ASEN 2012 Calorimetry Project Fall 2020

Linus C. Schmitz
University of Colorado Boulder, Boulder, Colorado, 80309, USA

Given the temperature readings a least squares fit was used to plot the data and get accurate values for the specific temperatures needed to determine the specific heat constant and compare the results to a list of possible values. It was concluded that sample B was most likely made of Aluminum 6061.

Nomenclature

$C_{s,av}$	=	Specific heat of the sample [J/(g°C)]
$C_{c,av}$	=	Specific heat of the calorimeter [J/(g°C)]
T_0	=	Initial temperature of the calorimeter [°C]
T_1	=	Initial temperature of the sample [°C]
T_2	=	Final temperature of the calorimeter and sample at equilibrium [°C]
m_c	=	Mass of the calorimeter [grams]
m_s	=	Mass of the sample [grams]
t	=	Time vector [seconds]
t_T	=	Testing time [seconds]
y	=	Temperature vector [°C]
δx_n	=	Error in *x* value [units of the *x* value]
σ_y	=	Error in *y* value [°C]
N	=	Length of either time or temperature vector [unitless]

I. Introduction

Calorimetry is a technique used to determine the specific heat capacity of a material through a process in which you identify the amount of heat transfer from a test piece of the material to the calorimeter. This is done by means of the following equation the derivation of which can be found in the appendix

$$C_{s,av} = \frac{m_c C_{c,av}(T_2 - T_0)}{m_s(T_1 - T_2)} \tag{1}$$

Once the $C_{s,av}$ of the test sample is calculated it can be referenced with a table of known values to determine what the material most likely is, given the $C_{s,av}$value and based on the determined error from those calculations.

For this project, the resultant data from a calorimetry experiment was provided and it asked to find the $C_{s,av}$ value for a given sample. From the data, a least-squares approximation was required to determine lines of best fit for the two key segments of the data. These lines were used to determine a theoretical instantaneous change in temperature of the calorimeter. The linear regression lines were used to find T_0, T_1 , and T_2 which are used in Equation 1. In addition, the least-squares calculations resulted in a known error which was used to determine the error in the final value using the general formula for error propagation:

$$\delta f = \sqrt{\left(\frac{\partial f}{\partial x_1}\delta x_1\right)^2 + \left(\frac{\partial f}{\partial x_2}\delta x_2\right)^2 + \cdots + (\frac{\partial f}{\partial x_n}\delta x_n)^2} \quad (2)$$

From the provided $C_{s,av}$ values for the possible four material test samples a reasonable determination could be made as to which sample was made of which material.

II. Experimental Method

The process for collecting the calorimetry data can be viewed in the video from 2016 as noted in the references. Given that the class did not in fact go through these steps in this project a detailed process of these techniques will be omitted from the experiment methods section of this report. Further explanation of this decision can be found in the discussion section.

The least-squares regression calculation is a matrix-based approach in which two vectors (time *t* and temperature *y* for a specific time interval) are passed into a coded function. Within the function, all the calculations were done and the *m* and *b* values for a linear equation such as

$$y = mx + b \quad (3)$$

were output in addition to the error in both of those two values. The function used the following equations to solve for values of Δ (Equation 4.1), *A (Equation 4.2)* and *B (Equation 4.3)***.** These were used in equation 5 to get the relative error for the entire value, σ_y. It is necessary to modify the following equations in order to apply them to matrices however an explanation of those modifications will not be covered in this report. The modifications can be seen in the coded function and in depth in Professor Nerem's lecture 6 slides.

$$\Delta = N\sum t^2 - (\sum t^2)^2 \quad (4.1)$$

$$A = \frac{\sum t^2 \sum y - \sum t \sum ty}{\Delta} \quad (4.2)$$

$$B = \frac{N\sum ty - \sum t \sum y}{\Delta} \quad (4.3)$$

$$\sigma_y = \sqrt{\frac{1}{N-2}\sum_{i=1}^{N}(y_i - A - Bt_i)^2} \quad (5)$$

Selecting the appropriate terms from these matrices, the values of *A*, *B*, δA and δB can be found. These calculations produced two key lines used to calculate the T_0 and T_2 values.

In order to solve Eq 1 values of T_0, T_1 and T_2 was needed. A time was chosen (t_T) which was roughly halfway between the time that the sample was placed into the calorimeter and when the calorimeter and sample were at equilibrium. T_1 was found from the data provided for the sample temperature at t_T. T_0 and T_2 were calculated by evaluating the linear equations output by the function in the format of Equation 3. Which resulted in a solution for the calculations.

Finally, an analysis was required to determine how accurate the calculations were. This was done by solving the general error formula (Equation 2) for the variables in our equation T_0 , T_1 , T_2 , m_c, and m_s.

$$\delta C_{s,av} = \sqrt{\left(\frac{\partial C_{s,av}}{\partial T_o}\delta T_0\right)^2 + \left(\frac{\partial C_{s,av}}{\partial T_1}\delta T_1\right)^2 + \left(\frac{\partial C_{s,av}}{\partial T_2}\delta T_2\right)^2 + \left(\frac{\partial C_{s,av}}{\partial m_c}\delta m_c\right)^2 + \left(\frac{\partial C_{s,av}}{\partial m_s}\delta m_s\right)^2} \quad (6)$$

III. Results

The specific heat capacity of the sample and the modified error in those calculations were as follows.

$$C_{s,av} = 0.831 \text{ J/(g°C)} \quad (7)$$

$$\delta_{C_{s,av}} = 0.066 \text{ J/(g°C)} \quad (8)$$

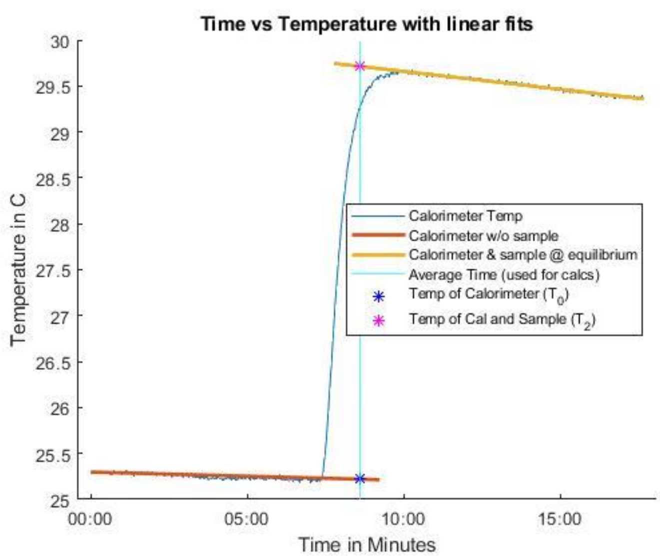
The reasoning for a modified error is provided in the discussion portion of this paper. From the provided specific heat capacities for the various test samples,

$$C_{acrlyic,av} = 1.47 - 1.5 \text{ J/(g°C)} \quad (9.1)$$

$$C_{Zinc,av} = 0.402 \text{ J/(g°C)} \quad (9.2)$$

$$C_{Al\ 6061,av} = 0.895 \text{ J/(g°C)} \quad (9.3)$$

$$C_{Copper,av} = 0.261 \text{ J/(g°C)} \quad (9.4)$$



thus, the sample could be made of Aluminum 6061 (Equation 9.3) based on the calculated value and error for the specific heat capacity (Equations 7 & 8). The figure 1 is a graphical representation of the results given the least squares fit and how T_0 and T_2 were found. Fig 1 can also be seen in greater detail in the code.

(Fig 1)

IV. Discussion

Aluminum is the only possible candidate for the material of the provided test sample (sample B), within that range with the $C_{s,av}$ ± the error values which were calculated. $C_{s,av} + \delta_{C_{s,av}}$ (Equation 7 + Equation 8) is roughly 0.002 J/(g°C) off from the $C_{Al\ 6061,av}$ value provided for Aluminum. This places the possible true value for the calculations comfortably within the calculated error range.

The initial error calculation in which all the variables were considered produced an error in the range of ~ ±1300 for a calculated value which was less than 1. Upon examination of the variables, it was discovered that the error for two of the variables (T_1 and T_0) was causing this massive increase in total error. After a discussion with other students and Teaching Assistants it was discovered that the σ_y(Equation 5) calculation was incorrect. This led to the decision that in order to get a reasonable error for the calculations the $\sigma_y$variable would be overwritten from the error calculation with a value which would be more reasonable given the calculated values of T_1 and T_0 at t_T. It is unclear where exactly the problem with the error calculations is stemming from, however, it can be assumed that there is an issue with the function used to calculate the linear regression and error values. The overwriting of the $\sigma_y$value causes the entire error calculation to be slightly off. Given however, that a reasonable total error is relatively small this change should not affect the total error calculation and thus the additional error from this change can be neglected.

The omission of the video analysis in the experimental methods section is given that the report outlines the steps taken by the author for this project. Since the author did not complete these steps it would not be accurate to list these as part of the methods used.

V. Conclusion

The objective of the lab was to use least-squares fit and calorimetry to determine what material the assigned sample was made of using Equation 1. This was done by analyzing the data provided, determining cut off points for the three stages of the experiment, matching a linear regression to those sections, and then extrapolating specific temperatures in order to calculate the specific heat capacity of the material being tested. Finally, this value was compared against a list of possible values and the most similar material was determined. After taking into consideration the additional error due to assumptions in the code, it can be concluded that sample B was made of Aluminum 6061.

VI. References

Hodgkinson, B. (2020, September 24). Thermocouple Calorimeter. Boulder: Ann and H.J. Smead AES Laboratory and Shops Videos.

Nerem, R. (2020). Lecture 6: Least Squares Curve Fitting . *ASEN 2012* , (pp. 12, 20-24,27,29,30).

Taylor, J. R. (1997). *An Intordution to Error Analysis.* Boulder : University Science Books .

Unknown. (2016, September 28). Calorimeter Demo 9/28/2016. Boulder: Ann and H.J. Smead AES Laboratory and Shops Videos.

VII. Appendix

Analytical derivation of error propagation:

$$\delta C_{s,av} = \sqrt{\left(\frac{\partial C_{s,av}}{\partial T_o}\delta T_0\right)^2 + \left(\frac{\partial C_{s,av}}{\partial T_1}\delta T_1\right)^2 + \left(\frac{\partial C_{s,av}}{\partial T_2}\delta T_2\right)^2 + \left(\frac{\partial C_{s,av}}{\partial m_c}\delta m_c\right)^2 + \left(\frac{\partial C_{s,av}}{\partial m_s}\delta m_s\right)^2}$$

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

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

These partial derivatives combined with the error values for each of the variables which were calculated from the least squares fit function and significant figures values for the provided constants resulted in the value in Equation 8 in the report. The error in each variable was found by summing the errors in *A* and *B* (Equation 4.2 and 4.3) in quadrature for T_0 , T_1 and T_2. The error in m_c, and m_s were found by taking half of the final significant figure provided for each of the measurements.

$$\delta T_0 = \sqrt{\delta A_0{}^2 + \delta B_0{}^2} \quad \delta T_1 = \sqrt{\delta A_1{}^2 + \delta B_1{}^2} \quad \delta T_2 = \sqrt{\delta A_2{}^2 + \delta B_2{}^2}$$

Derivation of Calorimetry equation (Equation 1):

By expanding and rewriting the first law of thermodynamics it can be seen how Equation 1 is derived.

$$\Delta u = mC_{c,av}\Delta T$$

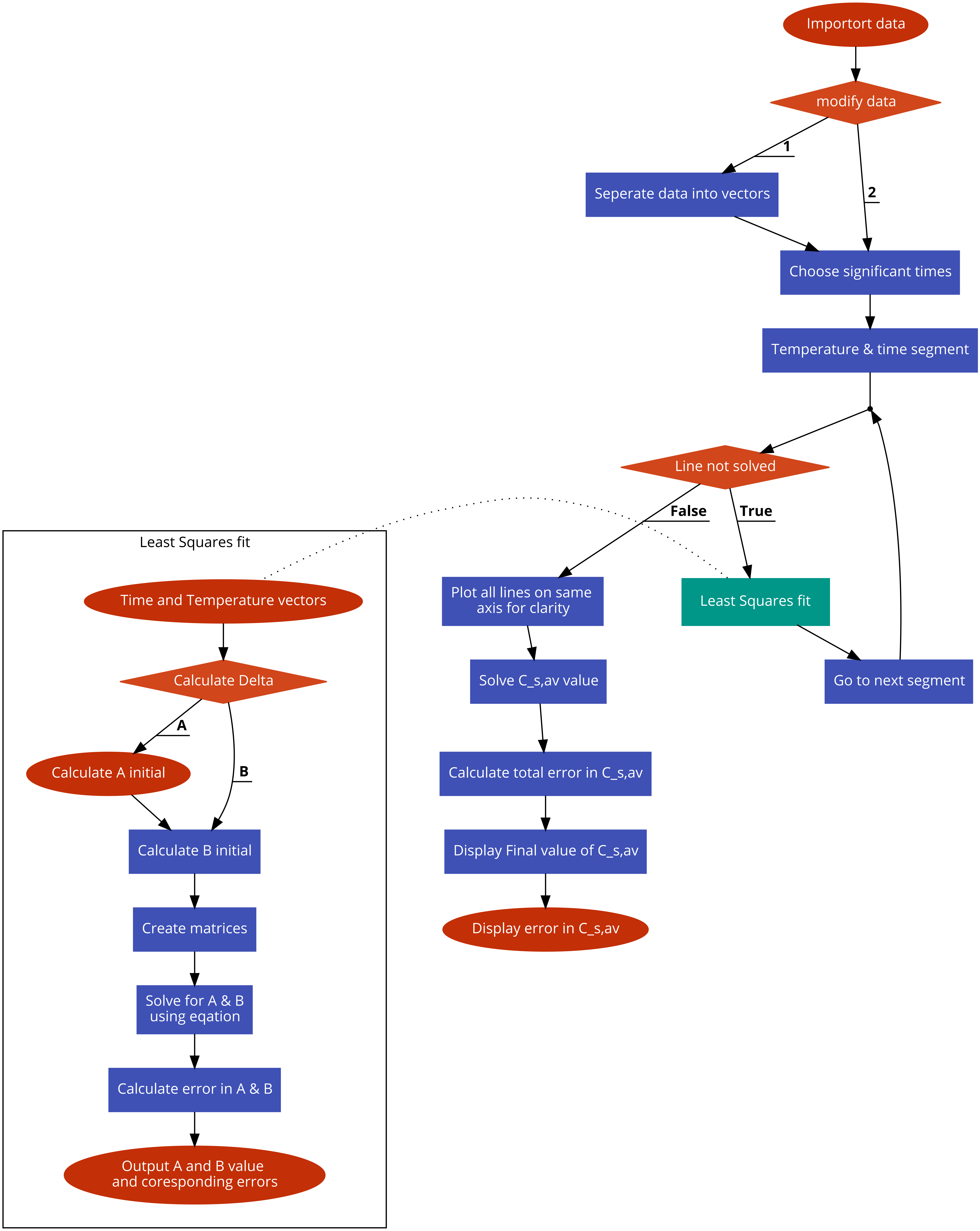
$$u_{c,f} - u_{c,i} = m_c C_{c,av}(T_2 - T_0) \;\&\; u_{s,f} - u_{s,i} = m_s C_{s,av}(T_2 - T_1)$$

Given that the system is adiabatic we know the following:

$$u_f = u_i$$

From which we can set the two equations equal and solve for $C_{s,av}$ which is our unknown getting:

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


Importort data
modify data
1
2
Seperate data into vectors
Choose significant times
Temperature & time segment
Line not solved
False
True
Plot all lines on same
axis for clarity
Least Squares fit
Go to next segment
Solve C_s,av value
Calculate total error in C_s,av
Display Final value of C_s,av
Display error in C_s,av
Least Squares fit
Time and Temperature vectors
Calculate Delta
A
B
Calculate A initial
Calculate B initial
Create matrices
Solve for A & B
using eqation
Calculate error in A & B
Output A and B value
and coresponding errors