Oblig 1 - FYS2160

Lasse Pladsen

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In this report I have analyzed the experimental data of the experiment measuring the temperatures of two thermos mugs with different features. I have found the melting temperature of the phase-change materal which makes up the special hotness-keeping properties of the Temperfect thermos. I have shown how one can create an algorithmic model to fit ths data by using a randomized heat conduction model originally used to model a different experiment of conduction between two metal blocks..

I. INTRODUCTION

This report will be a head first dive into the thermodynamics of a simple experiment. We will take a look at the data from "The Temperfect mug experiment" given in the oblig 1 exercise for the UiO course FYS2160. The Temperfect mug is a thermos mug where the insulatory material cools hot liquid to a drinkable temperature and keeps it there for a long period. The experiment compares temperature-keeping abilites of the Temperfect thermos and a Bodum thermos.

The report is divided into two parts; part A is about the experiment itself and analyzing its data while trying to predict what happened where. Part B is about creating algorithmic models to explain and fit the experiment, then comparing it to the actual experimental data. For this we will be using a model from a heat conduction/diffusion simulation between two metal blocks.

II. THEORY

The walls of the Temperfect mug contains a phase-change which result in water inside staying at a certain temperature for longer than an ordinary thermos. When its melting its temperature does not increase until its fully melted (phase change), instead the heat goes to melting the material. This energy is called the *latent heat* of the material. The same amount is released upon crystallization.

As far as I could find the Bodum mug only has a insulating layer of "vacuum" inbetween two layers of mug walls which provides its thermos effect, by reducing the medium in which conduction can occur. The following equations are provided in the oblig [1]. For this mug the water's temperature loses heat over the area A by the heat flux J_q as

$$AJ_q = mc_v \frac{dT}{dt} \tag{1}$$

where m and c_v are respectively the water's mass and specific heat capacity at constant volume. Assuming a stationary state after the mug's walls have been heated up we can write

$$J_q = -\lambda \frac{\Delta T}{\Delta x} \tag{2}$$

where λ is the mug's thermal conductivity and Δx is the width of the walls.

The amount of heat needed to completely melt the phase-change material in the Temperfect mug is called the latent heat:

$$L = Q_{\text{phase change}} \tag{3}$$

meaning $Q_{\text{phase change}}$ is the heat needed to completely melt or the heat released when completely crystallized. We can write a specific latent heat per unit mass as [2]

$$l = \frac{L}{m} = \frac{Q_{\text{phase change}}}{m} \tag{4}$$

To find the latent heat we just need to calculate the actual heat Q. If we know the head conduction property called the *heat capacity* C of the material then we can calculate the heat by

$$Q = C_v \Delta T = mc_v \Delta T \tag{5}$$

where $c_v = C_V/m$ is the specific heat capacity of the material at a fixed volume, and ΔT of course is the temperature change resulted by this heat Q [2]. Since there is no work done on the water in this experiment we will be using the heat conductivities at fixed volume $C = C_v$.

III. METHODS

A. The Temperfect mug experiment

The conducted experiment measured the temperatures of water inside two thermos mug; a Temperfect mug and a Bodum thermos mug. The mugs were filled with 3 dl of almost boiling water and the temperatures were seperately recorded over time. None of the mugs were closed off with a lid. In this report I am going to assume the following: 1) that the water temperature in each of the separate mugs are uniform in the entire volume of water. 2) that I have a stationary state in the phase-change material of the Temperfect mug. 3) that the heat loss is dominated by conduction through the walls.

I will plot the given data and attempt to analyze the different phases of the experiment. By reading off the plots and referencing the raw data I am going to attempt to find the phase-change material's melting temperature

T_m by where the material should be melting and crystallizing. Then using the data and (5) I am going to attempt to calculate the amount of heat that the phase-change material stored by how long the water's temperature was heated by the realeasing heat during the crystallization. For the values in the equation m and c_v I am going to use water's properties for the estimation because I do not have the information needed about the phase-change material itself.

If we assume that the water's heat loss is dominated by conduction through the Bodum mug's walls, sketched in fig 1, then I will derive the third equation given in the oblig to find an expression for the characteristic time τ for the ordinary Bodum thermos.

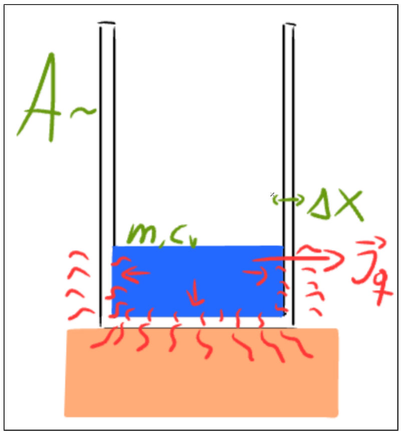

Figure 1. Sketch of Bodum thermos' heat loss by conduction through the mug walls.

By putting (2) into (1) we get

$$-A\lambda\frac{\Delta T}{\Delta x} = mc_v\frac{dT_w}{dt}$$

here we will assume that the room temperature T_a is constant over time, such that $\frac{d\Delta T}{\Delta t} = \frac{dT_w}{dt}$ so we get:

$$-A\lambda\frac{\Delta T}{\Delta x} = mc_v\frac{d\Delta T}{dt}$$
$$\frac{d\Delta T}{\Delta t}\frac{1}{\Delta T} = -\frac{a\lambda}{mc_v\Delta x} = D$$

where, for ease, I have introduced the constant $D = -\frac{a\lambda}{mc_v\Delta x}$. We solve this differential equation:

$$\Delta T = e^{Dt} + C_0 = C_1e^{Dt}$$

where C_i are some constants;

$$\frac{\Delta T}{C_1} = e^{Dt}$$

which we identify as equation three of the oblig, meaning that

$$C_1 = \Delta T_0 \tag{6}$$
$$D = -\frac{1}{\tau} \Rightarrow \tau = \frac{mc_v\Delta x}{A\lambda} \tag{7}$$

By using estimates for the Bodum mug's size we can then find a value for this τ using the water's properties m, c_v and steel's thermal conductivy λ.

B. Algorithmic models

In this report I will be using Python to do our numerical modelling of the experiment. I will be using the provided diffusion algorithm in the oblig along with data from the metal blocks experiment which shows temperature over time for two metal blocks in contact. Using the algorithm I am going to test different parameters `Ctb`, τ to fit the simulation to the data. The simulation is run with N number of heat packets with n amount of steps/iterations.

Furthermore I am then going to adjust the algorithm to simulate heat loss to the environment. In the time loop, after the diffusion calculations, I am going to add a randomized component which subtracts an amount of heat quanta decided by a new heat loss coefficient C_{loss}. This randomized loss will work in the same fashion as the diffusion simulation provided in the oblig. It takes a randomized number in $[-2, 2)$ and if it is less than the temperature difference between the surrounding air and the metal block, the block's temperature will subtract a given amount of heat packets as $\Delta T_i = T_i - C_{\texttt{loss}}/N$, where N is the total number of heat packets in the simulation.

Then to finish off the model I am going to adjust it to try to simulate the Temperfect mug itself with its phase-changing properties and compare it with the data.

IV. RESULTS

A. The Temperfect mug experiment

The temperatures were measured every 0.5 seconds over 6718.5 seconds/112 minutes, the data is plotted in figure 2. We see that the water was first added to the Bodum mug at $t = 6$ seconds, then to the Temperfect mug at $t = 22$ seconds. We can read off the melting temperature of the phase-change material in the Temperfect mug to be

$$T_m \simeq 62.9^\circ \text{ C}$$

from where the water's temperature stops cooling quickly and almost stays constant for a long period. More on this in the discussion section of the report. Using (5) and water's specific heat capacity $c_v = 4182\ \frac{J}{kgK}$ and mass density $\rho = 997\ kg/m^3 = 0.997\ kg/L$ [3] with the given volume of 3 dl water; I found an estimate for the heat that the phase-change material stored

$$Q = 346.92\ kJ = L_{\text{phase-change material}}$$

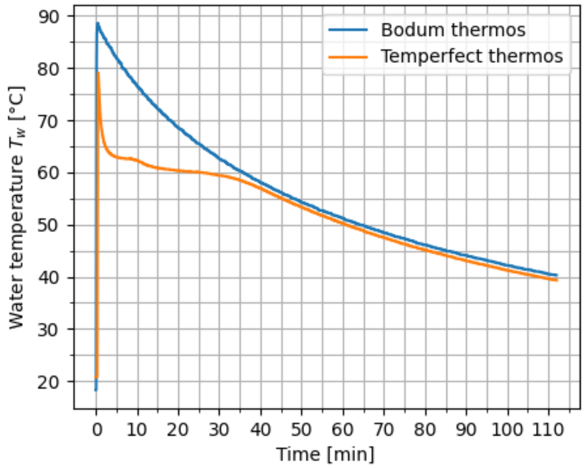

Figure 2. The temperature measurements of the water in the two thermos mugs.

using the temperature change during the slow cooling period from $t = 6.12$ minutes to $t = 35$ minutes of about $\Delta T = 4.2° \ C = 277.35° \ K$. Which is to say that this heat is the latent heat L of the phase-change material. More on why this is off in the discussion.

Using the estimates for the cylindrical Bodum thermos mug with no lid given in table I (assuming uniform cylindrical shape), along with the already discussed water properties and with the thermal conductivity of stainless steel $\lambda = 16.3 \ \frac{W}{m \ K}$ [4] I found

$$\tau = 6.26 \ s$$

Category	Estimated value
Radius r	3 cm
Height h	18 cm
Wall width Δx	0.3 cm
Area A	117 π cm^2

Table I. Used estimates for the Bodum thermos mug. Area is calculated as a cylinder without a top $A = 2\pi r h + \pi r^2$.

B. Algorithmic models

All scripts are provided in the canvas upload.

Using the provided algorithm I found that the parameters `Ctb` $= 1.96$ and $\tau = 150$ managed to almost exactly fit the simulation and the data. I used $N = 100\ 000$ total heat packets as a compromise between script run time and a smooth graph. The graphs are plotted in figure 3 with $n = 12N$ steps.

Simulating the heat loss to the environment in this algorithm I found the most fitting coefficient to be

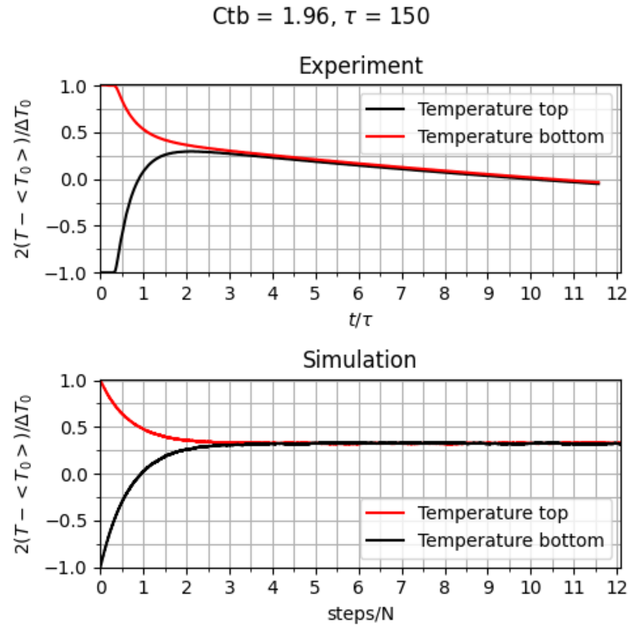

Figure 3. Plot of the metal blocks experiment and diffusion simulation *without* heat loss to environment. Here `Ctb` $= 1.96, \tau = 150$. The code `diffusion.py` is provided in the canvas upload.

$C_{\text{loss}} 1/25$. Figure 4 shows how well it fits the experimental data of the metal blocks.

For the Temperfect simulation I managed to somewhat simulate the quickly cooling part of the top metal block by using some if-logic and keeping track of the temperature and phase-change states. However, I did not really manage to simulate the slowly cooling part where the Temperfect mug kept the water hot longer, the plot is shown in figure (5).

V. DISCUSSION

A. The Temperfect mug experiment

Firstly in the graph (fig 2) it seems like the Temperfect's water temperature actually starts at a lower temperature than the Bodum mug, they peak at respectively 88.6° C and 79.1° C. I'm not sure if this is because the Temperfect's temperature quickly cooled while it was being poured, or if the experimental actually used different temperatures. Therefore I am going to give the benefit of the doubt and assume the former.

Initially the water in the Temperfect mug cools extremely quickly down to around $T_w = 62.7°$ C at $t = 6.12$ minutes, this should be where the phase-change material already was melting from the water's heat. While me heat equal to the materials latent energy is absorbed from the water. Afterwards the temperature levels out, assuming this is where the material has now fully melted,

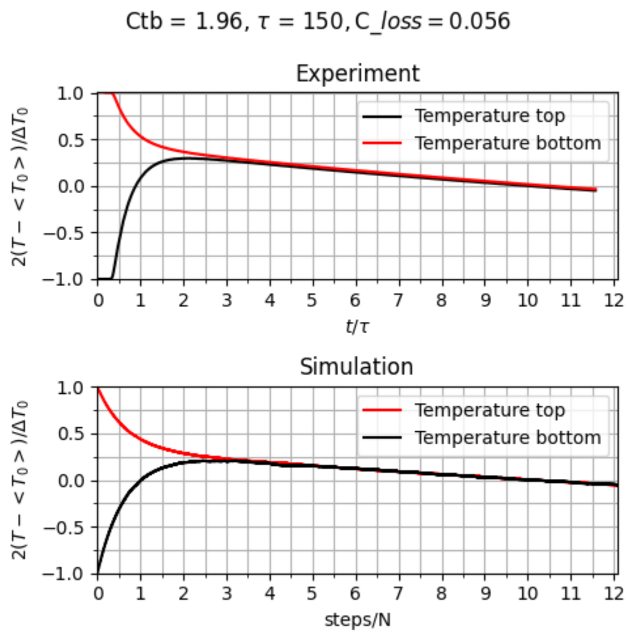

Figure 4. Plot of the metal blocks experiment and diffusion simulation *with* heat loss to environment. Here `Ctb` $= 1.96, \tau = 150$, $C_{\text{loss}} = 1/25$. The code `diffusion_with_loss.py` is provided in the canvas upload.

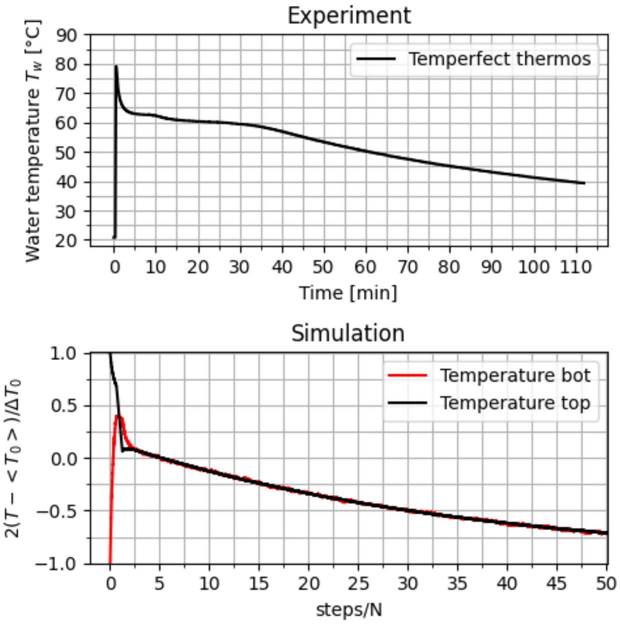

Figure 5. Simulation of the Temperfect mug with the diffusion model provided in the oblig. The code `temperfect_simulation.py` is provided in the canvas upload.

then stays at almost constant temperature for around 173 seconds (it cools by only 0.3° C). It would seem that this is where the crystallization is happening, but I am not sure if it makes sense for the material to crystallize instantly after melting. For it to happen the water must have reached the the melting temperature T_m during or right after the melting process. Meaning the material either stopped melting and started crystallizing instead, or it fully melted just as the water's temperature cooled to T_m.

At around $t = 10$ minutes the Temperfect's water actually starts to cool faster to around $T_w = 60.9°$ C for about 5 minutes, but then after this point the water cools slowly again for another 15 minutes until around $t = 30$ minutes. This could either be a hint to me being wrong, or some disturbance of the experiment itself.

The actual heat loss to the environment in both of the mugs could be different because they are designed different. Whereas I assume the Bodum thermos is a regular thermos with a vacuum insulation layer to reduce heat conduction, the Temperfect has the phase-change material. Both mugs however also lose some of the waters heat to the air circulating inside since the lids were not on. This heat loss part should be identical at least if the openings are around the same size.

To calculate how much heat was stored in the phase-change material is to find the latent heat L. If I knew which type of material it was I could look up the specific latent heat and calculate. Since I did not have this I used the water informatio n I had. I'm not convinced that this is accurate because this temperature difference is so small it could be just from the environmental heat loss. In summary ΔT in (5) should be from the heat Q, which I do not really have.

The value for $\tau = 6.26$ s sounds too low for the thermos. As we see in the graph (fig 2) it actually takes *longer* than the experiment of 110 minutes for the Bodum water's temperature to reach 37% (33° C) of its highest temperature (88.6° C), which is significantly off. I'm not sure what the oblig meant by asking me to fit the equation three model to the data.

B. Algorithmic models

The provided heat conduction algorithm works by randomly moving heat quanta from either the top to the bottom or vice versa in each step. It does this by generating a random number and selecting which direction to move heat quanta by checking this number to the temperature differences between the metal blocks. This creates a similar result to the data because the two temperatures will approach- and hover around each other because of the temperature difference being the factor choosing which direction to move heat to.

The parameters related to thermal conductivity is the heat capacity ratio between the two metal blocks `Ctb` which decides how many heat quanta are moved in each time step. To then add a heat loss using the exact same logic as the conduction algorithm itself I created a similar coefficient C_{loss} and it worked well to produce the same results as the experimental data, after tweaking its value a bit.

For the Temperfect simulation I managed to get halfway there, I could not really figure it fully out. I did manage to get the quickly cooling part in. The way I mplemented this was to use variables to keep track the phase states and initiate phase-changes from the bottoms temperature. I also implemented latent heat to almost delay the phase-changes a certain amount of steps so get/release more heat. For this I had to create parameters for the total latent heat L_b, the current steps latent heat L_i, and the simulated melting temperature T_{bm}. All this you can check out in the code `temperfect_simulation.py`.

C. General feedback

I want to express my feelings for this oblig. I know this is meant to be a deep dive head first as we learn to solve our problems, but just in general I, and some of my friends on this course, feel like this oblig was way too vague and poorly written for what you actually wanted us to do. This entire oblig became mostly guesswork and we became way too reliant on group assistants to literally point us in the direction that the oblig paper itself really should have done. And I know for fact that this wasn't just us as the group session didn't even have time to help everyone in the two hour session. This was either just too early (I know that was the intention...), or just too poorly written. It enden with us being so frustrated and confused on the last day that we just finished it up and delivered it to be done with it.

In general I also struggled to keep under the 2000-word limit as I had to delete tons of discussion and otherwise filling information, hopefully it didn't affect the readability too much.

VI. CONCLUSION

In this report I have analyzed, modelled, and simulated the Temperfect experiment. I found the melting temperature of the phase-change of the thermos to be around $T \simeq 62.9°$ C, however the latent heat stored in the material I do not believe I managed to calculate correctly ($L = 346.92\ kJ$). I esimated the characteristic time for the Bodum thermos to be $\tau = 6.263$ s which I also am not convinced is right.

Appendix A: Answers to concept questions

1. (a) Because the compression both increases the particle density and decreases the volume, the gas pressure increases.

   (b) The change in total thermal energy of the system equals $\Delta U = Q+W = 0.5Nfk_b\Delta T$. Here there is no heat $Q = 0$ but we do a positive work on the gas system by compressing it with the piston, so the change in temperature is also positive meaning the temperature increases.

   (c) The molecules will be more dense resulting more frequent collisions. Because gas pressure is just the molecules hitting the inside of the bottle walls this means that this happens more frequenty so the pressure has increased (a).

   Compressing the system increases the average kinetic energy of the gas molecules, which is what temperature is defined as ($1.5k_bT = \bar{K}_{translational}$). So the temperature increased (b).

   (d) As mentioned the volume of the system decreases, but I wouldn't say that this is a property of the gas. Its more a property of the gas' container. The thermal energy increases since we do a positive work on the gas. I'm not entirely sure on this point which other properties to perhaps evaluate.

2. (a) Quasistatic compression. The average kinetic energy of the molecules stays the same, the difference in this situation is that the particles on average lose the same amount of kinetic energy that it gains from the compression work increasing the density, by heat conduction through the bottle's walls.

   (b) We can see from the ideal gas law that a fixed temperature, but decreasing volume means that the pressure has to increase by the same amount that the volume decreases (I mean so that the product remains fixed) $PV = Nk_bT$.

   (c) In this case, yes the gas is more dense, but the molecules on average have the same kinetic energy. However, since the volume still is decreasing, this means that the molecules still hit the walls more often than before meaning the pressure still has to increase.

   (d) The thermal energy being proportional to the temperature ($U = 0.5Nfk_bT$) stays the same this time.

3. (a) Being in equilibrium is when $q_a/N_a = q_b/N_b$ where q can be assosiacted with energy and N with molecule count, so that literally means that they have the same energy per molecule when in equilibrium.

   (b) I'm not entirely sure what potential energy to evaluate here, but if we just look at $E_{\text{mech}} = E_{\text{pot}} + K$ then because of the reasoning in the next exercise (3d), then the water molecules must have more potential energy per molecule.

   (c) Since temperature is proportional to the average kinetic energy of the molecules this means (since they have the same temperature) each air and water molecule have on average the same kinetic energy, but water is more dense meaning more molecules in the same volume. So the air molecules must then have more kinetic energy per molecule regardless of the volume sizes.

(d) Once place in the bottle together they will transfer heat by conduction ($Q/\Delta t = -k_t A dT/dx$) and this will continue until they are the same temperature which is the equilibrium state. Also convection will play a role such that the temperatures becomes uniform in the entire mediums.

(e) While they are getting heated up they will still conduct heat to each other, so they will still continue to be at equilibrium. The pressure will change assuming the volume stays the same, since its proportinal to the temperature by the ideal gas law. The molecules are getting more and more average kinetic energy (temperature) from the "heated" particles bumping into them. The pressure must then increase beacuse the molecules bumping into the walls would be more frequent/have more momentum.

(f) As the ice's temperature is much lower than the water (ice below 0° C and water above of course) heat will flow from the water to the ice. Its temperature will only increase up to the melting point of 0° C and then the rest of the energy will go into the phase change of melting the ice into water. It melts because it reached its melting temperature, where the molecules have enough kinetic energy to break the rigid solid/crystal overall shape and can flow around each other more easily.

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[1] UiO, Oblig 1 FYS2160 (2023).

[2] D. V. Schroeder, *An Introduction to Thermal Physics* (Oxford University Press, 2021).

[3] Wikipedia contributors, "Properties of water — Wikipedia, the free encyclopedia," https://en.wikipedia.org/w/index.php?title=Properties_of_water&oldid=1172399722 (2023), [Online; accessed 2-September-2023].

[4] Wikipedia contributors, "List of thermal conductivities — Wikipedia, the free encyclopedia," https://en.wikipedia.org/w/index.php?title=List_of_thermal_conductivities&oldid=1172910180 (2023), [Online; accessed 6-September-2023].