Investigating the effect of increasing mass of alcohol on the enthalpy of combustion of ethanol and isopropanol.

Introduction:

In the modern world, cars have become an integral mode of transportation. Transportation of people and merchandise has allowed the world to run faster and as a result, the productivity of an average day has increased, however as a result, fossil fuel reserves are being burned everyday by combustion engines of cars. This has a negative effect not only on the environment but also on the economy. Because of depleting fuel reserves, the supply of everyday diesel petrol cannot cater for the increasing demand, in turn forcing the petroleum industries and governments to increase the price of petrol. In addition, the petroleum created from fractional distillation creates problems for the environment as the resultant combustion products aids the global warming process. Thus, a lot of today's scientific research is going towards the development of alternative fuels.

Alcohols are organic molecules that contain a hydroxyl group, –OH. Alcohols form a homologous series with the general formula, $C_nH_{2n+1}OH$. Alcohols are grouped into three categories based on their structure: primary, secondary and tertiary. In primary (1˚) alcohols such as ethanol, the carbon atom bonded to the –OH functional group is attached to only one alkyl group. In secondary (2˚) alcohols such as propan-2-ol (isopropanol), the carbon atom bonded to the –OH functional group is attached to two alkyl groups. In tertiary (3˚) alcohols, the carbon atom bonded to the –OH functional group is attached to three alkyl groups, such as 2-methylpropan-2-ol (Ryan and Norris, 2014). The more carbon atoms added to the homologous chain, the more complex the structure becomes, and their physical and chemical properties will also differ and follow a certain pattern.

In this experiment, I'll be investigating two fuels; ethanol and isopropanol (propan-2-ol). Ethanol is used extensively as a solvent in the manufacture of varnishes and perfumes; as a preservative for biological specimens; in the preparation of essences and flavorings; in many medicines and drugs; as a disinfectant and in tinctures (e.g., tincture of iodine); and as a fuel and gasoline additive. Isopropanol is an isomer of propan-1-ol that is used in rubbing alcohol, as a solvent in cosmetics such as hand lotions and after shave lotions, and as a chemical in the degradation of ethanol. As we can see, the above listed alcohols have a wide range of uses and are very common in the world today. However, in this experiment, I will only measure the enthalpy change of the alcohol, because, with the need to search for alternative fuels, understanding the enthalpy change of a potential fuel is a very important factor in deciding whether the fuel will truly be used commercially.

The combustion of alcohol is exothermic which produces a lot of energy. Alcohols burn in excess oxygen to produce carbon dioxide and water.

Ethanol: $C_2H_5OH\ (l) + 3O_2\ (g) \rightarrow 2CO_2\ (g) + 3H_2O\ (l)$

Isopropanol: $C_3H_7OH\ (l) + 4\frac{1}{2}O_2\ (g) \rightarrow 3CO_2\ (g) + 4H_2O\ (l)$

Due to the complete combustion of alcohol, it only gives water and carbon dioxide as the products, so they make good fuels that burn cleanly and quickly (Wooster and Eccles, 2008) Alcohols also give out a lot of energy, are readily available and can be easily stored.

The standard molar enthalpy of combustion (ΔH°_{c}), is the enthalpy change when one mole of a substance is burned in excess oxygen under standard conditions with the reactants and products in their standard states (Lister and Renshaw, 2009). Enthalpy changes are all measured under standard conditions in which the reactants and products are in their standard states at 100 kPa and 298 K (25˚C). It is measured in kilojoules per mole, kJ mol^{-1}. (Enthalpy is a measure of the heat content in a system.)

As the reaction involves the release of energy, it is exothermic in nature and thus the products are more stable than the reactants. Exothermic reactions are those reactions in which the amount of energy released (bonds formed) is more than the energy absorbed (bonds broken). An exothermic reaction releases energy to the surroundings, therefore causing the temperature of the surroundings to increase. Therefore, the enthalpy change can be measured by the heat transferred to the surrounding. This can be done by using a calorimeter. The enthalpy change can be measured by burning a known mass of a substance and using the heat released to raise the temperature of a known mass of water.

Enthalpy change can be measured by using the following formula:

$$\Delta H = mc\Delta T$$

Where m is the mass of water, c is the specific heat capacity of water, and ΔT is the temperature change $(T_{final} - T_{initial})$°C.

The specific heat capacity of water is given as 4.18 J g^{-1} K^{-1}. This means that it takes 4.18 joules to raise the temperature of one gram of water by one Kelvin.

Research question:

How does increasing the mass (50 g, 60 g, 70 g, 80 g, 90 g) of ethanol and propan-2-ol (isopropanol) affect its enthalpy change (using a constant-pressure calorimeter)?

Hypothesis:

I hypothesize that increasing the mass of ethanol and isopropanol will lead to an increase in the calculated enthalpy change for each mass of the alcohol.

This proportionality is due to the fact that increasing the mass of the alcohols means that more heat energy will be released to the surroundings on combustion. Therefore, water would experience a large temperature change. Hence, the calculated value of the alcohol's enthalpy of combustion (ΔH°_{c}) would be higher.

This will work because of an extremely exothermic reaction with oxygen known as combustion; the heat energy generated from the substance is released by the molecules of the substance. Increasing the mass of the alcohol sample is correlated with an increase in the amount of thermal energy released by combustion, as there are more molecules in the substance.

Variables:

For this experiment, I will be using an online constant-pressure calorimeter simulation provided by Pearson (https://media.pearsoncmg.com/bc/bc_0media_chem/chem_sim/calorimetry/Calor.php)

Independent: Mass of the alcohol (ethanol and isopropanol) **-** 50 g, 60 g, 70 g, 80 g, and 90 g.

Dependent: The enthalpy of combustion of each alcohol (by finding out the temperature change for each mass).

Controlled: The following variables were kept constant to ensure consistency and fairness in each trial.

Table 1: Controlled variables and methods to control them

Variables	**Method to control the variable**
Mass of water	The same mass of water was taken for each trial, which is 100 g. Changing the mass of water will affect the calculated value of the enthalpy change. Therefore, it is important to keep the mass of water constant. In terms of controlling this variable, the simulation uses a mass adjustment slider that can be adjusted to the required mass, so the mass of water was adjusted to 100 g for each trial.
Initial temperature of water	The initial temperature of water needs to be kept constant so that the temperature change of water can be calculated against a constant reference point. This variable is controlled by setting the temperature adjustment slider in the simulation to 20°C for each trial.

Temperature of ethanol and isopropanol*	The temperature of ethanol and isopropanol (propan-2-ol) was kept constant at 70°C and 80°C respectively. This variable was controlled by setting the temperature adjustment slider to 70°C for ethanol and 80°C for isopropanol for each trial. This was done so that the effect of mass on the change in enthalpy could be accurately observed.
Pressure inside the calorimeter	Since this a constant-pressure calorimeter, the pressure inside is constant and, therefore, it has to be an isobaric process (thermodynamic process in which the pressure stays constant). This is controlled as the calorimeter in the simulation automatically keeps it constant.
Apparatus used	The same type of calorimeter (700 mL capacity), beaker (300 mL), weighing balance (200 g), hotplate and digital thermometer was used in the simulation for each trial.

*The temperature of ethanol and isopropanol used in this simulation refers to the boiling point of each alcohol. The actual values of these boiling points have not been used in the simulation (78.37°C and 82.5°C respectively) because the simulation uses constant intervals between values (on the temperature adjustment slider).

Table 2: Apparatus used in the simulation

Sr. No.	Apparatus	Quantity	Capacity
1	Beaker	1	300 ml
2	Hotplate	1	-
3	Weighing balance	1	200 g
4	Digital thermometer	1	0°C to 100°C
5	Constant-pressure calorimeter	1	700 mL

Table 3: Chemicals used in the simulation

Sr. No.	Chemicals used
1	Ethanol (C_2H_5OH)
2	Propan-2-ol (C_3H_7OH)
3	Water (H_2O)

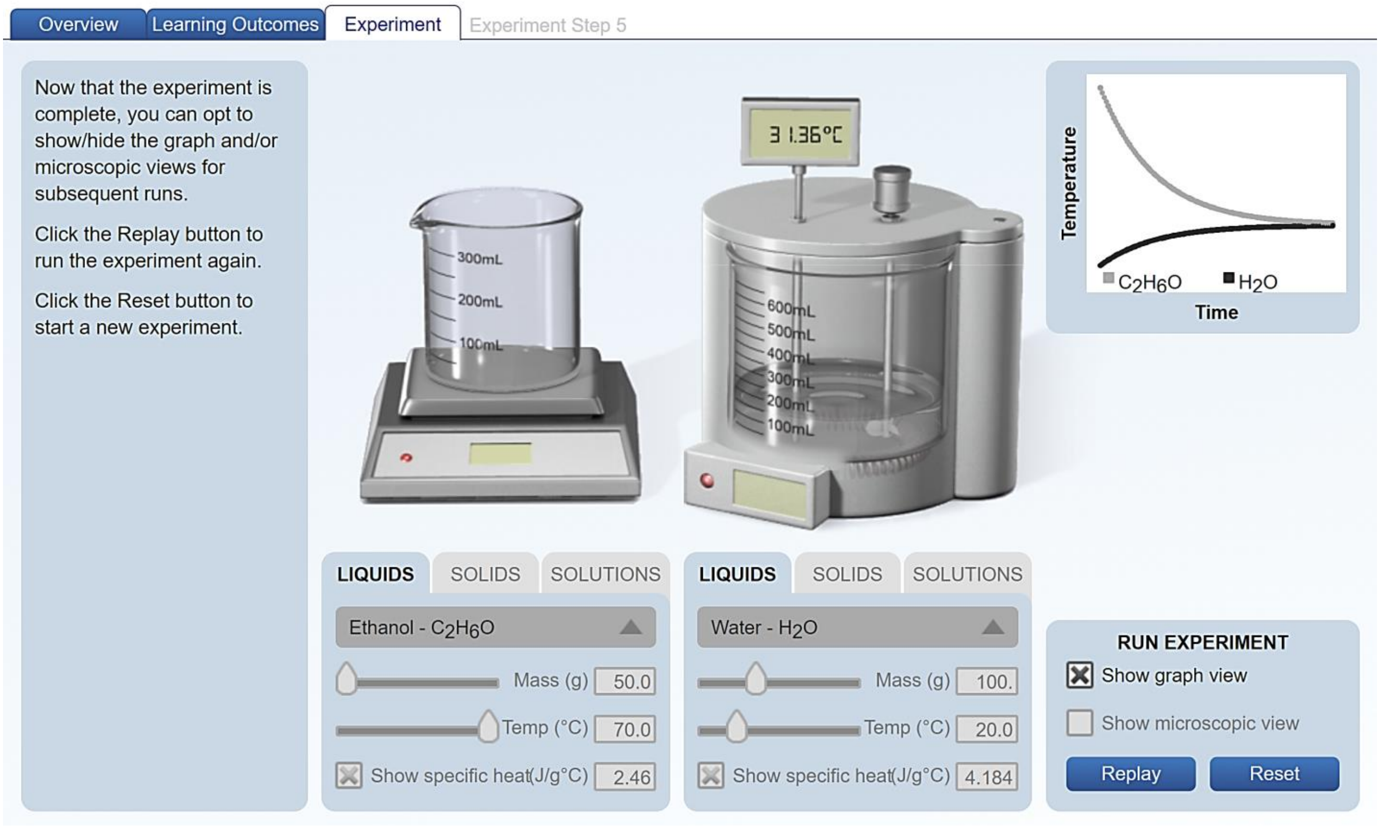
Methodology:

I chose to do a simulation as we could not conduct our experiment in school due to the pandemic. I thoroughly searched for other simulations as well, however, this is the only simulation that was user-friendly and free to use.

1. Open the Pearson simulation and click on “Run experiment” under the “Experiment” tab.
2. First, a substance has to be chosen from the pre-set list of chemicals. Start by selecting “ethanol” from the list.
3. Now set the mass adjustment slider to 50 g and its temperature adjustment slider to 70˚C. Then click on “Next”.
4. Now a second substance is to be chosen, which would go into the calorimeter. For all the trials, select “water” from the pre-set list of substances.
5. Mass is adjusted to 100 g of water and the temperature to 20˚C. Note that for all the trials, the above two steps will remain the same.
6. Click on “Next” and then “Start” to run the experiment and wait till thermal equilibrium between the ethanol and water in the calorimeter has been reached.*****
7. Once the experiment is over, record the final temperature of the water in the calorimeter and subtract the initial temperature (20˚C) to get temperature change (ΔT). Record the value of the temperature change (ΔT).
8. Click on “Reset” and repeat the above steps for 60 g, 70 g, 80 g, and 90 g of ethanol.
9. Once the temperature change for each mass of ethanol has been collected, repeat the above steps for the second alcohol, isopropanol, for 50 g, 60 g, 70 g, 80 g, and 90 g.
10. Once all the temperature change data has been collected, substitute the value of ΔT in the formula ($Q = mc\Delta T$) to calculate the enthalpy change for each mass of the alcohol (ethanol and isopropanol).

*****One point to be noted is that a constant-pressure calorimeter measures enthalpy change, unlike a bomb calorimeter which measures the heat of combustion. In this experiment, since enthalpy change is being measured, the heat released (upon heating the alcohol to its boiling point) is absorbed by the water and is equal to the change in enthalpy.

Figure 1: Experimental set-up



Now that the experiment is complete, you can opt to show/hide the graph and/or microscopic views for subsequent runs.

Click the Replay button to run the experiment again.

Click the Reset button to start a new experiment.

Ethanol - C_2H_6O
Mass (g) 50.0
Temp (°C) 70.0
☒ Show specific heat(J/g°C) 2.46

Water - H_2O
Mass (g) 100.
Temp (°C) 20.0
☒ Show specific heat(J/g°C) 4.184

☒ Show graph view
☐ Show microscopic view

Safety/Ethical considerations:

Since no actual chemicals were used, there was no wastage or environmental concern of any sort. Furthermore, the simulation didn't use any living organisms, and hence had no ethical concern.

Results:

Raw data table:

TABLE 4: Temperature change of water for different masses of Ethanol

Mass (g)	Initial temperature of water (°C)	Final temperature of water (°C)	Temperature change of water [Final temp. - Initial temp.] (°C)
50	20	31.36	11.36
60	20	33.04	13.04
70	20	34.58	14.58
80	20	35.99	15.99
90	20	37.30	17.30

TABLE 5: Temperature change of water for different masses of Isopropanol

Mass (g)	Initial temperature of water (°C)	Final temperature of water (°C)	Temperature change of water [Final temp. - Initial temp.] (°C)
50	20	34.22	14.22
60	20	36.30	16.30
70	20	38.19	18.19
80	20	39.92	19.92
90	20	41.52	21.52

Data processing:

Processed data table:

TABLE 6: Calculated enthalpy change for different masses of Ethanol and Isopropanol

Alcohol	Mass of alcohol (g)	Temperature change of water (^{0}C)	Calculated enthalpy change (kJ mol^{-1})
Ethanol	50	11.36	4.753
	60	13.04	5.456
	70	14.58	6.100
	80	15.99	6.690
	90	17.30	7.238
Isopropanol	50	14.22	5.950
	60	16.30	6.820
	70	18.19	7.611
	80	19.92	8.335
	90	21.52	9.004

Sample calculation: (*All of the calculations below are for 60 g of ethanol)*

To calculate the change in enthalpy for each mass of alcohol, this formula was used:

$$\Delta H = mc\Delta T$$

Where m is the mass of water, c is the specific heat capacity of water, and ΔT is the temperature change of water $\left(T_{final} - T_{initial}\right)$.

Temperature change of water = Final temperature of water (°C) − Initial temperature of water (°C)

Initial temperature = 20°C

Final temperature = 33.04°C

Temperature change = 33.04°C − 20°C ⇒ 13.04°C

The specific heat capacity of water (c), used in this simulation, is 4.184 J/g°C and a mass of 100 g of water was taken for each trial. The calculation is as follows:

ΔH = 100 g × 4.184 J/g°C × 13.04°C

ΔH = 5455.936 J

Convert to kilojoules = $\frac{5455.936}{1000} \Rightarrow$ 5.456 kJ

To calculate the standard deviation of temperature change and enthalpy change:

The formula for standard deviation is:

$$\sqrt{\frac{(X-\mu)^2}{n-1}}$$

where μ is the mean, X is the different values from each trial and n is the number of values.

Because this was a simulation, only 1 trial had been conducted for each alcohol. If 5 trials had been taken, the same temperature change would have been observed for all the trials. Hence, this indicates that there is no variation in the data set, therefore, the standard deviation for this data set is zero.

To calculate the percentage error in the enthalpy change values, the following formula can be used:

$$\frac{theoretical\ value - experimental\ value}{theoretical\ value} \times 100$$

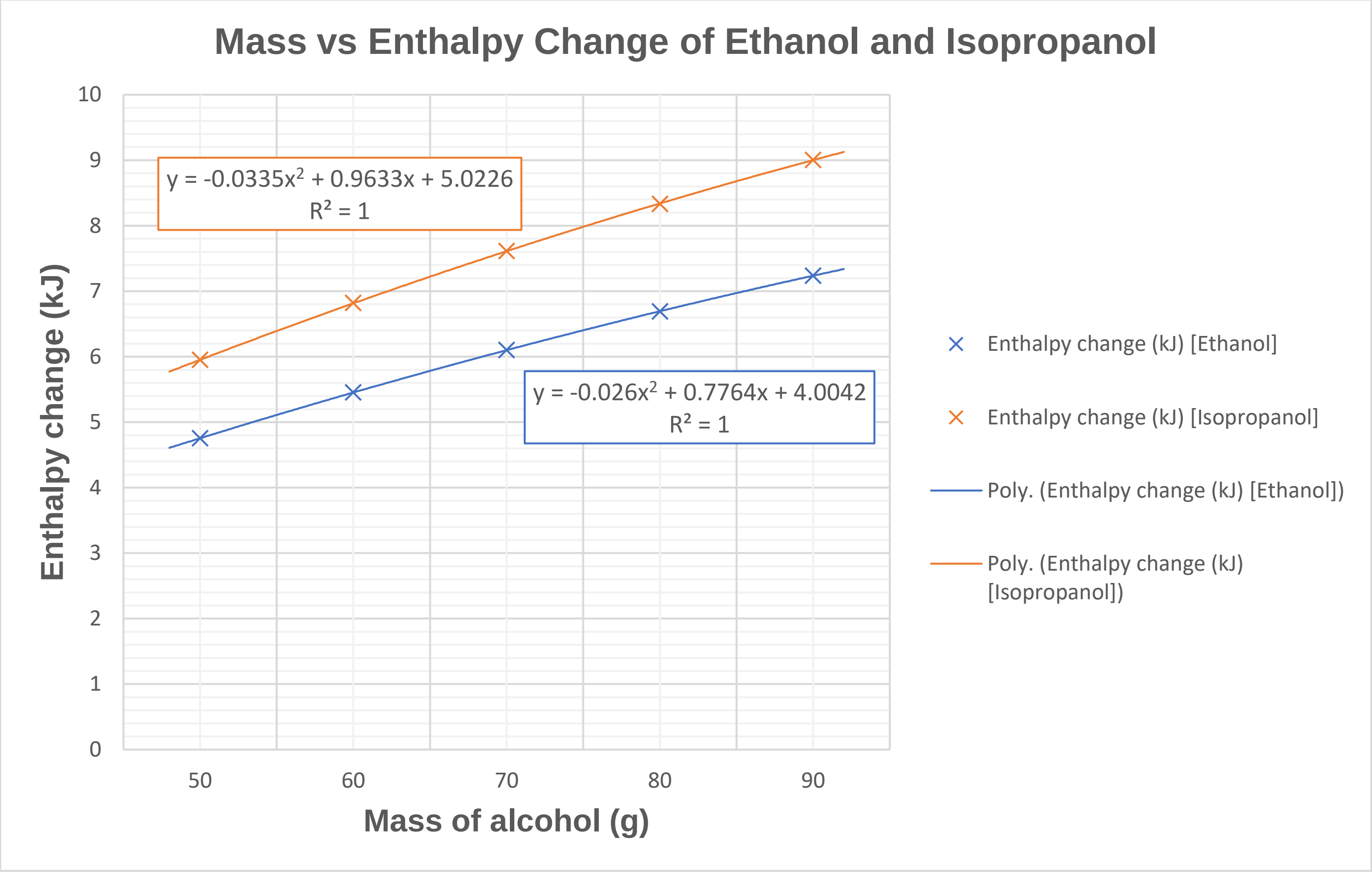
To calculate the percentage uncertainty in the enthalpy change values, the following formula can be used:

$$\frac{Absolute\ uncertainty}{Measured\ value} \times 100$$

The percentage uncertainties of the change in temperature of water and mass of alcohol can be added to get the overall percentage uncertainty of the enthalpy change values.

Again, since this was a simulation, there was little to no uncertainty in the readings and apparatus, therefore, there is no scope for uncertainty calculations for this experiment.

GRAPH: Mass vs. Enthalpy change of Ethanol and Isopropanol



Interpretation of graph and statistical analysis:

When analyzing the processed quantitative data, we can see an indistinct, non-linear relationship between the mass of the alcohol and the change in enthalpy for each mass of alcohol. This trend is evident as the values for enthalpy change increase as the mass of alcohol increases, however, the rate of change decreases with an increase in enthalpy change. The highest enthalpy change value recorded is 9.004 kJ for isopropanol and the lowest value is 4.753 kJ for ethanol.

Firstly, the polynomial (quadratic) trendline created for both series is extremely accurate as it suggested a perfect R^2 value: $R^2 = 1$ for Isopropanol Series and $R^2 = 1$ for Ethanol Series, which proposes that the given equation for each series is the best model and perfects suits the data. The R^2 values were calculated using MS Excel.

Secondly, we can see from the graph that the rate of change for the isopropanol series is higher than the rate of change for the ethanol series (the graph for the isopropanol series is steeper than the graph for the ethanol series). This could suggest that every molecule of isopropanol has a higher enthalpy change as compared to that of an ethanol molecule. This could be due to a higher number of carbon and hydrogen atoms in isopropanol than ethanol and/or the fact that isopropanol is branched while ethanol is unbranched.

Impact of uncertainties:

As mentioned above, there are little to no uncertainties in the experiment since this was a simulation. Therefore, uncertainties were of no significance in this experiment. There are 2 types of errors: random and systematic. In theory, a calorimeter reduces heat loss, but not all of it, i.e., there will always be some heat loss. However, this simulation uses an ideal constant-pressure calorimeter, i.e., there is no heat loss to the surroundings. Therefore, there is no scope for random errors as there are no statistical fluctuations in the measured data because a simulation can easily maintain ideal conditions, hence, there were no unknown or unpredictable changes observed in the experiment. Additionally, there is no scope for systematic errors as an imperfect instrument calibration is highly unlikely in a simulation as well as other environmental influences on the readings because, as mentioned above, simulations can easily maintain ideal conditions such as perfect insulation and perfect vacuum environments.

Conclusion:

Through this experiment, it is evident that the highest value of temperature change recorded was for 90 g of isopropanol (21.52°C) and the lowest value of temperature change recorded was for 50 g of ethanol (11.36°C). Therefore, 90 g of isopropanol had the greatest enthalpy change value (9.004 kJ) and 50 g of ethanol had the lowest enthalpy change value (4.753 kJ). Additionally, isopropanol had consistently higher enthalpy change values than ethanol.

My hypothesis that increasing the mass of ethanol and isopropanol will lead to an increase in the calculated enthalpy change was partially validated through this experiment. I can conclude that there is a non-linear relationship between the mass of alcohol and its calculated change in enthalpy, however, the rate of change of both graphs is decreasing (hence they are decreasing functions). For complete validation of my hypothesis, perhaps more data might have provided a more definite and clearer trend between the two variables.

Evaluation:

Strengths and weaknesses:

Weaknesses	Improvements
The biggest weakness was the fact that this was a simulation experiment. So, the data may or may not be accurate and reliable since only 1 trial was taken.	This could be well performed in real life, with proper uncertainties and errors as there would be more trials for each mass of alcohol, hence, the data would be more accurate.
The simulation only had 2 alcohols to experiment with, therefore, it led to the production of incomplete data.	A larger variety of alcohol samples can be taken and experimented with, so that trends could be clearer.
Another weakness was that there was a small range of the independent variable (mass of alcohol). (50 g, 60 g, 70 g, 80 g, and 90 g)	A wide range of values could be taken so that a more holistic and complete set of data can be obtained. (Possibly starting from 10 g to 100 g)

Strengths	
Random errors were reduced or not there at all since it was a simulation and systematic errors were negated as well (due to ideal conditions).	It allowed us to explore how the calorimeter works in ideal conditions, i.e., perfect insulation (no heat loss), therefore, the results achieved tend to be more precise.

Extensions:

- One possible extension to this experiment could be to investigate the effect of different independent variables on the same dependent variable. For example, one could investigate how concentration, carbon-chain length, or functional group, could affect the enthalpy change of the substance.
- One could also investigate the impact of a change in mass of compounds in other homologous series such as alkanes.
- Another possible extension would be to take a larger sample of alcohols and calculate the enthalpy of combustion for one mole of each alcohol. These values could then be used to compare which fuels or substances release the most energy when they are burned. In this case, a bomb calorimeter could be used to measure the heat of combustion.

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