SPECIFIC ENERGY OF FUELS

Specific energy is the amount of energy stored in a given system or region of space per unit mass. Often only the extractable energy is measured; and thus chemically inaccessible energy, such as rest mass energy, is ignored.

Herein, we estimate specific energy of fuels by analyzing the energy release when burning. In all of the following, we assume complete fuel combustion in oxygen.

GUESSTIMATIONS

Fuels are fat

Food fat burns, so it is a fuel. When it burns, fat releases *ca.* 40 kJ/kg, [6]. So, roughly estimate the specific energy of *all* fuels as 50 kJ/kg.

Average value

Find a *typical* specific energy value by averaging the lowest and the highest values of the burning energy spectrum. Choose, for instance, wood ($\sim$ 20 kJ/kg) and hydrogen ($\sim$ 150 kJ/kg) as estimators, see fig. 1:

$$e = \sqrt{20\,\mathrm{kJ/kg} \times 150\,\mathrm{kJ/kg}} \sim 54.77\,\mathrm{kJ/kg}\,.$$

So, estimate fuel specific energy as 50 kJ/kg (consistent with the fuels-are-fat guesstimate).

GASOLINE SPECIFIC ENERGY

In this section, we estimate the gasoline specific energy value using the 1.5 eV/reaction *rule*, [4].

Unless we are capable of photosynthesis, we get most of our energy from chemical reactions: from eating food and from burning hydrocarbon fuels. In a typical chemical reaction, one electron is exchanged between two atoms. The energy of this exchange is about 1.5 eV . If you want more precision than that, ask a chemist or look it up. To convert this to a useful number, we need to know two things:

1. The conversion from electron volts to joules: $1\,\mathrm{eV} \sim 2 \cdot 10^{-19}\,\mathrm{J}$.
2. The number of molecules involved in the reaction.

To determine the second, we need to introduce a little chemistry. We will be concerned primarily with hydrocarbons and therefore will limit ourselves to the reactions $C + O_2 \longrightarrow CO_2$ (carbon plus oxygen reacts to form carbon dioxide) and $2H_2 + O_2 \longrightarrow 2H_2O$ (hydrogen plus oxygen reacts to form water). All the oxygen for these reactions comes from the atmosphere.

We know this because batteries convert chemical energy to electrical energy. Common batteries provide an electrical potential of 1.5 V. Therefore, each single electron flowing through the battery gains an energy of 1.5 eV and each coulomb of electricity (a coulomb is a LOT of electrons, $1\,\mathrm{C} = 6 \cdot 10^{18}$ e) flowing through the battery gains an energy of 1.5 coulomb volts (or 1.5 J).

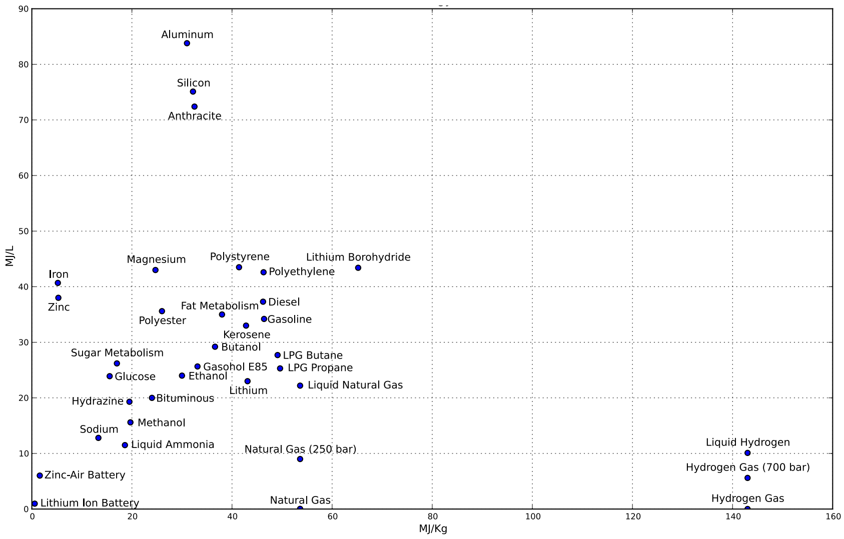

Figure 1 Specific energy and energy density of common fuels, [5]

In this book, there are only three hydrocarbons: coal (pure carbon), natural gas (methane or CH_4), and everything in between (including gasoline), which we will call CH_2. One mole of carbon has a mass of 12 g (the atomic weight of carbon) and contains $k_{\mathrm{av}} = 6 \cdot 10^{23}$ atoms. Burning that will result in k_{av} chemical reactions. One mole of methane has a mass of 16 g (the atomic weight of the carbon plus four hydrogens) and contains $k_{\mathrm{av}} = 6 \cdot 10^{23}$ molecules. Burning that will result in $3k_{\mathrm{av}}$ reactions (one CO_2 and two H_2O).

How much chemical energy (in joules) can be released by burning 1 kg (about 1 L) of gasoline? What is its energy density (in J/kg)?

Since we know that the energy we get for each chemical reaction is 1.5 eV, we need to estimate the number of chemical reactions that occur when we burn 1 kg of gasoline. To do this we need to estimate the chemical composition.

We will assume that the hydrogen to carbon ratio in gasoline is two (since it is more than zero [pure carbon] and less than four [pure methane]). Thus, we will assume that gasoline is made of CH_2 molecules. The atomic masses of carbon and hydrogen are 12 and 1, respectively, so that the molecular mass of CH_2 is 14. This means that one mole of CH_2 has a mass of 14 g or $1.4 \cdot 10^{-2}$ kg. Thus, 1 kg of gasoline contains

$$n = \frac{1\,\mathrm{kg}}{1.4 \cdot 10^{-2}\,\mathrm{kg/mole}} = 70\,\mathrm{mol}\,.$$

Each of these CH_2 « molecules » will give us two reactions: the carbon atom will oxidize and form CO_2 and the two hydrogen atoms will oxidize and form H_2O. Thus, each CH_2 molecule will provide 3 eV. The total energy released by burning (oxidizing) 1 kg of gasoline will be

$$70\,\mathrm{mol/kg} \cdot 6 \cdot 10^{23}\,\mathrm{reaction/mol} \cdot 3\,\mathrm{eV/reaction} \frac{1\,\mathrm{J}}{6 \cdot 10^{18}\,\mathrm{eV}} = 2 \cdot 10^{7}\,\mathrm{J/kg}\,.$$

Then, we estimate that 1 kg of gasoline will release $2 \cdot 10^{7}$ J.

Looking this up on the web, we find that gasoline has an energy density [*sic*] (specific energy) of about $4.5 \cdot 10^7$ J/kg so we are only off by a factor of two. Not bad, considering the approximations we made.

Note also that gasoline has a density of about $3/4$ that of water. This is definitely close enough to one for this book. However, if you need to be precise, you should use am energy density of $3 \cdot 10^7$ J/L.

Note that 1 kg of TNT contains only $4 \cdot 10^6$ J, which is only 10% of gasoline. However, the TNT can release that energy MUCH more rapidly.

[Correction: the balanced chemical equation for CH_2 burning is $2\,CH_2 + 3\,O_2 \longrightarrow 2\,CO_2 + 2\,H_2O$. With this, the number of molecules that are exchanged is 6 (2 carbons and 4 hydrogens, $2\,CH_2$). Then, the energy released is $1.5\,\text{eV} \cdot 6 \sim 9\,\text{eV}$ and, finally, the total energy becomes 60 MJ/kg.]

METHANE SPECIFIC ENERGY

In this section, we estimate methane specific energy values by several methods: eV per reaction rule, binding energy and Born-Habern cycle for methane combustion in oxygen.

eV per reaction rule

When methane burns in oxygen, $CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O$, one carbon and four hydrogens react, releasing $5 \cdot 1.5\,\text{eV} \sim 10\,\text{eV/reaction}$.

The molecular mass of methane is $16\,\text{g/mol} \sim 20 \cdot 10^{-3}\,\text{kg/mol}$. So, one kilogram of methane has $1\,\text{kg}/20 \cdot 10^{-3}\,\text{kg/mol} \sim 50\,\text{mol}$.

The specific energy of combustion of methane in oxygen is then

$$50\,\text{mol/kg} \cdot 6 \cdot 10^{23}\,\text{reaction/mol} \cdot 10\,\text{eV/reaction} \frac{1\,\text{J}}{6 \cdot 10^{18}\,\text{eV}} = 5 \cdot 10^7\,\text{J/kg}\,.$$

Thus, we estimate that burning methane in oxygen will release 50 MJ/kg.

On the web, [1], we find that the specific energy of methane ranges from 50 MJ/kg to 55 MJ/kg.

Binding energy

[Taken from [3]]

Combustion produce energy by burning stable (usually) molecule to more stable end products. (Note: O_2 binding energy is zero.)

In combustion: reaction conserves number of each atom species; compute energy per standand number of molecules (mol) and not weight.

On weight basis, methane produces the most energy.

Conserve number of atoms of each element

Consider methane CH_4 burning in oxygen O_2: $CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$.

Balancing the equation: number of each atom species is conserved in reaction.

Note: every molecule in reaction is stable. And yet we get energy. How?

First we need to define binding energy of a molecule.

Binding energy of a molecule

Molecular *binding energy* is difference between energy of molecule and its elements in their most stable state.

Chemists call this *enthalpy of formation*; the complete definition prescribes the measurement. Measurements are hard; in 30 years numbers have changed 1/2 percent.

Set binding energy zero for most stable oxygen state O_2. Binding energies of other stable molecules are negative. (really?)

Units: kJ/mol. What is a mol? Standard number of molecules ($\sim 6 \cdot 10^{23}$). Unit eases balancing chemical equations; imagine using kJ/kg. ($\sim$ 20 mol in Dasani [335 mL].)

Sample combustion calculation

Combustion Energy from Methane (0.016 kg/mol):

$$\mathrm{CH_4} + 2\mathrm{O_2} \longrightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + \text{heat}\,.$$

Looking at thermochemical data for the species (binding energies in kg/mol), we find that heat $= 394 + 2(242) - 75 = 803$ kJ/mol, which yields our estimate for the combustion energy of methane as 50 MJ/kg.

Born-Haber cycle

[Taken from [2]]

The combustion of all fossil fuels follows a very similar reaction:

Fossil Fuel (any hydrocarbon source) plus oxygen yields carbon dioxide and water and *energy*.

The world and modern society are driven by the need to produce energy to make products (manufacturing), to move around (transportation), to heat homes and buildings, and to create light (electricity). At least 75% of these needs are met by the combustion of fossil fuels. Energy is stored in chemical compounds in the bonds that bind atoms to each other.

$$\mathrm{CH_4(g)} + 2\mathrm{O_2(g)} \longrightarrow \mathrm{CO_2(g)} + 2\mathrm{H_2O(g)} + \text{energy}\,.$$

A chemical reaction occurs by the rearrangement of atoms and molecules in the reactant (starting) molecules and the end product molecules. Some bonds are broken while others are reformed. The process of breaking and forming bonds results in a net energy needed or given off for a reaction.

In fig. 2, the combustion reaction of methane and oxygen to form carbon dioxide and water is shown broken into steps to show the entire energy « using » and « forming » process. First it takes energy to break bonds, all four of the C—H bonds in methane must be broken. The energy units are kilojoules, a positive sign means that the process is *endothermic* or energy is required to break the bonds.

In a similar fashion, two diatomic oxygen molecules are broken apart which requires more energy. Now all of the individual atoms in the reactant molecules have been broken apart.

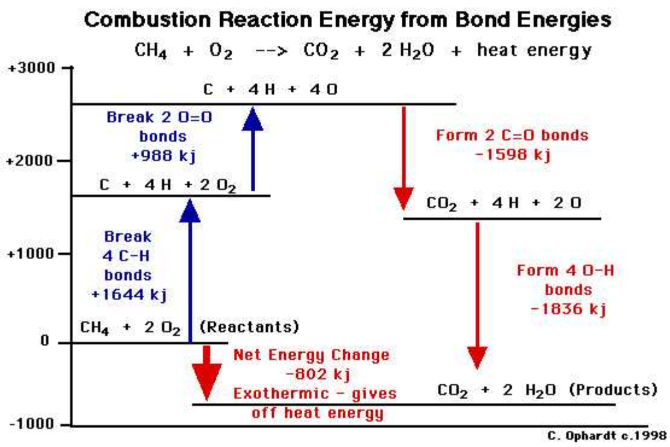

Figure 2 Born-Haber cycle for the combustion of methane in oxygen. [2]

On the right side of the diagram in a second step, the various atoms form new bonds in new molecules of carbon dioxide and water. The formation of new bonds is an exothermic process where heat is given off. Again the energy given off is totaled to form new bonds in carbon dioxide and water molecules.

Finally, the overall reaction yields an excess of energy given off −802 kJ. (the minus sign means that this is an *exothermic* process). In more familiar units this is equivalent to 191 kilocalories per 16 grams of methane. This is a little more than the 150 calories in a can of Coke.

The excess of energy given off is mainly in the form of heat. Chemical energy stored in the bonds of molecules is transformed into heat and light energy. Most chemical reactions are of this type and thus are exothermic. Less energy is required to break old bonds than is given off in the process of forming new bonds.

[1] Edited by Glenn Elert. Energy density of methane, July 2014. URL http://hypertextbook.com/facts/2004/BillyWan.shtml.

[2] Charles E. Ophardt. Energy of combustion, July 2014. URL http://www.elmhurst.edu/~chm/vchembook/512energycombust.html.

[3] Ohio State University. Getting energy from combustion, July 2014. URL http://www.physics.ohio-state.edu/~wilkins/energy/Resources/Lectures/combenergy-land.html.

[4] Lawrence Weinstein and John A. Adam. *Guesstimation*. Princeton University Press, 2008.

[5] the free encyclopedia Wikipedia. Specific energy, July 2014. URL http://upload.wikimedia.org/wikipedia/commons/c/c6/Energy_density.svg.

[6] the free encyclopedia Wikipedia. Specific energy, July 2014. URL http://en.wikipedia.org/wiki/Specific_energy#Energy_density_of_food.