

Calculating Fuel Values and Other Interesting Information about Fuels

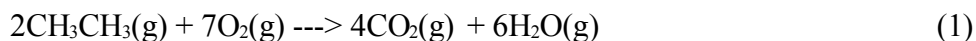
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Fuel Values

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 $\Delta H^\circ = \Delta H_f^\circ(\text{products}) - \Delta H_f^\circ(\text{reactants})$). 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.



$$\Delta H^\circ_{\text{RXN}} = 6\{\Delta H_f^\circ(\text{H}_2\text{O}(\text{g}))\} + 4\{\Delta H_f^\circ(\text{CO}_2(\text{g}))\} - 2\{\Delta H_f^\circ(\text{CH}_3\text{CH}_3(\text{g}))\} - 7\{\Delta H_f^\circ(\text{O}_2(\text{g}))\} \quad (2)$$

$$\Delta H^\circ_{\text{RXN}} = (6 \text{ mol H}_2\text{O})(-241.8 \text{ kJ/mol H}_2\text{O}) + (4 \text{ mol CO}_2)(-393.5 \text{ kJ/mol CO}_2) \\ - (2 \text{ mol C}_2\text{H}_6)(-84.7 \text{ kJ/mol C}_2\text{H}_6) - 0 = -2855. \text{ kJ/2 mol ethane} \quad (3)$$

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

$$\text{MM}(\text{C}_2\text{H}_6) = (2 \text{ mol C/mol C}_2\text{H}_6)(12.011 \text{ g/mol C}) + (6 \text{ mol H/mol C}_2\text{H}_6)(1.00794 \text{ g/mol H}) \\ = 30.007 \text{ g/mol C}_2\text{H}_6. \quad (5)$$

$$\text{Fuel Value (usually reported as a positive number)} = (1428 \text{ kJ/mol})/(30.007 \text{ g/mol}) = 47.49 \text{ kJ/g.} \quad (6)$$

Exercise 1: Calculation of the fuel value of ethanol.

Molecular Formula: $\text{CH}_3\text{CH}_2\text{OH}$.

$$\Delta H_f^\circ(\text{CH}_3\text{CH}_2\text{OH}) = -277.6 \text{ kJ/mol}$$

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 \rightarrow 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).

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

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

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

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 H₂ assuming STAP (25 °C, 1 atm).
The fuel value of H₂ = 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.

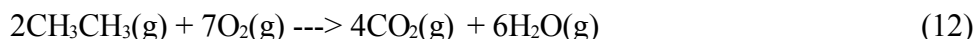
$$\text{Volumetric fuel value} = (26.8 \text{ kJ/g})(0.7937 \text{ g/mL}) = 21.3 \text{ kJ/mL or } 21.3 \times 10^3 \text{ J/L.} \quad (11)$$

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

CO₂ Intensity

This is just the amount of CO₂ per unit of energy (usually mol CO₂/J). Since CO₂ is a global warming gas the goal is to release as little as possible; thus the lower the CO₂ 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 CO₂ produced (J/mol or g CO₂). When this is done the higher numbers mean less CO₂ intensity.

Example 4: Calculation of CO₂ intensity for ethane.



The balanced equation (12) shows that we get 4 mol CO₂/2 mol C₂H₆ burned or 2 mol CO₂/mol C₂H₆. Along with the previously calculated kJ/mol C₂H₆ (see equation 4) we can use this to calculate mol CO₂/kJ.

$$(2 \text{ mol CO}_2/\text{mol C}_2\text{H}_6)(\text{mol C}_2\text{H}_6/1428 \text{ kJ}) = 1.400 \times 10^{-3} \text{ mol CO}_2/\text{kJ.} \quad (13)$$

Exercise 4: Calculation of CO₂ intensity for methane. Answer = 1.25 x 10⁻³ mol CO₂/kJ

Exercise 5: Calculation of CO₂ intensity for hydrogen. Answer = 0 mol CO₂/J.

The last exercise is why H₂ is considered the ideal fuel for many uses. It does not produce any by products other than water and produces no CO₂, 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 CO₂. Since you only get 1 mole of CO₂ for each mole of CH₄ burned burning methane causes 30 X less global warming than releasing the methane into the atmosphere.