

Running Engines for Maximum Power

Dr Owen Williams – University of Wales TSD:

The flame speed during combustion depends on the Air/Fuel ratio (AFR)



It is fastest when the mixture is slightly rich since this reduces the possibility of 'lean patches' in the cylinder which act to slow down the flame front.

Lean means Slow

When it is lean, there is too much O₂ and not enough fuel, so the flame temperature becomes low because the excess air takes up some of the heat energy from the previous burn (combustion cycle).

Lambda & the Fuel Equivalence Ratio

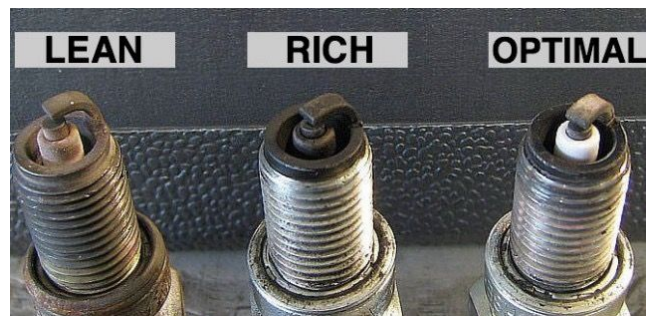
In terms of Lambda, we use the value of 'less than one' to indicate 'rich'

$\lambda = 0.9$ for example.

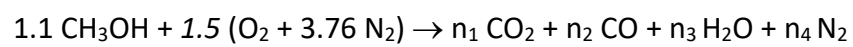
The fuel equivalence ratio is simply $\phi = \frac{1}{\lambda}$

So $\lambda = 0.9$ is simply $\phi = 1.1$

So, let's consider running the engine 10% rich,



Firstly, for Methanol:



C $\rightarrow 1.1 \times 1$	$n_1 + n_2 = 1.1$
H $\rightarrow 1.1 \times 4$	$2n_3 = 4.4$ so $n_3 = 2.2$
O $\rightarrow 3 + 1.1$	$2n_1 + n_2 + n_3 = 4.1$
N	$n_4 = 3.76 \times 1.5$

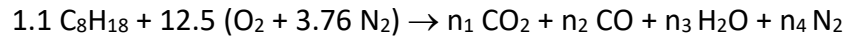
From this we can determine:

$$\begin{aligned}
 2n_1 + n_2 + n_3 &= 4.1 \\
 2n_1 + n_2 + 2.2 &= 4.1 \\
 2n_1 + n_2 &= 1.9 \\
 (\text{but we know } n_1 + n_2 &= 1.1, \text{ so } n_2 = 1.1 - n_1) \\
 2n_1 + 1.1 - n_1 &= 1.9 \\
 n_1 + 1.1 &= 1.9 \\
 n_1 &= 0.8
 \end{aligned}$$

Therefore, $n_2 = 1.1 - 0.8$

So $n_2 = 0.3$

Gasoline – Iso-Octane (10% Rich)



C → 8.8	$n_1 + n_2 = 8.8$
H → 19.8	$2n_3 = 18$ so $n_3 = 9.9$
O → $2 \times 12.5 = 25$	$2n_1 + n_2 + n_3 = 25$
N	$n_4 = 3.76 \times 12.5$

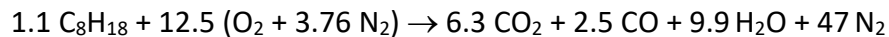
From this we can determine:

$$\begin{aligned}
 2n_1 + n_2 + n_3 &= 25 \\
 2n_1 + n_2 + 9.9 &= 25 \\
 2n_1 + n_2 &= 15.1 \\
 (\text{but we know } n_1 + n_2 &= 8.8, \text{ so } n_2 = 8.8 - n_1) \\
 2n_1 + 8.8 - n_1 &= 15.1 \\
 n_1 + 8.8 &= 15.1 \\
 n_1 &= 6.3
 \end{aligned}$$

$$\text{Therefore, } n_2 = 8.8 - 6.3$$

$$\text{So } n_2 = 2.5$$

So,



On a rolling road, we would be generally looking for 4% CO as an indication for Max Power...

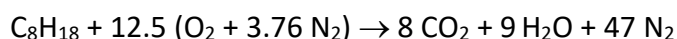
$$\frac{\text{Volume of CO}}{\text{Total Volume}} = \frac{2.5}{6.3 + 2.5 + 9.9 + 47} = 0.038 = 3.8\%$$

THIS SHOWS THE ASSUMPTION TO BE LOGICAL!

Flame Temperatures

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Let's look again at Iso-Octane, but stoichiometrically.



As we have established, the net enthalpy = 5065MJ

Molar Specific Heats – The heat required to make 1 kmol of substance 1K hotter

The flame is very thin and can expand as it heats, since its volume is not fixed, so we use 'constant pressure' specific heats.

All specific heats will increase with temperature as heat input will go into vibration modes as well as making the molecules move faster. Remember that the temperature is proportional to the translational kinetic energy (the movement of the gas molecules).

$\tilde{C}_p$ = Heat Required to Make 1kmol Hotter at CONSTANT PRESSURE

$\tilde{C}_p$	CO_2	H_2O	N_2
2000K	60.433	51.143	35.988
300K	37.28	33.468	29.07

You can clearly see the differences with CO_2 and H_2O being 'triatomic' molecules (having more degrees of freedom) resulting in much higher specific heat capacities at higher temperatures.

Remembering that:

$$dQ = dU + PdV$$

where dU is the internal energy and PdV is the WORK DONE due to moving boundaries

Enthalpy is simply:

$$H = U + PV \dots \text{(if constant pressure)}$$

Or

$$dH = dU + PdV$$

At constant pressure the change in heat is equal to the change in energy.

The net enthalpy released can be calculated from the 'enthalpy of formation' (H_f) at 298K.

This enthalpy release raises the temperature of the products from 298K to fuel flame front temperature, which we can calculate.

Using the fuel tables for CO_2 , H_2O and N_2 we get...

Try at 2300K ... Enthalpy needed: $H_f = (8 \times 109.66) + (9 \times 88.42) + (47 \times 66.99) = 4821.59 \text{ MJ}$

This is a bit of an underestimation.... We want 5065MJ

At 2500K ... Enthalpy needed: $H_f = (8 \times 122.94) + (9 \times 99.11) + (47 \times 74.3) = 5367.61 \text{ MJ}$

At 2400K ... Enthalpy needed: $H_f = (8 \times 115.79) + (9 \times 93.74) + (47 \times 70.64) = 5090.06 \text{ MJ}$

The enthalpy available (the 5065MJ) must lie between 2400K and 2500K

We can calculate the actual temperature quite easily:

$$\frac{T - 2400}{2500 - 2400} = \frac{5100 - 5090}{5367 - 5090}$$

$$\frac{T - 2400}{100} = \frac{10}{277}$$

$$T = 2400 + 100 \times \frac{10}{277}$$

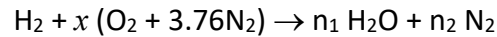
$$T = 2403.72\text{K}$$

So the flame front temperature in this particular case is 2403.72 Kelvin. The temperatures are very sensitive and need to be determined accurately if they are to be used as the basis for emissions modelling later on.

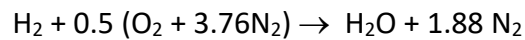
We can create a method to calculate the exact temperatures in Excel or MATLAB.

Calculate for: Isooctane C8H18				
0.99 C8H18 + 12.50 (O2+3.76N2) → 7.92 CO2 + 0.00 CO + 8.91 H2O + 0.13 O2 + 47.0 N2				
H2O (LHV)				
AFR by mass	kg CO2/kg fuel	Calorific Value (MJ/kg)	Enthalpy (MJ)	Flame Temp (K)
15.180	3.088	44.71786284	5049.099	2385.2

Let's take a look again at the combustion of hydrogen:



H → 2	n ₁ = 1
O → 2x	2x = 1 so x = 0.5
N → 0.5 (3.76)	= 1.88



The enthalpy analysis of this reaction yields $0 + 0 + 0 \rightarrow 241.8\text{MJ} + 0$

So the net heat released per kmol of H₂ = 241.8MJ

Looking again at our fuel tables, we can see that:

At 2500K →	H ₂ O + 1.88 x N ₂
	99.11 + 1.88 x 74.3
	= 238.794 MJ

So, you need 238.79MJ to get to 2500K. We have 241.8 available so the temperature must get to > 2500K

At 2600K →	H ₂ O + 1.88 x N ₂
	104.52 + 1.88 x 77.97
	= 251.1MJ

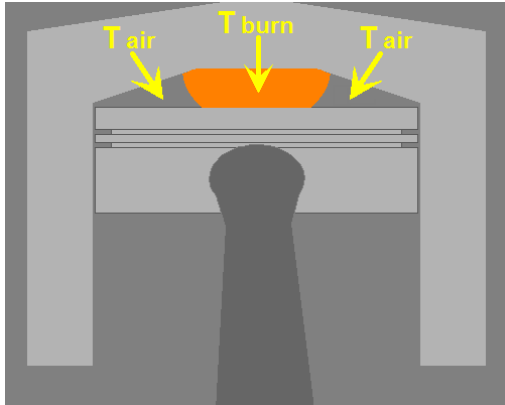
At 2600K, the enthalpy needed is more than we have available, so let's use this information to determine the correct temperature.

$$\frac{T - 2500}{2600 - 2500} = \frac{241.8 - 238.794}{251.1 - 238.794}$$

$$\frac{T - 2500}{100} = \frac{3.006}{12.306}$$

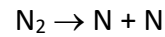
$$T = 2500 + 100 \times \frac{3.006}{12.306}$$

$$T = 2524.43\text{K}$$

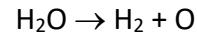


Rising cylinder pressure increases the burn zone temperature beyond the flame temperature.

In the burn zone, when the temperatures are $>2500\text{K}$, the nitrogen gas begins to split into its constituent atoms. The hotter it is, the more likely this is to occur.

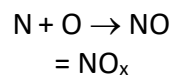


also

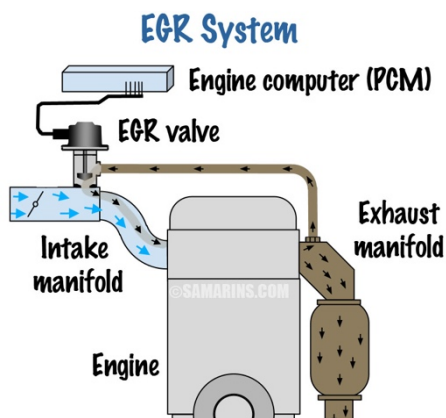


This process is called DISSOCIATION

Stable molecules start to dissociate into less stable radicals at temperatures $> 2500\text{K}$. These dissociations can lead to some other chemical reactions and the formation of undesirable combustion products. For example:



In atmospheric chemistry, NO_x is a generic term for the nitrogen oxides that are most relevant for air pollution, namely nitric oxide (NO) and nitrogen dioxide (NO_2). These gases contribute to the formation of smog and acid rain, as well as affecting tropospheric ozone. It is important for us to find ways to minimise the production of these molecules.



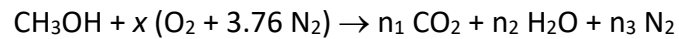
At part load in a drive-cycle, the cylinder is not full of air, due to the fact that you have limited the amount by which the cylinder can fill by the operation of the throttle. (you have throttled it). The burn zone temperature T_B can be determined from the ideal gas law.

$$PV_B = m_B R_B T_B$$

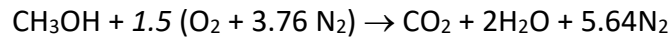
Adding EGR (Exhaust Gas Recirculation) allows you to increase the mass in the burn zone, thereby dropping the burned zone temperature. (An EGR to water intercooler can help here too).

$$M_B = M_{\text{total}} \times \text{MFB (Mass Fraction Burned)}$$

Let's now take a look again at the combustion of Methanol:



C → 1	$n_1 = 1$
H → 4	$2n_2 = 4 \rightarrow n_2 = 2$
O → 2x + 1	$2x + 1 = 2n_1 + n_2 = 2 + 2 = 4 \rightarrow x = 1.5$
N	$n_3 = 3.76 \times 1.5$



The enthalpy analysis of this reaction yields
 $201.2 + 0 + 0 \rightarrow 393.5 + 2 \times 241.8 + 0$
 $201.2 \rightarrow 877.1$

So the net heat released per kmol of $\text{CH}_3\text{OH} = 877.1 - 201.2 = 675.9 \text{ MJ}$

Looking again at our fuel tables, we can see that:

At 2300K →

$$\begin{aligned} &\text{CO}_2 + 2\text{H}_2\text{O} + 5.64\text{N}_2 \\ &109.6 + (2 \times 88.4) + (5.64 \times 66.9) \\ &= 663.7 \text{ MJ} \end{aligned}$$

So, you need 663.7MJ to get to 2300K.

At 2400K →

$$\begin{aligned} &\text{CO}_2 + 2\text{H}_2\text{O} + 5.64\text{N}_2 \\ &115.8 + (2 \times 93.7) + (5.64 \times 70.6) \\ &= 701.38 \text{ MJ} \end{aligned}$$

At 2400K, the enthalpy needed is more than we have available, so let's determine the correct temperature.

$$\frac{T - 2300}{2400 - 2300} = \frac{675.9 - 663.7}{701.38 - 663.7}$$

$$\frac{T - 2300}{100} = \frac{12.2}{37.6}$$

$$T = 2300 + 100 \times \frac{12.2}{37.6}$$

$$T = 2332.45 \text{ K}$$

Brazil runs E95 as a fuel, but this is difficult to start in winter due to the fact that it does not vaporise as easily as gasoline. It needs more heat to make it vaporise so needs heating to get it to start. E95 also needs to be poisoned, otherwise people will drink it!

The advantages of Alcohol!

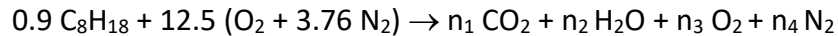
1. Both methanol and ethanol burn cooler than gasoline.
2. Alcohols need more heat to vaporise and thus cool things down
3. You need more mass of it, so the ideal gas law shows ... $T = \frac{PV}{mR}$
4. Alcohol fuels are lighter, and the molecules move faster thereby increasing the flame speed, so combustion is quicker with less heat loss. MBT timing is closer to TDC which reduces negative work.
5. It has a higher octane rating because the molecule is smaller and more stable, therefore less likely to split. This allows higher compression ratios or boost pressures without the likelihood of knock.



The Lean NO_x Model

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Let's look at gasoline, 10% lean...

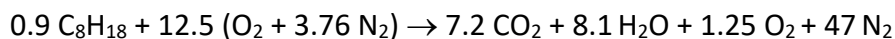


C → 7.2	$n_1 = 7.2$
H → 16.2	$2n_2 = 16.2$ so $n_2 = 8.1$
O → $2 \times 12.5 = 25$	$2n_1 + n_2 + 2n_3 = 25$
N	$n_4 = 3.76 \times 12.5$

From this we can determine:

$$\begin{aligned} 2n_1 + n_2 + 2n_3 &= 25 \\ (2 \times 7.2) + 8.1 + 2n_3 &= 25 \\ 2n_3 &= 2.5 \\ n_3 &= 1.25 \end{aligned}$$

So,



The enthalpy analysis of this reaction yields

$$\begin{aligned} (0.9 \times 259.2) + 0 + 0 &\rightarrow (7.2 \times 393.5) + (8.1 \times 241.8) + 0 + 0 \\ 233.28 &\rightarrow 4791.78 \end{aligned}$$

So, the net heat released per 0.9 kmol of C₈H₁₈ = 4558.5 MJ

While burning 90% of the fuel, this is 90% of the enthalpy released at stoichiometric, so

$$\begin{aligned} 0.9 \times 5065 \text{ MJ} \\ = 4558.5 \text{ MJ} \end{aligned}$$

This is because burning 10% lean creates 10% less net heat released and uses 10% less fuel, so the calorific value stays constant when lean.

Looking again at our fuel tables, we can see that:

$$\begin{aligned} \text{At } 2200\text{K} \rightarrow & 7.2 \text{ CO}_2 + 8.1 \text{ H}_2\text{O} + 1.25 \text{ O}_2 + 47 \text{ N}_2 \\ & (7.2 \times 103.5) + (8.1 \times 83.1) + (1.25 \times 66.7) + (47 \times 63.3) \\ & = 4476.8 \text{ MJ} \end{aligned}$$

So, you need 4476.8 MJ to get to 2200K.

$$\begin{aligned} \text{At } 2300\text{K} \rightarrow & 7.2 \text{ CO}_2 + 8.1 \text{ H}_2\text{O} + 1.25 \text{ O}_2 + 47 \text{ N}_2 \\ & (7.2 \times 109.6) + (8.1 \times 88.4) + (1.25 \times 70.6) + (47 \times 66.9) \\ & = 4737.7 \text{ MJ} \end{aligned}$$

At 2300K, the enthalpy needed is more than we have available, so let's determine the correct temperature.

$$\frac{T - 2200}{2300 - 2200} = \frac{4590 - 4476.8}{4737.7 - 4476.8}$$

$$\frac{T - 2200}{100} = \frac{113.2}{260.9}$$

$$T = 2200 + 100 \times \frac{113.2}{260.9}$$

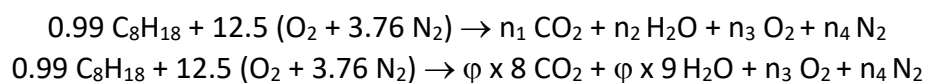
$$T = 2243.38K$$

As can be seen, the combustion temperature is lower running lean (2243.38K compared to 2403.72K for stoichiometric), but it **burns more slowly** therefore there is more time for heat transfer and the engine runs hotter.

We can do these calculations from any **fuel equivalence ratio** (ϕ)

$\phi = 1$ means stoichiometric

$\phi = 0.99$ means 1% lean



So for n_3

$$25 = 2.8\phi + 9\phi + 2n_3$$

$$2n_3 = 25 - 16\phi - 9\phi$$

$$2n_3 = 25 - 25\phi$$

$$n_3 = \frac{25(1 - \phi)}{2}$$

$$n_3 = x(1 - \phi)$$

Hint:

Flame temp is when $8\phi \times \text{Poly CO}_2 + 9\phi \times \text{Poly H}_2\text{O} + x(1-\phi) \text{ Poly O}_2 + 47 \text{ N}_2$

Burn Zone Temperatures

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Flame temperature is not equivalent to the burn zone temperature. The flame temperature represents the initial temperature at the start of combustion, whereas the burn zone temperature increases as the cylinder pressure rises and can be calculated using the ideal gas law, in addition to the ratio of specific heats.

$$PV = mRT$$

Molar specific heat is known as the heat required to make 1 kmol of a substance increase its temperature by 1°K. The two types of specific heats are at constant pressure and constant volume, and the ratio of specific heats is the ratio between these two values, also known as the polytropic index:

$$n = \frac{C_p}{C_v}$$

A process can be considered polytropic if the relationship between the pressure and volume of an ideal gas undergoing compression or expansion follows:

$$PV^n = \text{constant}$$

We can easily derive a formula to find the temperature that follows the flame temperature after the rise in pressure.

$$PV = mRT \quad \therefore V = \frac{mRT}{P}$$

$$PV^n = \text{constant} \quad \therefore P_1 V_1^n = P_2 V_2^n$$

$$P_1 \left(\frac{mRT_1}{P_1} \right)^n = P_2 \left(\frac{mRT_2}{P_2} \right)^n$$

$$\therefore P_1 \left(\frac{T_1}{P_1} \right)^n = P_2 \left(\frac{T_2}{P_2} \right)^n$$

$$P_1 \frac{T_1^n}{P_1^n} = P_2 \frac{T_2^n}{P_2^n}$$

$$\frac{T_1^n}{P_1^{n-1}} = \frac{T_2^n}{P_2^{n-1}}$$

$$\frac{T_2^n}{T_1^n} = \frac{P_2^{n-1}}{P_1^{n-1}}$$