

The upper limit of specific impulse for various
rocket fuels

Tom Myers

July 10, 2016

1 Abstract

A quick calculation to find the upper limit on specific impulse for various rocket fuels, based on the energy density of these fuels. We find that for Hydrogen/Liquid Oxygen, the upper limit is 532.5s, for Methane/Liquid Oxygen, the limit is 458.7s, and for Kerosene/Liquid Oxygen, the limit is 470.2s.

2 Hydrolox

To find the upper limit is a simple matter of equating the chemical energy stored in the fuel with the kinetic energy of the exhaust. Specifically:

$$E = \frac{1}{2}mv_e^2 \quad (1)$$

$$\sqrt{\frac{2E}{m}} = v_e \quad (2)$$

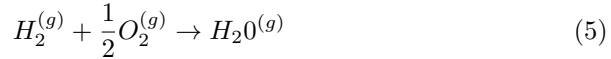
$$\frac{\sqrt{\frac{2E}{m}}}{g} = \frac{v_e}{g} = I_{sp} \quad (3)$$

Where E is the total chemical energy in a mass m of the fluid, v_e is the exhaust velocity, g is the acceleration due to gravity on the surface of planet Earth, and I_{sp} is the specific impulse.

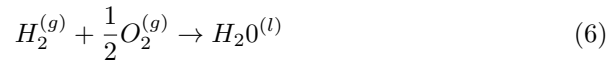
We work out $\frac{E}{m}$ (chemical energy density) as a single number - call this u :

$$I_{sp} = \frac{\sqrt{2u}}{g} \quad (4)$$

u is then the chemical energy in the following reaction:



In practice, combustion tables usually give the energy (called enthalpy change of combustion, ΔH) for



So to get the correct answer we must factor in the enthalpy change of



Which is called ΔH_{vap} Energy of this is called ΔH .

Thus, $u = \frac{(\Delta H - \Delta H_{vap})}{m_m}$, where m_m is the molar mass, and the complete equation is:

$$I_{sp} = \frac{\sqrt{\frac{2(\Delta H - \Delta H_{vap})}{m_m}}}{g} \quad (8)$$

Putting numbers in (all readily found on Wolfram Alpha, or elsewhere), for hydrogen and oxygen to water:

$$\begin{aligned}\Delta H &= 285.8 \text{ kJ/mol} \\ \Delta H_{vap} &= 40.2 \text{ kJ/mol} \\ m_m &= 18 \text{ g/mol} \\ g &= 9.81 \text{ m/s}^2\end{aligned}$$

We obtain:

$$I_{sp} = 532.5\text{s}$$

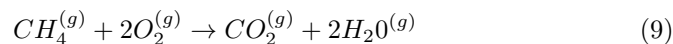
For reference, the Space Shuttle Main Engines (some of the most complex hydrolox engines ever built) had an I_{sp} of 452.3s (85.1% of the theoretical maximum). They ran the engine slightly fuel-rich (for every three hydrogen molecules burnt, one was left unburnt), which gives an effective molar mass of $18\frac{2}{3}$ g/mol. Factoring that in gives a theoretical I_{sp} of 522.9s for that engine (so the real value is now 86.6% of theoretical).

Where does the remaining energy go? Some is stored in the motion of the exhaust: in intramolecular vibrations and rotations, and kinetic energy in directions perpendicular to the rocket's travel. Some is also used to heat (and boil) the two cryogenic liquids from their stored temperature to their combustion one (a quick estimate factoring in only latent heat of vaporisation of oxygen brings the upper bound down to 520s).

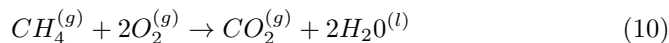
Some fuel is also tapped off to run the turbopumps, but (in the steady state) the work done by those turbopumps is ultimately converted back into heat, which warms the propellents and is thus not wasted by the engine. Some heat probably leaves the surface of the rocket, but in the vacuum of space, over the course of an 8 minute burn, this is likely to be quite small.

3 Methalox

Our previously derived formula for I_{sp} still applies, but we have to think carefully about the reaction to obtain the right values.



Again, combustion tables usually give values for



So we have to factor in vaporising 2 moles of water for every mole of methane we burn. As for the molar mass, this is simply $44 + 2 \times 18$, for one CO_2 and two H_2O . Thus (again, readily available on Wolfram Alpha):

$$\Delta H = 890.3 \text{ kJ/mol}$$

$$\begin{aligned}\Delta H_{vap} &= 2 \times 40.2 \text{ kJ/mol} \\ m_m &= 80 \text{ g/mol} \\ g &= 9.81 \text{ m/s}^2\end{aligned}$$

Hence, the upper limit for a stoichiometric methalox mixture ratio is:

$$I_{sp} = 458.7s$$

4 Kerolox

In the case of kerosene, the fuel is not a single molecule but rather a mixture of different hydrocarbons. This forces us to approach the calculation a little differently, to accommodate the combustion data being in kJ/kg rather than kJ/mol. Our reference shows the typical amount of carbon and hydrogen in kerosene, which allows us to work out the amount of liquid oxygen needed to combust the kerosene. According to our reference, kerosene is 86.5% carbon, 13.2% hydrogen by mass; for this analysis we neglect the trace elements making up the remaining 0.3%.

In one kilogram of kerosene, there is therefore:
865g of carbon:



Carbon weighs 12g/mol, and each mole of carbon needs one mole of O_2 (32g/mol), so we need

$$\frac{865}{12} \times 32 \approx 2300g \tag{12}$$

of oxygen to combust all the carbon in a kilogram of kerosene.
There is also 132g of hydrogen:



Hydrogen gas weighs 2g/mol, and each mole of hydrogen needs half a mole of O_2 (32g/mol), so we need

$$\frac{1}{2} \times \frac{132}{2} \times 32 \approx 1060g \quad (14)$$

of oxygen to combust all the hydrogen in a kilogram of kerosene

In total, therefore, each kilogram of kerosene needs 3.36 kilograms of oxygen to burn. The reference gives energy per unit mass of kerosene - we can thus convert this to energy density of kerolox by dividing by (1+3.36).

Equation (3):

$$\frac{\sqrt{\frac{2E}{m}}}{g} = \frac{v_e}{g} = I_{sp} \quad (15)$$

$$\frac{E}{m} = 46400/(1 + 3.36) \text{ kJ/kg (see reference for 46400 value)}$$

$$g = 9.81 \text{ m/s}^2$$

Hence the upper limit for Kerolox is:

$$I_{sp} = 470.2s$$

5 References

Most of the values here can be found through appropriate queries on Wolfram Alpha (wolframalpha.com).

Kerosene specific heat can be found on page 61, table 2.2 of Flagan, Richard C., and John H. Seinfeld: 'Fundamentals of air pollution engineering' (Courier Corporation, 2013). <http://authors.library.caltech.edu/25069/4/AirPollution88-Ch2.pdf>