Calorimetry Extrapolations on Sample D

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1) Abstract

Calorimetry is used to find quantities of thermodynamic properties by measuring the voltage difference that occurs between a thermocouple of two different densities at the same temperature. Inside a well-insulated box, we can insert a heated sample that can be analyzed using computer software to create temperature data as it changes with time; The data can later be used with different equations in thermodynamics to provide many quantities. In our case, we will be looking to figure out our sample material from the specific heat of the object placed in the calorimeter. Corresponding to given values, we are to use the temperature measurements in combination with the first law of thermodynamics, least-squares extrapolation, and error propagation in order to estimate a value within reasonable certainty and pick the sample material we are testing.

2) Introduction

For proper thermodynamic calculations, five rows of data gave us the variables: Time, Temperature in Calorimeter 1, Temperature in Boiling Water, Temperature of Room, and Temperature in Calorimeter 2. While all of these data columns are useful, it is important to know exactly where they will fit in in the various equations that we will be using. The first equation we will be looking at is given to us and solves for the specific heat of the sample, Eq(2), but in order for it to truly be useful, it is necessary to derive it from the first law of thermodynamics Eq(1).

$$\Delta E = E_{in} - E_{out} \tag{1}$$

Assuming that the calorimeter and everything in the system is adiabatic, we can assume that the energy in the system does not change, $\Delta E = 0$, allowing us to equate our energy in (from the heated sample) to the energy out (from the calorimeter). We know from our thermodynamics background that energy has the units Joules [J], and if we look at our units for specific heat, $[\frac{J}{g \cdot °C}]$, multiplying our specific heat by the change in temperature in Celsius [℃] and our mass in grams [g], we will be able to set the changes in energy in the sample and the calorimeter equal to each other as shown below. With this understanding and use of the given equations, further units and calculations will be more clear.

$$E_{Sample} = E_{Calorimeter}$$

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

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

First, it is important to get the best use of our data, the temperature values for calorimeter 1 and calorimeter 2 were averaged for slightly increased accuracy. The averaged calorimeter data will be used for the rest of the calculations, starting by finding regression lines using the Least Squares method at the bottom and top linear portions before and following the temperature fluctuation. As directed in the assignment protocol also shown in appendix 2, we will analyze the given data to find our different temperatures for the specific heat calculation (Eq.2).

3) Experimental method

3.A) Regression lines and temperature calculations

MATLAB is an invaluable tool when it comes to handling and manipulating data sets, and will come in handy with our 714 element data vectors we will be using from the calorimeters. First off, using MATLAB to easily average the data from Calorimeter 1 and 2, it is required that we find fit lines using Least Squares interpolation (Eq.3) for the top and bottom linear portions of the temperature data. Using combined if and for loops, the vector is indexed through while looking for the location where the time scale (now in minutes) reaches 10 minutes where the sample is first introduced. Then, using time as our 'X' variable and temperature as our 'Y' variable, we calculate our Least Squares interpolation (Eq.3) using equations 4-6 in MATLAB to find the regression lines for both linear regions mentioned.

$$Y_i = Mx_i + B \tag{3}$$

$$B = \frac{\sum_{i=1}^{N} x^2 \sum_{i=1}^{N} y - \sum_{i=1}^{N} x \sum_{i=1}^{N} xy}{\Delta} \tag{4}$$

$$M = \frac{N \sum_{i=1}^{N} xy - \sum_{i=1}^{N} x \sum_{i=1}^{N} y}{\Delta} \tag{5}$$

$$\Delta = N \sum_{i=1}^{N} x^2 - (\sum_{i=1}^{N} x)^2 \tag{6}$$

Once the regression lines have been fitted, we can look for all of the points needed to be extrapolated from the assignment to find the values of $T_0,\ T_1,\ and\ T_2$. T_0. The direct process given from the instructions at the bottom of our assignment document are included in appendix 2. With all of these temperatures found, there is a clear path towards calculating our specific heat from equation 2 in the introduction. But before the values are taken with 100% certainty, it is important to consider the uncertainty of our measurements and how they propagate throughout all of our calculations. So it is encouraged to look at the equations referenced and general rationale for the uncertainty and error propagation choices made in appendix 3.

4) Results

The first calculations made that build the framework for further calculations are the regression fit lines constructed with the Least Squares method (Eq.3-6). The bottom regression line chosen to model the starting calorimeter data T_0 has a slope or M value of -0.0387℃, and an initial temp or B value of 28.8℃. Our top regression line later used to calculate our T_2 value was found to have a M value of -0.0483℃ and a B value of 33.2℃. Using the equation for linear regression error (Eq.7), the error found for our top and bottom regression lines respectively are 0.237 ℃ and 0.715℃. Plugging our M and B values into equation 3, regression lines were constructed with associated error lines as shown below in Figure 1.

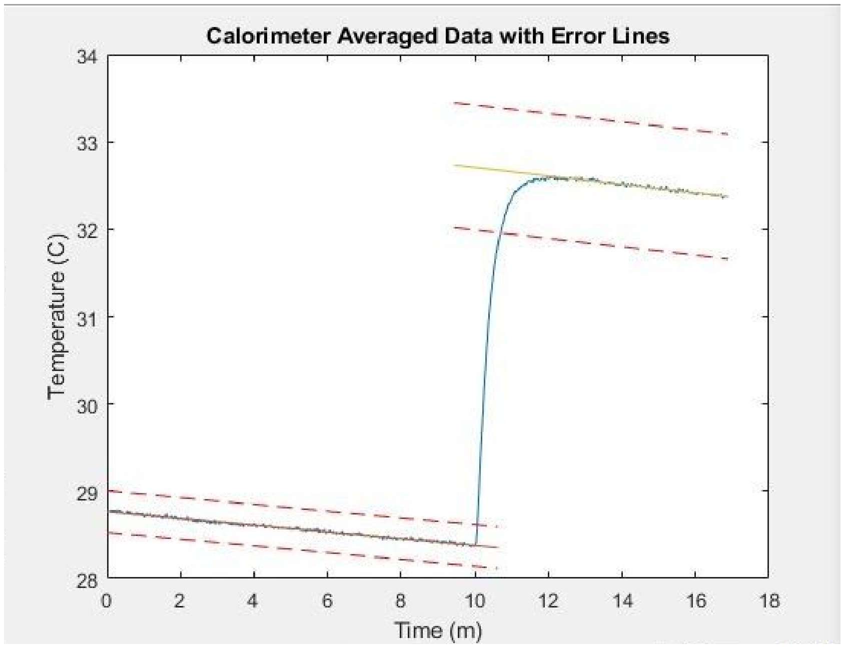


Figure. (1)

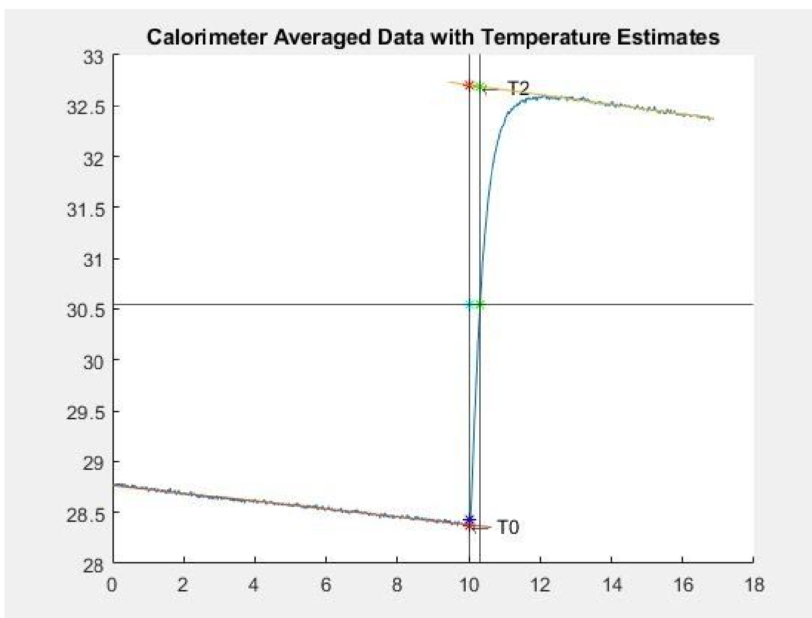


Figure. (2)

From these regression lines, the required calculations can be made to make our T_2 estimation. To start our calculations based on the process in appendix 2, the estimated time before insertion was 10.127 minutes from the beginning of the temperature readings. This point was picked after direct analysis of the charted temperature data, finding the initial data spot of the temperature spike right before the large temperature change characterized from ~10-11 minutes into the readings. As displayed on figure 2, the initial temperatures are taken on the bottom and top regression line right before the moment of insertion at 28.375℃ and 32.699℃. Upon finding the temperatures at 10.127 minutes, they were averaged to a value of 30.537℃. This temperature actually occurs 11.6 seconds later at 10.321 minutes, and from this time point, the temperature from the top regression line is pulled to represent our final graphical calculation for T_2 at 32.690℃. All of these temperatures calculated, plugged into equation 2, provide a specific heat value of 0.3587 $[\frac{J}{g \cdot ℃}]$. Wrapping up our estimations with propagation of our errors and calculating the partial derivative using MATLAB for our specific heat calculation using equation 8, the error in the samples specific heat value was found to be 0.0636 $[\frac{J}{g \cdot ℃}]$.

5) Discussion

Throughout the process of picking proper windows for accessing error, it was deemed necessary to account for a window not only the size used for the regression lines, but slightly larger for the estimates at or just after the time of sample insertion. This affects the size of our errors in one way in particular. Looking at the trend of the line, these error windows include parts of the large temperature jump that would make an error larger than the much smaller errors that would occur from including the fit line windows exclusively. This choice will give us errors that are more characteristic of the various estimates we calculate. We can further affirm this decision from looking at the specific heat and its error propagated from the different temperature errors.

6) Conclusion

From mathematical derivation and error analysis, the sample chosen from the candidates to be most likely the mystery sample is zinc. The calculated specific heat value was found to be 0.3587 $[\frac{J}{g \cdot ℃}]$ with an error of 0.0636 $[\frac{J}{g \cdot ℃}]$. From the given calorimeter candidate materials, zinc has a specific heat value that is the closest to our estimate at 0.402 $[\frac{J}{g \cdot ℃}]$. Not only is it the closest in value, but the added error to our estimate makes zinc the only sample that is within our range of error as well. Over all, the estimates integral to choosing our sample seem to lead to results that are well within reason. The calculated fit lines using Least Squares fitting appear to fit well to the given data window, and the errors displayed on figure 1 are reasonable enough. This leads to the conclusion that the described method and error choices provide a good direct path for analyzing calorimetry data, as well as making calculations off of the different temperature values desired for use in calculating thermodynamic properties such as specific heat.

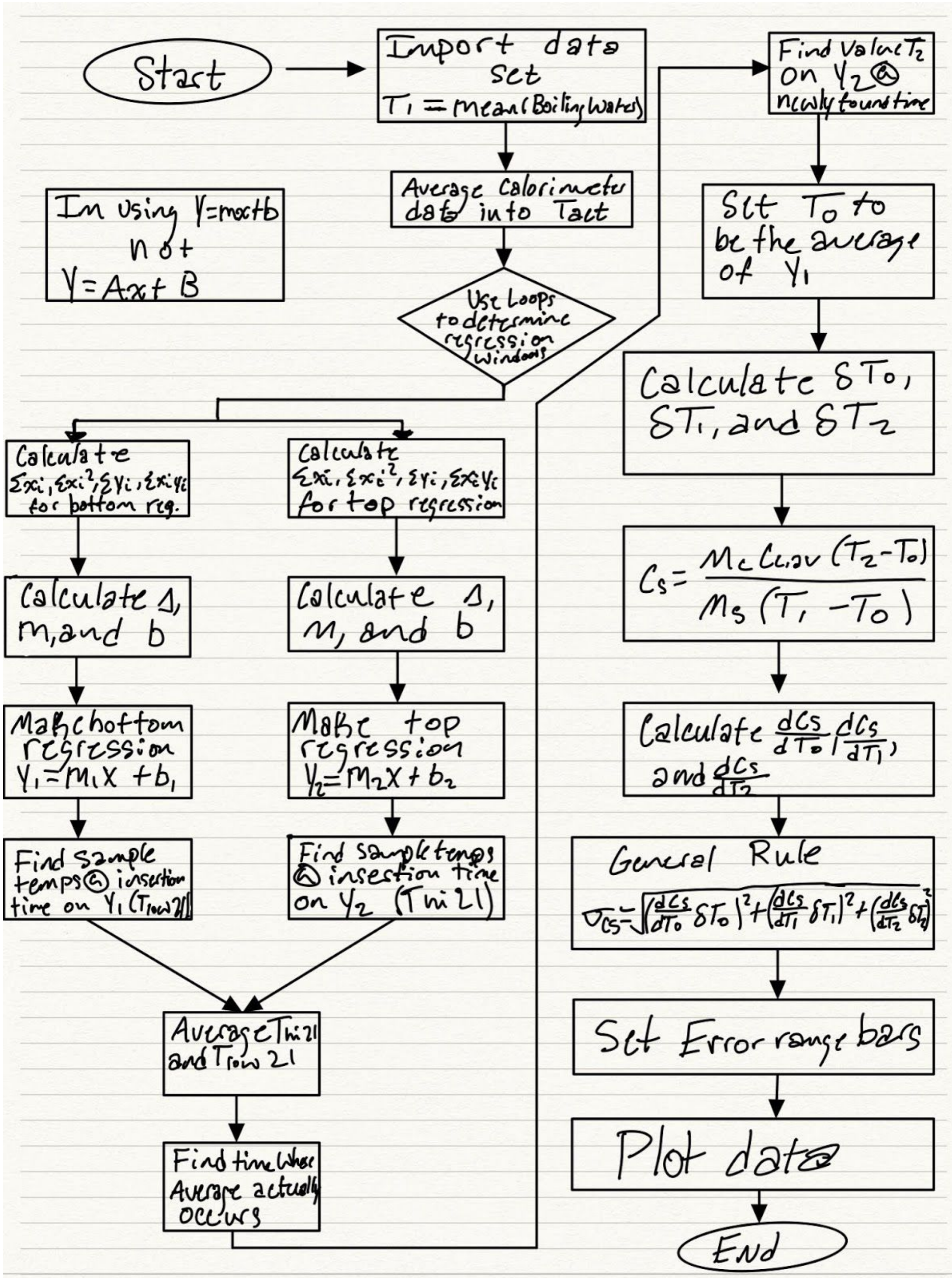
7) References

1.“Reference Style and Format.” *Www*, www.aiaa.org/publications/journals/reference-style-and-format.

2. Given materials and methods from the instructional team for ASEN 2012

8) Appendix

1.



2.

The starting calorimeter temperature is set to be the average value of our bottom regression line that is fit through the data before our sample is added. The initial sample temperature T_1, is assumed to be at a temperature equilibrium with the boiling water it is submerged in, so T_1 can be declared to be the average value of the boiling water. Finally, the final temperature equilibrium achieved between the calorimeter and the sample T_2, is extrapolated on the top regression line from the average temperature time index. IT is found from averaging the temperatures on the top and bottom regression at the time of the sample insertion, finding where the average truly occurs, and then extrapolating on the top regression from that time index.

3.Uncertainty and Error Propagation

It is important to account for the error in calculations to make sure that the estimates made are within an acceptable range. To show this from our base data alone, the error in the averaged calorimeter data was calculated to be up to 2.65 ℃. Since the whole range of the data is just under 5℃, it would be fair to say an error of 2.65℃ would be much larger than should be comfortable for good data. Regardless, the main uncertainties needed to revolve around our specific heat calculation, mainly the uncertainties with our regression lines and the data they were fit to. With Least Squares interpolation, there is a formula for calculating the uncertainty (Eq.7).

$$y = \sqrt{\frac{1}{N-2}\sum_{i=1}^{N}(y_i - B - x_i)^2} \qquad (7)$$

With the given equation, our y_i value will be replaced by our top and bottom fit lines, and the average temperature of the water data we chose to represent T_1. In place of our $-B-x_i$ term, we will be subtracting the actual temperature values over each different time range corresponding to our fit lines and T_1 data. Once the uncertainties are calculated, they are propagated into the uncertainty of the specific heat calculation using the general form for error propagation Eq.(8).

$$\delta q = \sqrt{(\left|\frac{dq}{dx}\right|\delta x)^2 + (\left|\frac{dq}{dy}\right|\delta y)^2} \qquad (8)$$

First, before the general formula can be used, it is necessary to calculate the partial derivatives of equation 2 with respect to our different temperature values we have already found our error in. By just adding a term to equation 8, MATLAB is utilized in order to plug in our partial derivatives and associated errors to calculate the error of the specific heat equation. With the given framework set out, the specific heat can be calculated with a given range of error to make an accurate guess at what our sample material is.