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Final Project

The concept of the Carbon Footprint has become a significant consideration in our lives. A large majority of this issue resides in carbon dioxide, an unfortunate byproduct of energy generation. Here, we will use a gallon of gasoline to determine which energy sources create the most considerable amount of carbon dioxide and provide respective ranks. In each case, the fuel is being burnt via combustion, which is merely burning in the presence of oxygen. Various combustion sources contain gasoline, ethanol, butane, propane, and methane. Each of these contains approximately 120 million Joules of energy and operate at a 30% efficiency. There are also forms of non-combustion sources that we will be looking at. These are hydrogen and electricity. They have 60% efficiency and 77% efficiency, respectively. For the sake of calculations, we can assume that the source of electricity generation is the burning of bituminous coal and that this has a 34% efficiency.

Knowing all of these calculations, we can begin to theorize what the process of calculations should be. First, we must find the proper chemical reactions for each fuel source. Next, we must balance the equation to find the proper molarity of the products and reactants. Afterward, we use a series of conversions to convert joules into moles of CO_2 . From there, we rank the sources from the least moles of CO_2 to the greatest moles of CO_2 .

Combustion Sources:

Gasoline:
$$2 C_8 H_{18} (l) + 25 O_2 (g) \rightarrow 18 H_2 O (l) + 16 CO_2 (g)$$

$$\Delta H^{o}_{rxn} = H^{o}_{products} - H^{o}_{reactants}$$

$$\text{H}^{\text{o}}_{\text{products}} = [18 \text{ moles of H}_{2}\text{O} (-285.5 \frac{kJ}{mol \, H_{2}O})] + [16 \text{ moles of CO}_{2} (-393.8 \frac{kJ}{mol \, CO_{2}})]$$

$$H_{products}^{o} = -11439.8 \text{ kJ}$$

$$H_{\text{reactants}}^{\text{o}} = [2 \text{ moles of } C_8 H_{18} (-249.73 \frac{kJ}{mol C_8 H_{18}})] + [25 \text{ moles of } O_2 (0 \frac{kJ}{mol O_2})]$$

$$H_{\text{reactants}}^{\text{o}} = -449.46 \text{ kJ}$$

$$\Delta H_{rxn}^{o} = -11439.8 \text{ kJ} - (-449.46 \text{ kJ}) = -10940.34 \text{ kJ of combustion energy}$$

$$1.2 \times 10^8 J * \frac{100 \, J \, of \, combustion \, energy}{30 \, J \, of \, kinetic \, energy} * \frac{1 \, kJ}{1000 \, J} * \frac{2 \, moles \, C_8 H_{18}}{10940.34 \, kJ} * \frac{16 \, moles \, of \, CO_2}{2 \, moles \, of \, C_8 H_{18}} = 584.99 \, moles \, of \, CO_2$$

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

$$\Delta H^{o}_{rxn} = H^{o}_{products} - H^{o}_{reactants}$$

$$\text{H}^{\text{o}}_{\text{products}} = [3 \text{ moles of H}_{2}\text{O} (-285.5 \frac{kJ}{mol H_{2}O})] + [2 \text{ moles of CO}_{2} (-393.8 \frac{kJ}{mol CO_{2}})]$$

$$H_{products}^{o} = -1644.1 \text{ kJ}$$

$$H_{\text{reactants}}^{\text{o}} = [1 \text{ mole of } C_2H_5OH (-277.6 \frac{kJ}{mol C_2H_5OH})] + [3 \text{ moles of } O_2(0 \frac{kJ}{mol O_2})]$$

$$H_{\text{reactants}}^{\text{o}} = -277.6 \text{ kJ}$$

$$\Delta H^{o}_{rxn} = -1644.1 \text{ kJ} - (-277.6 \text{ kJ}) = -1366.5 \text{ kJ of combustion energy}$$

$$1.2 \times 10^8 J * \frac{100 \text{ J of combustion energy}}{30 \text{ J of kinetic energy}} * \frac{1 \text{ kJ}}{1000 \text{ J}} * \frac{1 \text{ mole } C_2 H_5 OH}{1366.5 \text{ kJ}} * \frac{2 \text{ moles of } CO_2}{1 \text{ mole of } C_2 H_5 OH} = 585.44 \text{ moles of } CO_2$$

Butane:
$$2 C_4 H_{10}(g) + 13 O_2(g) \rightarrow 10 H_2 O(l) + 8 CO_2(g)$$

$$\Delta H^{o}_{rxn} = H^{o}_{products} - H^{o}_{reactants}$$

$$H_{products}^{o} = [10 \text{ moles of } H_2O (-285.5 \frac{kJ}{mol H_2O})] + [8 \text{ moles of } CO_2(-393.8 \frac{kJ}{mol CO_2})]$$

$$H_{products}^{o} = -6005.4 \text{ kJ}$$

$$H_{\text{reactants}}^{\text{o}} = [2 \text{ moles of } C_4 H_{10} (-124.7 \frac{kJ}{mol C_4 H_{10}})] + [13 \text{ moles of } O_2 (0 \frac{kJ}{mol O_2})]$$

$$H_{\text{reactants}}^{\text{o}} = -249.4 \text{ kJ}$$

$$\Delta H^{o}_{rxn} = -6005.4 \text{ kJ} - (-249.4 \text{ kJ}) = -5756 \text{ kJ}$$
 of combustion energy

$$1.2 \times 10^8 J * \frac{100 \text{ J of combustion energy}}{30 \text{ J of kinetic energy}} * \frac{1 \text{ kJ}}{1000 J} * \frac{2 \text{ moles } C_4 H_{10}}{5756 \text{ kJ}} * \frac{8 \text{ moles of } CO_2}{2 \text{ moles of } C_4 H_{10}} = 555.94 \text{ moles of } CO_2$$

Propane:
$$C_4H_8(g) + 5 O_2(g) \rightarrow 4 H_2O(l) + 3 CO_2(g)$$

$$\Delta H^{o}_{rxn} = H^{o}_{products} - H^{o}_{reactants}$$

$$\text{H}^{\text{o}}_{\text{products}} = [4 \text{ moles of H}_{2}\text{O} (-285.5 \frac{kJ}{mol H_{2}O})] + [3 \text{ moles of CO}_{2} (-393.8 \frac{kJ}{mol CO_{2}})]$$

$$H_{products}^{o} = -2323.4 \text{ kJ}$$

$$H_{\text{reactants}}^{\text{o}} = [1 \text{ mole of } C_4 H_8 (-103.8 \frac{kJ}{mol C_4 H_8})] + [3 \text{ moles of } O_2 (0 \frac{kJ}{mol O_2})]$$

$$H_{\text{reactants}}^{\text{o}} = -103.8 \text{ kJ}$$

$$\Delta H_{rxn}^{o} = -2323.4 \text{ kJ} - (-103.8 \text{ kJ}) = -2219.6 \text{ kJ of combustion energy}$$

$$1.2 \times 10^8 J * \frac{100 \, J \, of \, combustion \, energy}{30 \, J \, of \, kinetic \, energy} * \frac{1 \, kJ}{1000 \, J} * \frac{1 \, mole \, C_4 H_{10}}{2219.6 \, kJ} * \frac{3 \, moles \, of \, CO_2}{1 \, mole \, of \, C_4 H_8} = 540.64 \, moles \, of \, CO_2$$

Methane:
$$CH_4(g) + 2 O_2(g) \rightarrow 2 H_2O(1) + CO_2(g)$$

$$\Delta H^{o}_{rxn} = H^{o}_{products} - H^{o}_{reactants}$$

$$\text{H}^{\text{o}}_{\text{products}} = [2 \text{ moles of H}_{2}\text{O} (-285.5 \frac{kJ}{mol H_{2}O})] + [1 \text{ mole of CO}_{2} (-393.8 \frac{kJ}{mol CO_{2}})]$$

$$H_{products}^{o} = -964.8 \text{ kJ}$$

$$H_{\text{reactants}}^{\text{o}} = [1 \text{ mole of } CH_4 (-74.8 \frac{kJ}{mol \ CH_4})] + [2 \text{ moles of } O_2 (0 \frac{kJ}{mol \ O_2})]$$

$$H_{\text{reactants}}^{\text{o}} = -74.8 \text{ kJ}$$

$$\Delta H^{o}_{rxn} = -964.8 \text{ kJ} - (-74.8 \text{ kJ}) = -890 \text{ kJ of combustion energy}$$

$$1.2 \times 10^{8} J * \frac{100 J \text{ of combustion energy}}{30 J \text{ of kinetic energy}} * \frac{1 kJ}{1000 J} * \frac{1 \text{ mole } C_{4}H_{10}}{890 \text{ kJ}} * \frac{1 \text{ mole of } CO_{2}}{1 \text{ mole of } CH_{8}} = 449.44 \text{ moles of } CO_{2}$$

Non-combustion Sources:

Coal:
$$C_{137}H_{97}O_9NS$$
 (s) + 633/4 O_2 (g) \rightarrow 137 CO_2 (g)+ 97/2 H_2O (l) + SO_2 (g)+ NO (g) -28.3 kJ/g * 1933.41 g/1 mol of coal = -54713.55 kJ/mol.

Electricity:

$$1.2 \times 10^{8} J * \frac{100 J \text{ of combustion energy}}{34 J \text{ of kinetic energy}} * \frac{1 \text{ kJ}}{1000 J} * \frac{1 \text{ mole coal}}{54713.55 \text{ kJ}} * \frac{137 \text{ mole of } CO_2}{1 \text{ mole of coal}} = 883.75 \text{ moles of } CO_2$$

$$883.75 \text{ moles of } CO_2 * \frac{100 J \text{ of electrical energy}}{77 J \text{ of kinetic energy}} = 1147.73 \text{ moles of } CO_2$$

With a 77% efficiency, 883.75 moles of CO₂ becomes 1147.73 moles of CO₂.

Hydrogen:

883.75 moles of
$$CO_2$$
* $\frac{100 \, J \, of \, electrical \, energy}{75 \, J \, of \, kinetic \, energy} = 1178.33 \, moles \, of \, CO_2$

With a 75% efficiency on the electrolysis reaction, 883.75 moles of CO2 becomes 1178.33 moles of CO₂.

1178.33 moles of
$$CO_2$$
* $\frac{100 \text{ J of electrical energy}}{60 \text{ J of kinetic energy}} = 1963.88 \text{ moles of } CO_2$

With a 60% efficiency on the Hydrogen Fuel Cell cars, 1178.33 moles of CO_2 becomes 1963.88 moles of CO_2 .

Conclusion

To start each combustion-sourced reaction, the equation must be balanced to [x] [Source] $+ [x] O_2 -> [x] H_2 O + [x] CO_2$. Once this equation is balanced, we must then determine the heat of the reaction. This is done by referencing a heat of formations table. We then use the delta heat of the reaction to determine our energy of combustion. Next we apply a conversion from Joules to moles of CO_2 . This conversion is as follows:

$$1.2 \times 10^8 \ J * \frac{100 \ J \ of \ combustion \ energy}{30 \ J \ of \ kinetic \ energy} * \frac{1 \ kJ}{1000 \ J} * \frac{[x] \ moles \ [source]}{[combustion \ energy] \ kJ} * \frac{[x] \ moles \ of \ CO_2}{[x] \ moles \ of \ [source]} = moles \ of \ CO_2$$

We are given 120 Million joules in a machine that has a 30% efficiency and turned into kilojoules. Next we use the amount of moles of the source from the balanced equation and the determined combustion energy from the heat of the reaction. Lastly we must turn the moles of source to moles of CO₂. Using this method, it was determined that Methane had the lowest amount of moles of CO2 at 449.44 moles. Next, in order, came Propane at 540.64 moles, Butane at 555.94 moles, Gasoline at 584.99 moles, and lastly Ethanol at 585.44 moles had the greatest amount produced CO₂ moles.

Now we can move onto the non-combustion sources. Like the previous sources, we know we are supposed to keep 120 million Joules as a constant to maintain accuracy. However we are told that a form of coal must be burnt in order to generate electricity for the car and the electrolysis procedure for Hydrogen Cells. Next we have to find out the moles of CO₂ produced via electricity with the burning of coal. There is also a 34% efficiency rating on the burning of coal which must be factored in. From there, we must also consider that in order to turn the joules created via coal into joules created via electricity to power an electric car, which has a 77% efficiency rating of its own. Moving on to Hydrogen power, we know that the process of creating hydrogen power only has a 75% efficiency rating, so the moles of CO₂ increase again. Lastly, the Hydrogen Fuel Cell cars have a 60% efficiency rating, so the moles increase yet again.

Finalizing the ratings and calculations, we learn that electricity produces 1147.73 moles of CO₂ and that hydrogen produces 1963.88 moles of CO₂ per 120 million joules. This completes the ranking of least to greatest moles of CO₂ as Methane, Propane, Butane, Gasoline, Ethanol, Electricity, and Hydrogen. This list also remains the same when we decide to determine the order of size of carbon footprint of number of joules of kinetic energy.

Sources

Enthalpies for Ethanol, Butane, Propane, Methane, Oxygen, Carbon Dioxide, and Water:

Anne Marie Helmenstine, Ph.D. *Thermochemistry Heat of Formation Table for Common Compounds*. www.thoughtco.com/common-compound-heat-of-formation-table-609253.

Enthalpy for Gasoline (Octane):

ATcT Thermochemical Values Ver. 1.118.

www.atct.anl.gov/Thermochemical%20Data/version%201.118/.