

Calorimetry Analysis an Unknown Substance

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The objective of this analysis was determine the composition of an unknown material sample used in a calorimetry experiment. The temperature changes of the sample were collected by two different thermocouples and recorded via a Cold Junction Compensation (CJC) software and exported to a .txt file. Our analysis focused on the .txt file utilizing linear best fit approaches and error analysis to identify the substance. Our comparison was based on the specific heat capacities for substances. Based on the results obtained, we determined that the material we are analyzing is very likely to be Tellurium Copper.

Nomenclature

$C_{s,av}$	=	Specific heat of the sample ($\frac{J}{g \cdot K}$)
$C_{c,av}$	=	Specific heat of the Calorimeter ($\frac{J}{g \cdot K}$)
T_O	=	Initial temperature of the Calorimeter (K)
T_1	=	Initial temperature of the Sample (K)
T_2	=	Initial temperature of the calorimeter and sample at equilibrium (K)
m_c	=	Mass of the Calorimeter (g)
m_s	=	Mass of the Sample (g)

I. Introduction

We could then use that data to determine what the material sample was based on the determination of its specific heat. The importance of the experiment and analysis is to show that a calorimeter can be used to determine an unknown material substance based on the thermodynamic properties of all known substances.

II. Experimental Method

The experimental method was used to set up the process that would allow us to find the unknown sample.

A. Purpose

The purpose of the analysis is to use a calorimeter to obtain a temperature profile, which then will be analyzed to determine the specific heat of an unknown sample. The result will be compared to that of given material. We received the specific heats for four(4) candidate materials in which one material was chosen for our unknown sample. The specific heats of the four samples was treated as exact numbers. Furthermore, we received calorimeter's specific heat and mass. To determine the unknown material, we used the given data to calculate the specific heat of the substance to find its unique thermodynamic properties.

B. Assumptions

In order to find the specific heat of the unknown substance based on a linear relationship, we will assume a perfectly insulated calorimeter. Many calorimeters also have a stirring apparatus to keep the calorimeter at the same average temperature. This, however, can also lead to adding energy to the system which will cause a change in temperature of the water, instead of only measuring the effects of the change in temperature of the water based on the sample. The temperature change due to the stirring mechanism will therefore be neglected. Finally, the potential and kinetic energies of the system are negligible since there is no change in elevation and the calorimeter is not stationary and closed. As a result, the change in the temperature of our sample can assumed to be only due to the heat transfer process that happens due to the difference in temperatures.

C. Schematic

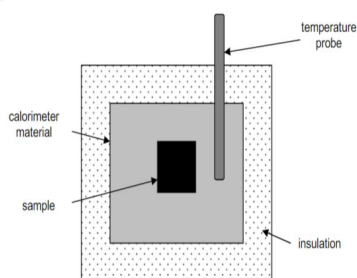


Fig. 1 Free-body Diagram of initial state and final state of the calorimeter and sample.

D. Fundamental Laws and First Law of Thermodynamics

We can apply the First Law of Thermodynamics to the system. The first Law of thermodynamics states that energy is conserved. Based on our assumptions, we can analyze the system we have assuming that all the change in energy will be represented by change in the internal energy, which is represented by change in sensible energy (i.e. temperatures). The internal energy is directly related to the specific heats. Thus, any energy gained by the sample will be lost by the water, and thus, it is possible to equate the two changes in energies between the calorimeter and the sample.

E. Process

To determine the specific heat of the sample, we used least square regression methods utilizing linear algebra methods. The goal is to model the change in the temperature profile of the unknown sample, and analyze it.

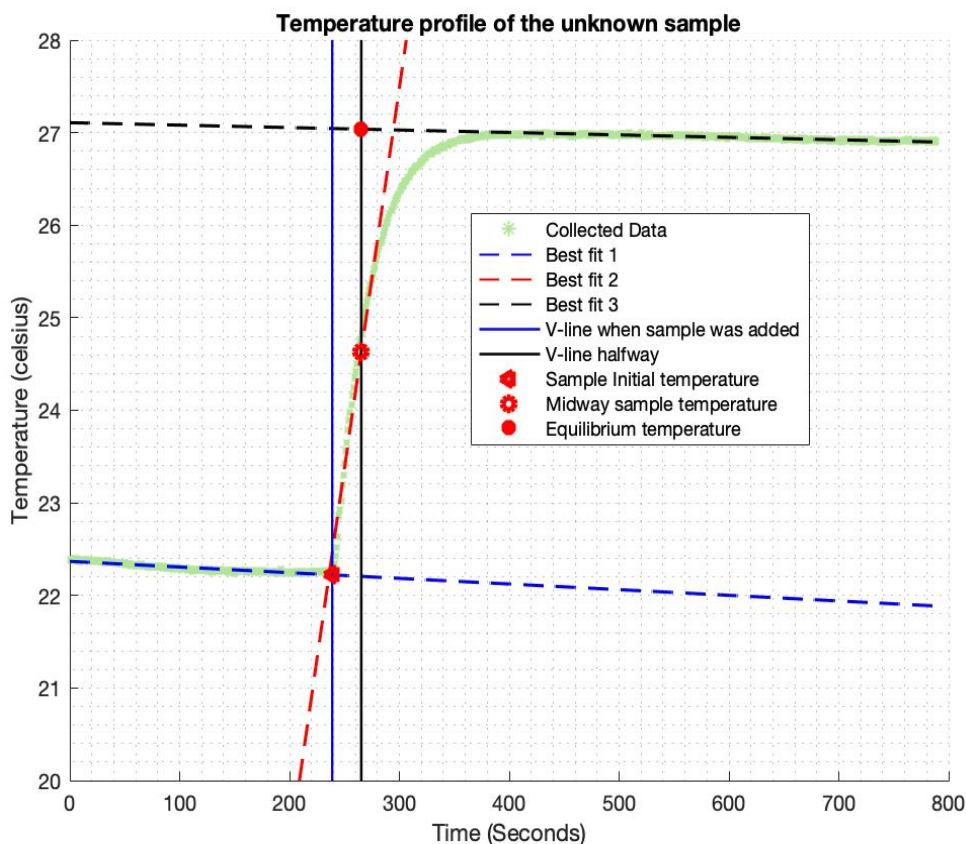


Fig. 2 Linear determination of change in sample temperature

Using the least square regression method, we determined three linear best fit lines on the graph for three different regions. The first region was from the initial time to the time the sample was inserted. The second region is the region where the heat transfer happened, represented by a change in temperature. Lastly, the third region is where the sample reached equilibrium temperature. All the linear regressions are done via a local function that returns best fit

parameters (refer to the flow chart at the Appendix for more information). To find the linear best fit for initial temperature (figure1:Best fit 1), we chose the initial data point and the point at time value at 238.88 seconds where the sample appears to enter the calorimeter (figure2: sample initial temperature). We then determined the equilibrium linear best fit (figure2:Best fit 3) using the same method, this time where the sample appears to be at equilibrium and the final value of the data set. We then used the initial temperature and the initial equilibrium temperature estimation to determine the halfway temperature. The halfway temperature then is used to improve our equilibrium temperature estimation. A line for the change in sample temperature(figure1: Best fit 2) was then modeled. We found the midway point temperature from time the sample entered the calorimeter. The point of intersection of the equilibrium best fit line was used to obtain the upper bound of the midway point as the temperature of the sample rises (figure2:equilibrium temperature). This was determined by utilizing root finding built-in Matlab functions. Estimated temperature values can then be used to find the specific heat of the sample using equation (2) below.

Based on our assumptions, the equation for the first law of thermodynamics can be derived to calculate specific heat. the from the total change in internal energy is equal to the difference of the change in temperature and. Equating the internal energy will enable us to solve to the sample specific heat. The derivation is shown here:

$$\Delta U = Q - W$$

$$\Delta U = U_2 - U_1 = 0$$

$$(m_c U_{c2} + m_s U_{s2}) - (m_c U_{c1} + m_s U_{s1}) = 0 \quad (1)$$

$$(m_c C_c T_2 + m_s C_s T_2) - (m_c C_c T_0 + m_s C_s T_1) = 0$$

$$(m_c C_c T_2 + m_s C_s T_2) = (m_c C_c T_0 + m_s C_s T_1)$$

$$C_{s,av} = \frac{m_c C_{c,av}(T_2 - T_0)}{m_s(T_1 - T_2)} \quad (2)$$

$$\delta y_{new}^2 = [t_{new} 1] Q [t_{new}; 1] \quad (3)$$

Furthermore, the uncertainty in each measurement was estimated as follows:

1- Uncertainty in Initial temperature of water: we averaged the temperatures of the water and took the uncertainty of the mean (Taylor,188).

2- Uncertainty in sample initial temperature : we estimated the uncertainty to be equal to the uncertainty of the best fit dependent variable based on the equations of the matrix operations (Anderson,Clark,Least Square Sum)

3- Uncertainty in equilibrium temperature : we estimated the uncertainty to be equal to the uncertainty of new values in dependent variables (equation 3) (Anderson,Clark,Least Square Sum)

4- Uncertainty in masses: provided by the lab faculty.

III. Results

Temperature Values			
	Initial Temperature (C)	Midway Temperature (C)	Final Temperature(C)
Calorimeter	$22.22 \pm .01$	$24.63 \pm .19$	27.04 ± 0.003
Water	93.30 ± 0.011		
Sample	$22.22 \pm .017$	$24.63 \pm .19$	27.04 ± 0.003

Fig. 3 Free-body Diagram of initial state and final state of the calorimeter and sample.

Based on the data and the determined specific heat value, the sample material that most closely corresponds to Tellurium Copper. Our sample has a relative error of 13% with respect to Tellurium Copper, the smallest of all possible samples. Although our sample with its error estimations does not confirm that it is Tellurium Copper, we think that there is more than one possible reason to cause this to happen. The possible reasons are discussed below.

A. Code verification and reality check

The code was checked with all the other examples and compared with some of the other classmates who have different samples. Also, the linear function was checked with various examples that we know the analytic solutions to and compared outputs to see how will the function work. The linear fit and the code gave rational numbers and were pretty accurate.

Moreover, a dimensional analysis was run on every step to make sure that the results are accurate. There was one conversion unit made to convert between Cal/g*c and J/g*k to compare the results with the candidate alloys.

IV. Discussion

As explained above, our sample is most likely to be Tellurium Copper. There is more than one source for mistakes in error estimations. Fig 4 (below) visulaize the difference between the specific heats for our sample and each possible candidate. Although the error bars are represented there, they are so small and almost invisible. It is also worth to note that Pb value represented is the mean, for the values were given in a wide range (standard deviation of the mean was taken as its error). For the overall uncertainty analysis, after determining each term uncertainty, a step-by-step method was used to find the overall uncertainty ,treating the specific heat of the calorimeter as exact.

During the experiment, thermocouples were used to record temperature changes through the duration of the experiment. We believe finding the average of the temperatures gave us more accuracy due to the increased data points available and how close the data were. Systematic errors could have occurred with one or both thermocouples that

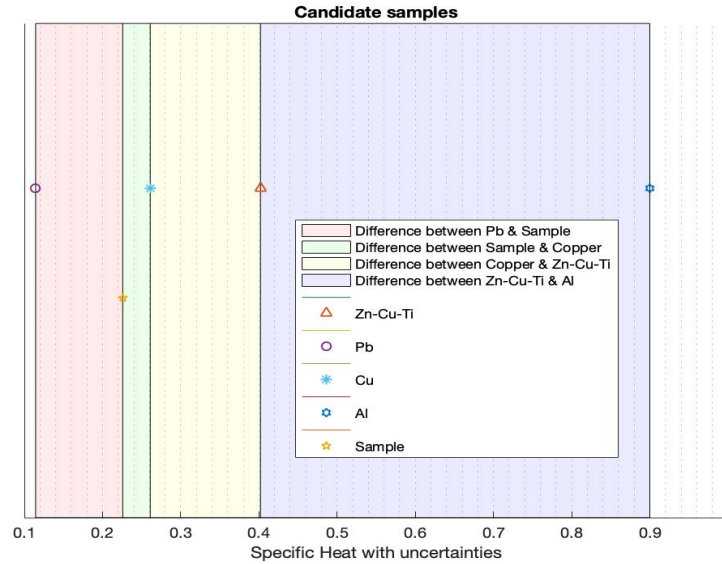


Fig. 4 Unknown sample and candidate samples' specific heats

could lead to bias when calculating the temperature values. Since there is extremely difficult to perfectly insulate a calorimeter, heat exchange likely occurred in the insulating walls causing another source of uncertainty. These biases were likely very negligible and were likely not a major contributor towards error based on the amount of data points we have. The contributors that did likely cause errors would be located in the least squares analysis. Since the value at which the sample was placed in the calorimeter was arbitrarily chosen (Figure 1: Sample initial temperature), Errors in the linear equation may be skewed. Similarly, this would also cause errors in the equilibrium best fit equation and the best fit connecting the two. In addition, we treated the time that the sample reached halfway temperature as an exact number, however it is not clear that this is the case. A Monte Carlo simulation could be a useful tool to find there errors in the lines of best fit which would allow for more precise time values and more precise values. In addition, it is not clear for us that the specific heat of the claroimeter is exact number as it has been treated. Furthermore, there might be some error in the given candidate sample values.

V. Conclusion

Based on the calculations made, we feel confident that the unknown sample was Tellurium Copper. We had a very small error, , meaning the sample would not likely as another sample as seen in the figure below:

VI. References

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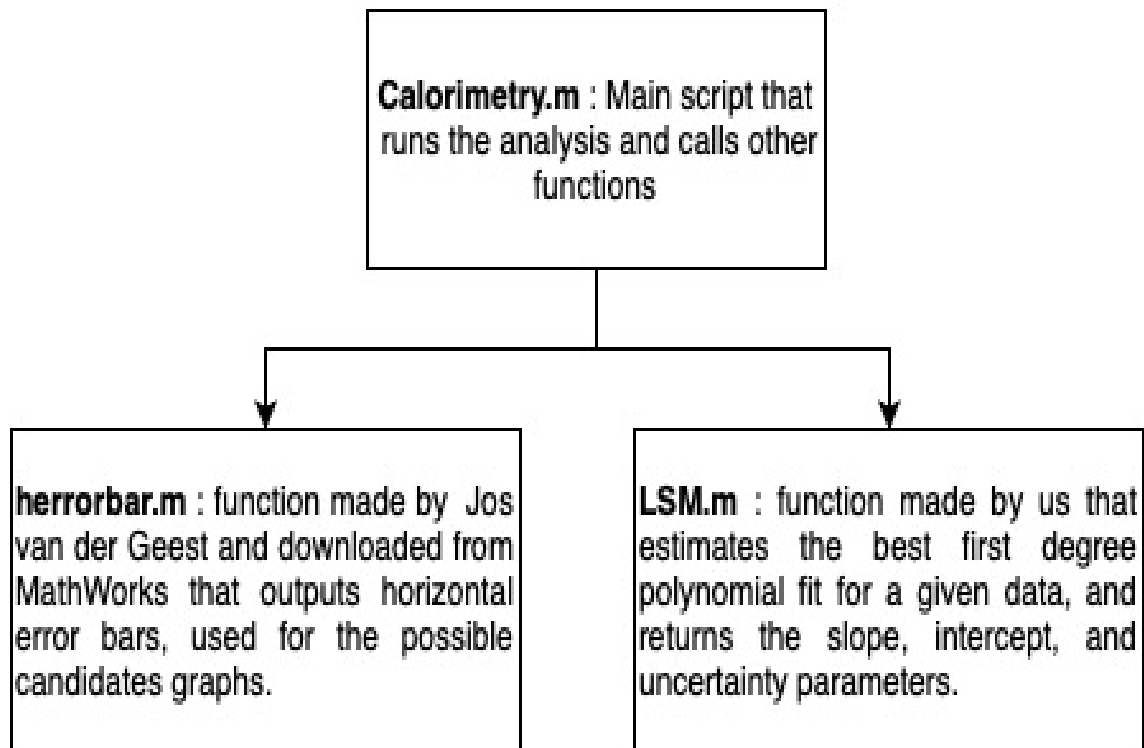
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VII. Appendix

Structural flow chart



Flow chart

