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Kenneth C. McGill
Georgia College

Michelle L. Yasechko
Georgia College

Wendy K. Nkari
Georgia College

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Dr. Kenneth C. McGill
Michelle L. Yasechko Chemistry Major
Wendy K. Nkari Chemistry Major

Dr. Kenneth C. McGill
Faculty Sponsor

The adiabatic bomb calorimeter has been an effective tool in facilitating heat transfer between molecules via combustion reaction.[1] Heat is released from the substance combusted and transferred into another, usually water. The heat transferred is measured and the enthalpy of combustion determined for the combusted material. One such classic experiment is the determination of combustion enthalpy of sucrose, obtaining the calorimeter constant with benzoic acid. The results of an adiabatic combustion experiment can be taken one step further to determine the combustion enthalpy in kcal/g by a simple conversion calculation. Since food nutrition labels report calories per grams of serving (note: 1 food caloric = 1 kcal), food can be combusted in an adiabatic bomb calorimeter and the results compared to its corresponding nutrition label. The food chosen for this experiment consisted of marshmallows and cheddar cheese.

Introduction

In 1881, a scientist named Berthelot invented a closed vessel in which a controlled combustion could take place, which he referred to as a bomb. He knew that many substances, particularly hydrocarbons, will combust in the presence of oxygen to form water and carbon dioxide. A general hydrocarbon combustion reaction can be written as follows:

$$C_xH_yO_z + O_2(g) \text{ -----> } CO_2(g) + H_2O(g)$$

The balanced version of this reaction would be:

$$C_xH_yO_z + (X+Y/4-Z/2)\ O_2(g) \text{ -----> } X\ CO_2(g) + (Y/2)\ H_2O(g)$$

Commonly, fuels such as gasolines usually come to mind when mentioning hydrocarbons. However, any organic compound can be referred to as fuel because any organic compound, whether gasoline, carbohydrates, sugars, or proteins, can be combusted in an oxygen rich environment, releasing energy as heat to its surroundings. Just as gasoline provides the energy to propel vehicles, food provides the energy to drive muscular functions. The common reaction that occurs in all fuel combustions follows:

organic compound + oxygen _ carbon dioxide + water + energy

And for proteins:

protein + oxygen _ carbon dioxide + water + ammonia + energy

The energy resulting from combustion reactions can be measured in an adiabatic bomb calorimeter. In an adiabatic bomb calorimeter the bomb, which is the vessel containing the sample and where the combustion takes place, is pressurized with O2 to ensure complete combustion, and then submersed in a known quantity of water. Both the bomb and the water are brought to temperature equilibrium before initiating combustion. To achieve sufficient heat for the combustion, the sample is in contact with a fuse wire, which ignites the sample when current is passed through the wire. The heat resulting from the combustion is transferred to the water surrounding the bomb and is measured with a thermometer or resistive temperature device, RTD.

Operation of the adiabatic bomb calorimeter is based on the First Law of Thermodynamics: heat lost (by the sample) = heat gained (by the water). 3 The heat gained by the water from the complete combustion of the sample is proportional to the temperature change of the water. Therefore, accurately recording the temperature of the water before and after the combustion is the key to success of this experiment. Since the temperature change, ΔT, will be determined, along with the calorimeter constant, C, the heat given off by the sample in the combustion, Q, can be calculated from the relation:

$$Q = C\Delta T \qquad \text{(equation 1)}$$

In order to compare the heat of combustion of food to its corresponding nutrition label value, its enthalpy of combustion must first be calculated. An equation for calculating the heat of combustion of food can be derived from equation 1. Since the combustion occurs at constant volume, equation 1 can be written as:

$$Q_V = Cv\Delta T \qquad \text{(equation 2)}$$

And, since at constant volume ΔU = Cv1, equation 2 can be written as:

$$U = Cv\Delta T \qquad \text{(equation 3)}$$

Also, enthalpy and internal energy are related in the expression:

$$H = \Delta U + \Delta(pV) \qquad \text{(equation 4)}$$

Since the contribution to $\Delta(pV)$ from the net change in pV of solids going from reactants to products is generally negligible, equation 4 can be written as:

$$H = \Delta U \qquad \text{(equation 5)}$$

Now, substituting ΔH in for ΔU in equation 3 gives:

$$H = C\Delta T \qquad \text{(equation 6)}$$

For enhanced accuracy of data, an RTD was used instead of a thermometer. An RTD outputs data in resistance (as the temperature increases, its resistance increases). It follows that equation [6] becomes:

$$H = C\_R \qquad \text{(equation 7)}$$

where ΔR is the change in resistance proportional to change in temperature.

<u>Benzoic Acid Combustion</u>

As mentioned previously, a sample with a known heat of combustion, benzoic acid, was combusted in order to obtain the calorimeter constant, C, in equations 1-7. Therefore, equation 7 is rearranged:

$$C = \Delta H/\Delta U \qquad \text{(equation 8)}$$

Since the sample must be in contact with a fuse wire for the combustion to take place, the fuse wire is combusted with the sample. The fuse wire therefore must be accounted for in all calculations. To incorporate the fuse wire into each combustion, equation 8 can be expanded:

$$C = \frac{(m_{bw} - m_w)*\Delta H_b + (m_w - m_{wa})*\Delta H_w}{R_f - R_i} \qquad \text{(equation 9)}$$

Where m_{bw} is the mass of benzoic acid + wire, m_w is the mass of the wire, $\_H_b$ is the enthalpy of combustion of benzoic acid, m_{wa} is the mass of the wire after the combustion, $\_H_w$ is the enthalpy of combustion of the wire and is also a known value, R_i is the initial resistance, and R_f is the final resistance.

Food Combustion

In this experiment marshmallows and cheese were combusted. To calculate each combustion, ΔH_{mm} and $\_H_{ch}$ takes the place of ΔH_b respectively, and m_{mmw} and m_{chw} takes the place of m_{bw} respectively in equation 9. Then, equation 9 is rearranged to give

$$H_{mm} = \frac{-(C^*R_f - C^*R_i - \Delta H_{wmw} + \Delta H_w{}^*m_{wa})}{(-m_{mmw} + m_w)} \quad \text{(equation10)}$$

and,

$$H_{ch} = \frac{-(C^*R_f - C^*R_i - \Delta H_{wmw} + \Delta H_{w^*mwa})}{(-m_{chw} + m_w)}$$

respectively. Finally, the resulting enthalpy of combustion, calculated in units of kilojoules/gram is converted to kilocalories/gram.

Experimental

Benzoic acid was employed to obtain the heat capacity of the calorimeter. First, approximately 1.00 g of benzoic acid was weighed, pressed into a pellet, and then re-weighed. A 10 cm piece of ignition wire was cut, cleaned with acetone, and also weighed. The fuse wire was carefully fused into the center of the benzoic acid pellet using a 9-volt battery. Next, the sample holder, previously cleaned with soap and water and then with acetone, was removed from the likewise cleaned bomb vessel. The benzoic acid pellet was then connected to the two terminals of the sample holder by carefully threading each end of the fuse wire through the terminals and then wrapping the excess fuse wire around the terminals on the sample holder. Caution was taken so that the ends of the fuse wire were turned inward and not touching the sides of bomb vessel in order to prevent shorting against the bomb vessel. The sample holder was gently lowered into the vessel and the bomb lid was properly assembled onto the bomb vessel, ensuring a good seal. The hose from an oxygen tank was firmly connected to the inlet valve located on top of the bomb. The bomb was slowly pressurized to 30 ± 1atm. By carefully opening the release valve, the bomb was slowly vented to 0 ±1 atm. The bomb was then re-pressurized and re-vented two more times. Finally, the bomb was pressurized again to 30 ±1 atm to ensure that as much pure oxygen as possible was contained in the bomb. Then the shutoff valve on the oxygen bottle was turned off, the oxygen line was vented, and removed from the bomb.

Using a digital multimeter, the continuity of the two terminals located on top of the bomb was read. The reading obtained should be 1 ohm or less.

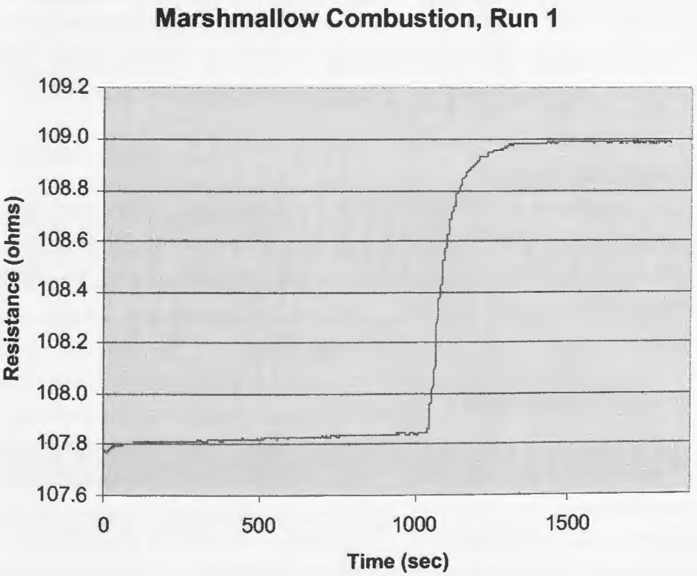
Next, the water bucket is filled with approximately 2000 ±1 ml of tap water, obtained by using a 1 L volumetric flask. To ensure the exact mass of water was for every bomb ignition, the water bucket was placed on a balance and balanced with weights. The weights needed to balance the water were recorded and the bucket removed. The bucket of water was then placed inside of the calorimeter. Bomb tongs were attached to the bomb vessel, and the bomb was lowered into the water. Electrodes of the apparatus were then plugged into their appropriate positions on top of the bomb. The bomb tongs were then carefully removed. (Note: ensure that no bubbling appears from the bomb, which could signal a leak.)

The adiabatic jacket cover was secured and its attached RTD was lowered into position. The electric stirrer was then lowered and the system was allowed to reach temperature equilibrium (approximately 10 minutes). Resistance readings were monitored via applicable software. The charging switch of the calorimeter was turned on. Then the ignition button was depressed until illumination of the ignition indicating light was observed. The button was then released (Note: the ignition button should not be depressed for more than 4 seconds otherwise damage may occur). The resistance was then observed for an increase, indicating successful combustion. Resistance readings were allowed to stabilize for approximately 10 ±1 minutes. The system was then turned off and the bomb was removed from the apparatus and vented. Using Microsoft Excel, the data collected were saved. The fuse wire remaining was then weighed.

The bomb was cleaned and the procedure was repeated two more times employing benzoic acid, three times with marshmallows, and three times with cheddar cheese cubes (Note: the weight of marshmallows was approximately 2 grams while that of cheese cubes was approximately 1 gram).

Employing the saved Microsoft Excel file, the output of the RTD was formatted into a graph. From the minimum and maximum resistance values on the graph, the initial and final resistance values were determined, along with standard deviations. In the absence of a minimum on any of the graphs, a linear regression was performed. Such a graph is displayed in Figure 1.

Table 1:
"Marshmallow Combustion Graph"



Results and Discussion

The calorimeter constant calculated from equation 9 was found to be 26.064 (± 0.986) kJ/Ω. The data employed for this calculation was recorded from the Benzoic Acid combustions and is shown in Table 1.

Table 1:
Benzoic Acid Combustion Data

	Run 1:	Run 2:	Run 3:
Mass of Benzoic Acid + wire, m_{bw} (grams):	1.1005(±0.001)	91.0625(±0.001)	0.9878(±0.001)
Mass of wire, m_w (grams):	0.0165(±0.0005)	0.0165(±0.0001)	0.0159(±0.0009)
Mass of wire after, m_{wa} (grams):	0.0077(±0.0007)	0.0056(±0.0006)	0.0107(±0.0007)
Initial resistance, R_i (ohms):	108.2650(±0.0024)	108.6680(±0.0018)	109.3772(±0.0017)
Final resistance, R_f (ohms):	109.3690(±0.0011)	109.7280(±0.0016)	110.3570(±0.0021)

The enthalpy of combustion from the label attached to the nichrome fuse wire and the literature value for enthalpy of combustion of Benzoic Acid1 were recorded as follows and incorporated into equation 9 as well:

H_w: -1400 (±1) cal/g
H_b: -3227 (±1) kJ/mol

Marshmallow Combustion

The results of the marshmallow combustion experiment successfully elucidated the approximate kilocalories/gram of marshmallows. The values from the following table, Table 2, were recorded and incorporated into equation 10:

Table 2:
Marshmallow Combustion Data

	Run 1	Run 2	Run3
Mass of wire before, m_w (grams):	0.0160 (±0.00009)	0.0164 (±0.0004)	0.0160 (±0.00009)
Mass of wire after, m_{wa} (grams):	0.0106 (±0.0006)	0.0108 (±0.0008)	0.0149 (±0.0009)
Mass of marshmallow + wire m_{mmw} (grams):	2.1127 (±0.0007)	2.1207 (±0.0007)	2.1263 (0.0003)
Initial resistance, R_i (ohms):	107.8278 (±0.0023)	106.9744 (±0.0024)	107.1524 (±0.0030)
Final resistance, R_f (ohms):	108.9970 (±0.0030)	108.1150 (±0.0018)	108.2990 (±0.0020)

Table 3 shows the results calculated from equation 10.

Table 3:
Marshmallow Combustion Enthalpy

	KJ/g	Kcal/g
Run1:	20.1(±1.7)	4.8(±1.7)
Run 2:	17.5(±1.7)	4.2(±1.7)
Run 3:	23.1(±2.1)	5.5(±2.1)

An average enthalpy of combustion for marshmallows was calculated to be 3.23(±0.99) kcal/g. Prior to comparing this result to the nutrition label, the theoretical value was obtained by dividing the calories per serving by the grams per serving found on the nutrition label. The calories per serving were 100, and the grams per serving were 28, giving a theoretical value of 3.6(±1.4) kcal/g and a percent difference of 9.5 percent.

Cheese Combustion

The result obtained for the cheese combustion proved to be less successful than the marshmallow experiment. A larger percent difference was calculated from the results. Contributing to the decreased success of this combustion experiment was the observation of a residue in the bomb after the cheese combustion consisting of hard, tiny, white beads, presumed to be calcium. Further analysis is required to properly account for the non-combustible material found in food, such as minerals. Continuation of the cheese experiment would consist of analyzing the water formed in the combustion as well as analysis of the residue. The analysis of water would be best accomplished using Gas Chromatography Mass Spectrometry methods to identify the other compounds present in the water formed from the combustion. Analysis of the residue can be done by doing various tests depending on the food label, for example in this case, a protein test and a lipid test can be done4.

The values from the following table, Table 4, were recorded and incorporated into equation 10:

Table 4:
Cheese Combustion Data

	Run 1	Run 2	Run3
Mass of wire before, m_W (grams):	0.0160 (±0.00009)	0.0158 (±0.0008)	0.0168 (±0.0008)
Mass of wire after, m_{Wa} (grams):	0.0132 (±0.0002)	0.0121 (±0.0001)	0.0108 (±0.0008)
Mass of cheese + wire, mchw (grams):	1.0687 (±0.0009)	1.0427 (±0.0011)	0.9013 (±0.0014)
Initial resistance, R_i (ohms):	108.0542 (±0.0014)	108.2888 (±0.0013)	108.2380 (±0.0016)
Final resistance, R_f (ohms):	108.8660 (±0.0018)	108.9800 (±0.0020)	109.0220 (±0.0020)

Table 5 shows the results calculated from equation 10.

Table 5:
Cheese Combustion Enthalpy

	KJ/g	Kcal/g
Run 1:	14.51(±0.99)	3.47(±0.99)
Run 2:	14.11(±0.99)	3.37(±0.99)
Run 3:	11.89(±0.99)	2.84(±0.99)

An average enthalpy of combustion for cheese was calculated to be 4.8(±1.8) kcal/g. Prior to comparing this result to the nutrition label, the theoretical value was obtained by dividing the calories per serving by the grams per serving found on the nutrition label. The calories per serving were 110, and the grams per serving were 28, giving a theoretical value of 3.9(±1.4) kcal/g and a percent difference of 22.9 percent.

The results of both marshmallow and cheese combustion experiments are shown in Table 6:

Table 6:
Combustion Enthalpy Comparison

Combustion:	Experimental Kcal/g:	Nutrition Label Kcal/g
Marshmallow	3.2(±1.7)	3.6 (±1.4)
Cheese	4.8(±3.3)	3.9(±1.4)

NB: The error analysis is an absolute value

Conclusion

The adiabatic bomb calorimeter provides a safe, simple, and effective means of measuring energies of combustion or many types of fuels, including food. Determination of calories in food, especially sugars and carbohydrates, is successfully accomplished via adiabatic calorimetry.

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