Bomb Calorimetry Simulation – Instructions

1. **Determination of the Calorimeter Constant**
   Each virtual Parr bomb calorimeter is associated with a 4-digit serial code, which can be input on the CHOOSE SAMPLE page. Each Parr bomb calorimeter has its own calorimeter constant C_{eq}. To ensure consistent results across multiple experiments, make sure you are using **THE SAME CALORIMETER SERIAL CODE** each time.

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

   (b) At the top of the page, enter a 4-digit code corresponding to your chosen calorimeter. Ensure you are using the same calorimeter serial code each time you run an experiment. Record the 4-digit code used, and ensure it is in your report. Click the button next to Benzoic Acid if it isn't already selected. Then, 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 20 and 30 ^{o}C.

   (d) Record the weight wire before igniting.

   (e) Recall that you need to add water and set the pressure of oxygen in the bomb calorimeter to 30 atm. Think about what might happen if these aren't added. Add 2.0 L of water and 30 atm of oxygen to the bomb calorimeter. Click on the IGNITE button.

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

   (g) To download the data, click DOWNLOAD DATA. Alternatively, click on VIEW RESULTS. The downloaded csv file contains bomb calorimetry data as time in seconds versus temperature in ^{o}C. The pop-up window contains the bomb calorimetry data in time in minutes versus temperature in ^{o}C. The csv file should directly be used for data analysis. This data 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 and csv file.

   (h) To perform extrapolations, students may perform a linear least squares regression of the first five and last six data points. A vertical line can be placed to equate the two enclosed areas as in Fig. 2 of the discussion. These extrapolated temperatures may change slightly.

   (i) Record the initial (T_i) and final (T_f) temperatures. Using a small Python or MATLAB script, students may plot their own figure. 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).

   (j) 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 $\frac{J}{K}$):

      $$C_{eq} = -\frac{E_{released}}{(T_f - T_i)}$$

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.

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

    (a) Repeat steps (a)-(j) above, choosing one of the other compounds in place of Benzoic Acid. Ensure that you are using the **SAME** 4-digit calorimeter serial code as previously

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

    $$n = \frac{\text{Sample Wt.}}{M}$$

    (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:

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

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

    $$\Delta \bar{U} = \frac{\Delta U}{n}$$

    (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/`