Bomb Calorimetry Simulation – Instructions

1. **Determination of the Calorimeter Constant**
   A new virtual calorimeter is created each time the web page for this web app is refreshed. Therefore, it is necessary to determine the calorimeter constant (C_{eq}) each time the program is run.

   (a) On the opening screen, click on CHOOSE SAMPLE.

   (b) Click the button next to Benzoic Acid if it isn't already selected. Click on TAKE IT TO THE SCALE.

   (c) Record the Sample Weight (about 1 gram). This may be adjusted to an approximate value between 0.1 and 2 grams by clicking on the arrows or entering a value directly in the text box. The initial water temperature may also be adjusted between 22 and 30 ^{o}C.

   (d) Record the weight wire before igniting.

   (e) Click on the IGNITE button.

   (f) Record the weight of the wire after ignition.

   (g) Click on EXTRAPOLATE. Extrapolations of the flat portions of the graph appear in dashed red (initial) and green (final). These extrapolations are based on Linear Least Squares Regression of the first five and the last six data points. The uncertainty in the extrapolation of T_i is approximately 0.0015 ^{o}C, and the uncertainty in T_f is approximately 0.0025 ^{o}C.

   (h) Hovering your mouse over the plot, position the vertical blue line so as to equate the two enclosed areas as in Fig. 2 of Discussion. The extrapolated temperatures may change slightly.

   (i) Record the initial (T_i) and final (T_f) temperatures. You can download the plot as a png file by clicking on the camera icon ( ).

   (j) Click on VIEW RESULTS. A pop-up window will appear that contains the bomb calorimetry data (time in seconds versus temperature in ^{o}C). This data can be copied and saved as a text file or directly copy and pasted into a spreadsheet for data analysis. The plot and extrapolations (data analysis and visualization) should be reproduced by students using this raw simulation data, which is representative of the data a student would get by doing a real bomb calorimetry experiment on a standard Parr Bomb Calorimeter. A summary of all of the other important parameters are also summarized on this pop-up page. After printing or copy-and-pasting this data and information, the window can be closed by clicking on the X in the top left.

   (k) Click on CONSTANTS to obtain the energy equivalents of benzoic acid and iron wire.

      i. Calculate the energy released ($E_{released}$ in Joules, J) in the combustion:

      $$E_{released} = (26425\ J/g)\times(\text{Sample Wt.})+(5858\ J/g)\times[\text{Wt. wire before}(g)-\text{Wt. wire after}(g)]$$

      ii. Calculate the Calorimeter Constant (C_{eq} in $^{J}/_{K}$):

      $$C_{eq} = {}^{E_{released}}/_{[T_i-T_f]}$$

   Note that there are two conversion factors above: 26425 J/g is the energy equivalent conversion factor for the standard (benzoic acid), while 5858 J/g is the energy equivalent for the iron (wire).

   In a research situation, the measurement of the Calorimeter Constant would be repeated many times to determine a very precise average of the Calorimeter Constant and its uncertainty. The visual plot of the data shown on the Bomb Calorimetry Simulator is not meant to provide final data analysis or visualizations for a students report. It is only designed to provide preliminary visualization of the data (it is a plot of the data provided after clicking VIEW RESULTS and serves as an example of what students should be able to plot themselves using the raw data from the simulation).

2. **Determination of the Enthalpy of Combustion (ΔH_{comb}) of a Compound**

   (a) Repeat steps (a)-(k) above, choosing one of the other compounds in place of Benzoic Acid.

   (b) Calculate the Molar Mass (M) of the compound from its chemical formula, and the number of moles (n) burned in the experiment:

   $$n = {}^{Sample\,Wt}/_{M}$$

   (c) Calculate the total energy released in the combustion (ΔU) in Joules (J), correcting for the change in mass (in grams, g) of the wire due to burning:

   $$\Delta U = -C_{eq}(T_i - T_f) + (5858\,J/g) \times [\text{Wt. wire before}(g) - \text{Wt. wire after}(g)]$$

   (d) Calculate the energy released per mole of compound burned ($\Delta\bar{U}$ in ${}^{J}/_{mole}$):

   $$\Delta\bar{U} = {}^{\Delta U}/_{n}$$

   (e) Balance the combustion reaction for one mole of compound, and calculate the change in the number of moles of gas (ΔN_{gas}):

   $$\Delta N_{gas} = [\text{moles of } CO_2 \text{ formed}] - [\text{moles of } O_2 \text{ consumed}]$$

   (f) Calculate the molar enthalpy of combustion ($\Delta\bar{H}$):

   $$\Delta\bar{H} = \Delta\bar{U} + \Delta N_{gas}RT$$

   (g) Divide by 1000 to obtain the molar enthalpy of combustion ($\Delta\bar{H}_{comb}$) in ${}^{kJ}/_{mol}$.

References

[1] `https://asu-molecular-sciences-cloud-lab.github.io/bomb_calorimetry_v2/`