Calculating Fuel Values and Other Interesting Information about Fuels

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Fuel Values

Fuel values are defined as the amount of energy generated by complete combustion of a particular mass of the fuel (usually one gram). It takes more energy to move larger amounts of mass; thus the higher the energy density (fuel value) the less energy is used transporting the fuel. This is particularly important for cars and trucks which have to carry their energy source.

This can be calculated from the energy change in the combustion reaction, which we can calculate from enthalpies of formation. The logic is that we find the change in enthalpy of the reaction as written by taking the enthalpies of formation of the products and subtracting the enthalpies of formation of the reactants. This gives us our standard delta value (final - initial or $\Delta H^o = \Delta H_f^o(\text{products}) - \Delta H_f^o(\text{reactants})$). This calculated enthalpy change is per the number of moles written in the equation. To convert to per gram we need to divide the enthalpy change by the number of moles and the molar mass.

Example 1: Calculation of the fuel value of ethane.

$$2CH_3CH_3(g) + 7O_2(g) \text{ ---> } 4CO_2(g) + 6H_2O(g) \quad (1)$$

$$\Delta H^o_{RXN} = 6\{\Delta H^o_f(H_2O(g))\} + 4\{\Delta H^o_f(CO_2(g))\} - 2\{\Delta H^o_f(CH_3CH_3(g)))\} - 7\{\Delta H^o_f(O_2(g)))\} \quad (2)$$

$$\Delta H^o_{RXN} = (6 \text{ mol } H_2O)(-241.8 \text{ kJ/mol } H_2O) + (4 \text{ mol } CO_2)(-393.5 \text{ kJ/mol } CO_2) \\ -(2 \text{ mol } C_2H_6)(-84.7 \text{ kJ/mol } C_2H_6) - 0 = -2855. \text{ kJ/2 mol ethane} \quad (3)$$

$$\Delta H^o_{RXN}(\text{per mol ethane}) = -2855. \text{ kJ/2 mol ethane} = -1428 \text{ kJ/mol ethane.} \quad (4)$$

$$MM(C_2H_6) = (2 \text{ mol C/mol } C_2H_6)\ (12.011 \text{ g/mol C}) + (6 \text{ mol H/mol } C_2H_6)(1.00794 \text{ g/mol H}) \\ = 30.007 \text{ g/mol } C_2H_6. \quad (5)$$

Fuel Value (usually reported as a positive number) = (1428 kJ/mol)/(30.007 g/mol) = 47.49 kJ/g. (6)

> Exercise 1: Calculation of the fuel value of ethanol.
> Molecular Formula: CH_3CH_2OH. $\Delta H^o_f(CH_3CH_2OH) = -277.6$ kJ/mol
> Answer: 26.8 kJ/g.

Volumetric Fuel Value

Volumetric fuel values are defined as the amount of energy generated by complete combustion of the fuel per unit volume (usually per mL or L). If a fuel has a high volumetric fuel value it requires less storage space for the same amount of energy. This is also important for cars and trucks which have to carry their energy source.

This can be calculated from the per mass fuel value as long as the density of the fuel is known. The conversion is from J/g —> J/mL. To do this conversion we need to multiply by a conversion constant with g on top and mL on the bottom (g/mL = density).

Example 2: Calculation of the volumetric fuel value of ethane gas assuming STAP (25 ˚C, 1 atm).

$$\text{Assume ideal} \Rightarrow V/n = RT/P = (0.8206 \text{ L}\cdot\text{atm}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})(298 \text{ K})/(1.00 \text{ atm}) = 24.5 \text{ L/mol.} \quad (7)$$

$$d = (30.007 \text{ g/mol})/(24.5 \text{ L/mol}) = 1.22 \text{ g/L.} \quad (8)$$

$$\text{Volumetric fuel value} = (47.49 \text{ kJ/g})(1.22 \text{ g/L}) = 58.2 \text{ kJ/L.} \quad (9)$$

Or not bothering to calculate the intermediate value of density we could have calculated it this way:

$$\text{Volumetric fuel value} = (47.49 \text{ kJ/g})(30.007 \text{ g/mol})/(24.5 \text{ L/mol}) = 58.2 \text{ kJ/L.} \quad (10)$$

Exercise 2: Calculation of the volumetric fuel value of H_2 assuming STAP (25 ˚C, 1 atm).
The fuel value of H_2 = 120. kJ/g. Answer = 9.87 kJ/L.

Example 3: Calculation of the volumetric fuel value of ethanol (liquid).
The density of ethanol = 0.7937 g/mL.

$$\text{Volumetric fuel value} = (26.8 \text{ kJ/g})(0.7937 \text{ g/mL}) = 21.3 \text{ kJ/mL or } 21.3 \times 10^3 \text{ J/L.} \quad (11)$$

Exercise 3: Calculation of the volumetric fuel value of octane.
The density of octane = 0.703 g/mL Answer = 28.8 kJ/mL

CO_2 Intensity

This is just the amount of CO_2 per unit of energy (usually mol CO_2/J). Since CO_2 is a global warming gas the goal is to release as little as possible; thus the lower the CO_2 intensity the better a fuel is for global warming. This quantity is not always specified as consistently. Some like to talk about the inverse quantity, amount of energy per unit of CO_2 produced (J/mol or g CO_2). When this is done the higher numbers mean less CO_2 intensity.

Example 4: Calculation of CO_2 intensity for ethane.

$$2CH_3CH_3(g) + 7O_2(g) \text{ ---> } 4CO_2(g) + 6H_2O(g) \quad (12)$$

The balanced equation (12) shows that we get 4 mol CO_2/2 mol C_2H_6 burned or 2 mol CO_2/mol C_2H_6. Along with the previously calculated kJ/mol C_2H_6 (see equation 4) we can use this to calculate mol CO_2/kJ.

$$(2 \text{ mol } CO_2/\text{mol } C_2H_6)(\text{mol } C_2H_6/1428 \text{ kJ}) = 1.400 \times 10^{-3} \text{ mol } CO_2/\text{kJ.} \quad (13)$$

Exercise 4: Calculation of CO_2 intensity for methane. Answer = 1.25×10^{-3} mol CO_2/kJ

Exercise 5: Calculation of CO_2 intensity for hydrogen. Answer = 0 mol CO_2/J.

The last exercise is why H_2 is considered the ideal fuel for many uses. It does not produce any by products other than water and produces no CO_2,, making its contribution to global warming negligible. However, if you go back to the calculation of volumetric energy density you will see a problem.

Methane is itself a greenhouse gas that is 30 X more effective at trapping energy in the atmosphere than CO_2. Since you only get 1 mole of CO_2 for each mole of CH_4 burned burning methane causes 30 X less global warming than releasing the methane into the atmosphere.