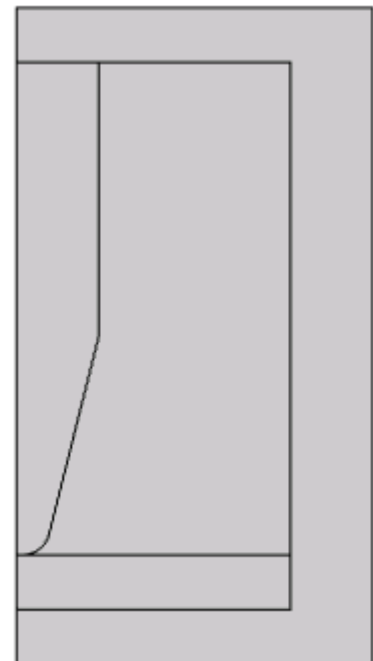
Duplicate the first polygon drawn for the Eppendorf tube and repeat the fillets to regain the Eppendorf tube area.

Draw a rectangle adjacent to the lower face of the PCM to represent the fuel pack area. Make this rectangle 10 x 2 mm, with the lower right corner located at (0, -2) mm



Draw three rectangles on the outer boundaries (lower, right, and top) of the model to represent insulation. Make these 3 mm thick, and whatever length is appropriate.

Use a Boolean operation to merge these three rectangles. Right click “Geometry 1”, then Booleans and partitions → Union. Deselect “Keep interior boundaries” in the Union settings.



Add the materials to the model. Right click “Materials” and choose “Blank Material”, create a blank material for each of the four different materials we will be modeling: 1) insulation, 2) PCM, 3) fuel pack and 4) reaction solution. Enter the material properties in each of the newly created materials and rename them as appropriate.

Table 1: Material properties used in finite element model

<b>Insulation</b>	Density	48.1 [kg/m <sup>3</sup> ]
	Thermal conductivity	0.033 [W/m-K]
	Specific heat	1,300 [J/kg-K]
<b>PCM</b>	Density	840 [kg/m <sup>3</sup> ]
	Specific heat	2,360 [J/kg-K]
	Thermal conductivity	1.5 [W/m-K]
<b>Fuel pack</b>	Density	990 [kg/m <sup>3</sup> ]
	Thermal conductivity	0.58 [W/m-K]
	Specific heat	4,181 [J/kg-K]
<b>Solution in tube</b>	Density	1000 [kg/m <sup>3</sup> ]
	Thermal conductivity	0.58 [W/m-K]
	Specific heat	4,181 [J/kg-K]

### Adapt the physics to the system being modeled.

Set the initial values: 20 [degC]

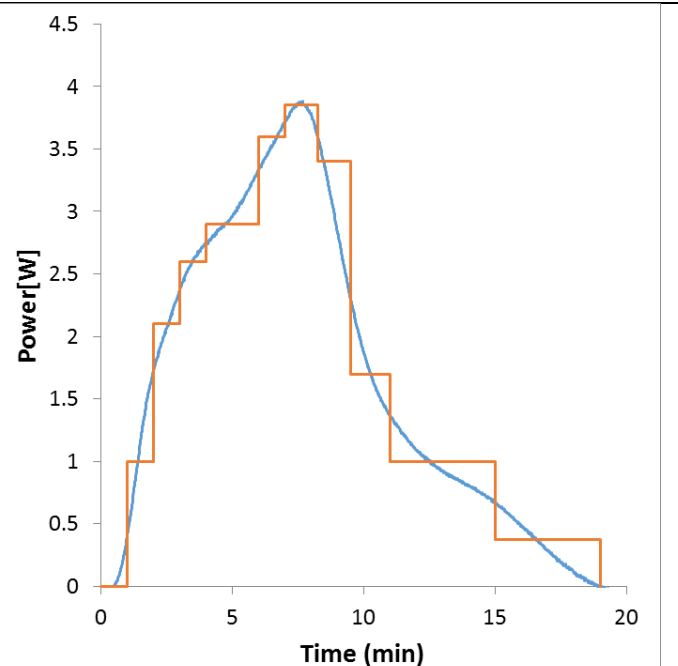
Add a heat source: Right click “Heat transfer in Solids” and choose “Heat Source”, setting it to an overall heat transfer rate corresponding with the power profile we determined earlier using the test fixture.

The power curve calculated using the test fixture can be approximated with a multistep function. In COMSOL, multiplying by a conditional can be used to vary an input parameter. For example, setting the input power to  $5*(t < 60)$  will set the power to 5 watts when  $t < 60$  is true, and zero watts otherwise.

These steps can be combined to approximate a more complicated curve, like the one showed on the right.

For this model, use the following as the “Overall heat transfer rate”:

$$0*(t < 60) + 0.5*(t > 60)*(t < 120) + 1.5*(t > 120)*(t < 180) + 2.25*(t > 180)*(t < 300) + 3*(t > 300)*(t < 420) + 3.375*(t > 420)*(t < 540) + 2.75*(t > 540)*(t < 600) + 1.675*(t > 600)*(t < 720) + 1*(t > 720)*(t < 840) + 0.675*(t > 840)*(t < 1020) + 0.125*(t > 1020)*(t < 1320) + 0*(t > 1320).$$



### Boundary conditions:

**Left boundary:** ( $r=0$ ) should already be set to “Axial symmetry”

**Lower boundary:** Temperature, 20 [degC]

**Right and upper boundary:** Heat flux: Change the type to “Convective heat flux”, using a heat transfer coefficient of 15 W/m<sup>2</sup>K and an external temperature of 20°C

## Part 2: Laboratory assignment

### 1: Mesh the model

Output an image of your mesh using the “Image Snapshot” button in the graphics window (it looks like a camera). Provide commentary on the mesh size distribution. Why are the mesh elements distributed like they are? Do you think this will matter in the model? What steps could you take to change the uniformity of the mesh?

### 2: Run the thermal model as described above (without phase change)

Change the maximum step size of the solver to 5 seconds, and model the simulation over the course of one hour.

2a: **Make an animation:** right click “Export” and select “Player”. Change the number of frames to 60. Take an “Image Snapshot” on the frame which appears to show the hottest temperatures.

2b: **Export a movie:** right click “Export” and select “Animation”. Give it a file name, and click “export”. Make sure you can view the exported movie in another program (VLC, Windows media player, etc.)

2c: **Create a temperature vs time graph for a single point in the tube.** Add a “cut point 2D” data set at  $r=0$ ,  $z=0.005$ . Create a 1D plot group with a point graph corresponding to this point. Based on the thermal gradients observed in the animation created in 2a, how representative do you think the temperature at this point will be?

### 3: Add phase change to the model

The PCM has the following properties:

Latent heat: 172 kJ/kg

Melt range: 60-62 °C

Model phase change as step up in heat capacity for the PCM material in the melting temperature range:

$$C_p = 2360 + (172000/2) * (T > 60[\text{degC}]) * (T < 62[\text{degC}])$$

3a: **Compare an image snapshot** from the phase change model captured at the same time as the image snapshot captured in 2a.

3b: **Interpret a temperature time graph** for the point used in 2c. Approximately how long does this design hold the solution temperature between ~59-64 °C? What could be changed to increase the amount of time the solution is held at temperature?

3c: **Export an image snapshot** at a time point which shows the largest temperature variations in the reaction solution. To simplify this model we modeled the reaction solution as a solid. What would happen if this were modeled as a liquid? How might you expect this temperature distribution to change if we added convection to the model?