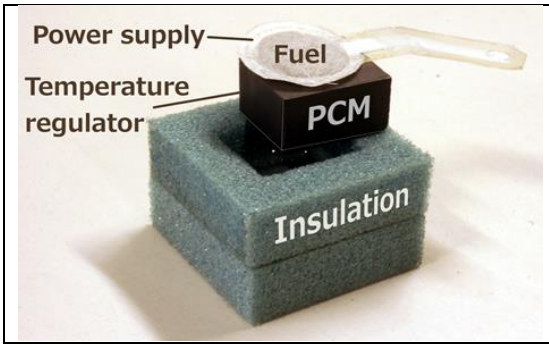
Lecture 14: Lab 7b, Thermal PDE for Phase Change Temperature Control

Robust, electricity-free diagnostics, including nucleic acid amplification tests (NAATs), show great promise to improve healthcare in low-resource settings. However, many challenges exist when designing to specific device temperature requirements, or accommodating harsh or variable environmental conditions. In this lab we will create a thermal partial differential equation model with phase change as a tool which can be used during device design.

This lab is based on research from the Yager group and PATH. The manuscript and supplemental information will be included in the lab 7b documents for reference.	Buser JR, Diesburg SP, singleton J, Guelig D, Bishop JD, Zentner C, Burton R, LaBarre P, Yager P, Weigl BH. (2015). Precision chemical heating for diagnostic devices. *Lab Chip*, *15*, 4423–4432. doi:10.1039/C5LC01053E

In these systems, an exothermic reaction is coupled with a phase change material (PCM). The exothermic reaction is contained in a fuel packet, shown below, and constitutes the power supply for the device shown below. The PCM regulates temperature while it melts and solidifies. This system can hold elevated, controlled temperatures for reactions such as isothermal nucleic acid amplification.

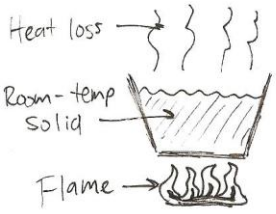
	Here is an exploded view of a chemical heater designed and built for use with isothermal NAATs. The fuel reacts with NaCl solution, resulting in a heat flux into the PCM. The heated diagnostic assay would sit beneath the temperature regulator (PCM block) within an appropriate cut-out in the insulation. Top insulation omitted for clarity, saline reservoir not shown.

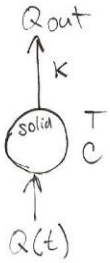
Thermal systems can be put in the same unified form as has been shown earlier in the course for electrical, fluidic, mechanical, and chemical systems.

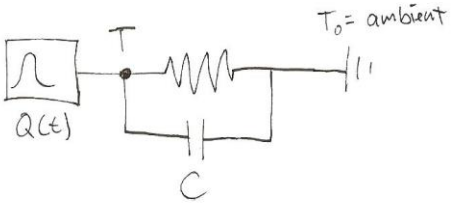
	Electrical	**Thermal**
Effort	**Voltage, V (volts)**	**Temperature, T (K)**
Flow	**Current, I (amps)**	**Flux, Q (J/s)**
Damping	Resistor, R (ohms = V/A) I = V/R	Thermal resistance (L/kA) Q = kAΔT/L
Storage	Capacitor, C (farad = As/V) I = CdV/dt	Specific heat, C Q = CdT/dt
Inertance	Inductance, L (henry = Vs/A)	None
Conservation of effort	ΣV = 0 on a loop	ΣT = 0 on a loop
Conservation of flow	ΣI = 0 on a node	ΣQ = 0 on a node

Ice baths are a commonly used temperature regulator where water is the PCM. Phase change temperature regulation is also commonly used in cooking: a boiling pot of water is a reliable way to hold your noodles somewhere around 100°C. The water on the stove top starts off as room temperature liquid, and heat is applied to the lower surface, raising the temperature of the water initially at a rate dependent on heat transfer into the pot, the specific heat of the pot and water, and the rate of heat loss to the environment.

Let's envision a pot on the stove filled with a room-temperature solid (chocolate probably), which we will refer to as the phase change material (PCM).

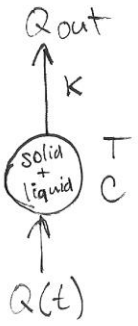


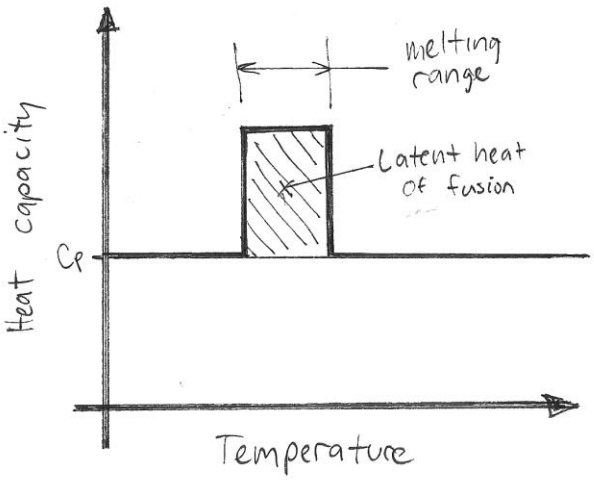




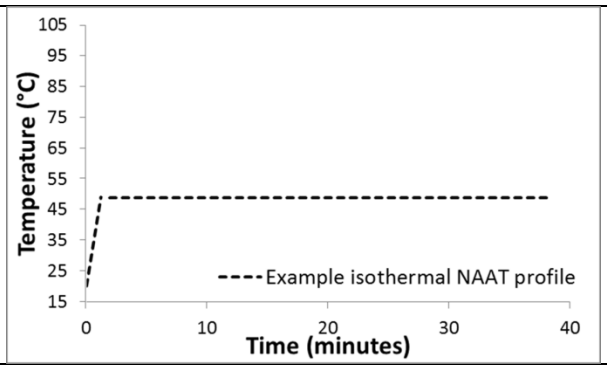
Heat flux into the system, Q(t), raises the temperature, T. As the system temperature rises, so does the heat flux lost to the environment. The dynamics of the system will depend on the values of the specific heat, C, and the thermal transfer coefficient, k (technically, k is for conduction, and here we're looking at convection, but bear with me). The equations given in the table above can create an ordinary differential equation model describing this system, which will be left as an exercise.

Things get more interesting when the room-temperature solid reaches its melting temperature. Once the solid begins to melt, it will take much more energy to raise T further. In a simplified view of the system, all of the chocolate must melt before T will rise further. One way to model the melting phenomena is to view the phase change as an increase in the specific heat of the system that occurs over a small temperature range. Here, instead of viewing the specific heat as a constant, we make it a function of temperature. A step function with an offset can be used, and the area above the flat line should be equal to the latent heat of fusion for the melting material.





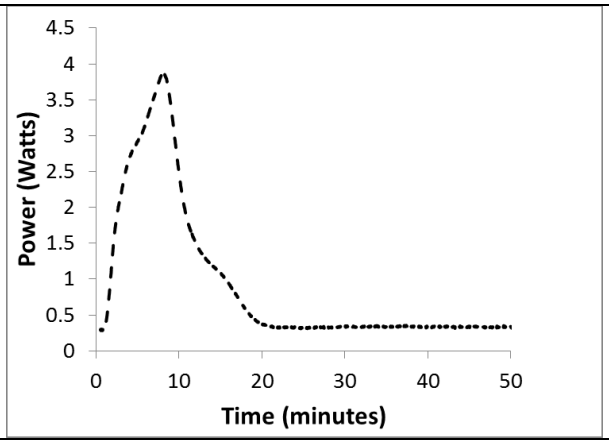
Now, let's consider how this type of system can be adapted to control temperature for isothermal nucleic acid amplification. The temperature requirements of an example assay are shown here.



To understand how a PCM system can be adapted to achieve a temperature profile that looks something like this, it is first necessary to design an appropriate heat source. A detailed tutorial of how a test fixture was designed and used to characterize the exothermic reaction fuel packs is given in the lab 7b document.

The fuel packs we've designed produce much of their power quickly, peaking around 10 minutes. There is a period of lower production following this, by ~20 minutes power production is mostly over.

Given that our isothermal nucleic acid amplification lasts around 30 minutes, the PCM melting/solidifying process must be used to buffer the temperature.



When this exothermic reaction of the fuel pack is coupled with an appropriately designed PCM temperature regulator, the thermal profile of the system begins to look like that shown below.

While heat flux is going into the system, the temperature rises. Before the PCM starts melting, the temperature rises quickly. Once the PCM starts melting, the temperature rises slower, since energy is being stored in the PCM. Around 20 minutes, heat flux into the system drops off, and the system temperature begins to drop. The PCM is solidifying during the process, which holds the temperature within tolerance.