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Nomenclature

atm	Atmosphere (standard atmospheric pressure; 101,325 Pa).
AFR	Air to fuel ratio by mass.
BMEP	Brake Mean Effective Pressure (Theoretical measure of efficiency).
cc	Cubic centimetres.
EGR	Exhaust gas recirculation.
GEM	Gasoline, Ethanol, Methanol fuel blend.
HCCI	Homogenous Charge Compression Ignition engine.
HHV	Higher heating value per mass of fuel.
ICE	Internal combustion engine.
LHV	Lower heating value per mass of fuel.
NEDC	New European Driving Cycle.
PPM	Parts per million.
Q	Heat added into the system.
RON	Research octane number.
SI	Spark ignition engine.
TDC	Top dead centre.
WLTP	World harmonised Light vehicle Testing Procedure.

Conversion equivalents.

1.1. Pressure

1.1.1. $\text{Bar} - \text{Pa} = \cdot 10^5$

1.1.2. $\text{Pa} - \text{Bar} = \cdot 10^{-5}$

1.2. Volume

1.2.1. $\text{cc} - m^3 = \cdot 10^{-6}$

1.2.2. $m^3 - \text{cc} = \cdot 10^6$

1.2.3. $\text{cc} - \text{L} = \frac{\text{cc}}{1000}$

1.3. Temperature

1.3.1. Kelvin to °C = -273.15

1.3.2. °C – Kelvin = +273.15

1.4. RPM

1.4.1. Revolutions - radians = $\cdot 2\pi$

1.4.2. Minute – seconds = $\div 60$

1. Introduction.

The following paper has been written with the intent of highlighting the potential impact the automotive world faces, regarding the emission produced as a by-product of using various fuels within an internal combustion engine (ICE). It will be shown that when based upon simple stoichiometric combustion and the idea of chemical equilibrium, it enables calculation of known chemical reactants in the form of harmful gases, for example; Carbon Dioxide [CO_2], Carbon Monoxide [CO], Nitric Oxides [NO_x].

The other unfortunate side of combustion of fuels, such as Iso-Octane and N-Decane, is the potential for reactants alike; unburnt hydrocarbons, particulate mass [soot, smoke] and sulphur oxides [SO_x]. All of which cause known health problems and contribute to the production of acid rain. (McAllister, Chen, & Fernandez-Pello, 2011)

Objectives -

- Outline the mathematics of blending fuel types to return; Mass percentages, AFR by mass, enthalpy of formation and then the LHV & HHV.
- Demonstrate an understanding of enthalpy of formation and how it can be manipulated to return values of Q .
- Develop a model with the use of "Zeldovich model" equation, to show NO_x production via adiabatic flame temperature propagation, during lean burn conditions of Iso-octane.
- Show the potential of reducing NO_x production, by introducing the idea of EGR into the system.

2. Fuel Blending.

Fuel Blending

Fuel blending is a well-known procedure in this day-in-age, there has been multiple benefits proposed from using 'GEM' fuels, these fuel types are presented as varying blends of gasoline [petrol], ethanol and methanol.

Studies have shown that within HCCI combustion style engines, using a blend of methanol and gasoline can significantly reduce the production of NO_x (Waqas, et al., 2017). Along with, when configured in an iso-stoichiometric form, certain blends of 'GEM' fuels demonstrate very similar LHV's, octane ratings (If set to constant stoichiometric AFR's) in comparison to solitary fuels. They also share a close relationship behind enthalpies of vaporisation (Turner, Pearson, Bel, Goede, & Woolard, 2012).

The major benefit is the sustainability and price, by blending hydrocarbon-based fuels with alcohol's it poses the idea that we, as a race, can improve energy security, aid the reduction in production of greenhouse gases and develop a cheaper "cost-per-unit-energy" fuel. This is brought about because methanol can be obtained from a wider range of feedstocks in a cost-effective manner (Turner, Pearson, Bel, Goede, & Woolard, 2012).

Mathematical modelling.

Regarding mathematical modelling under the condition of chemical equilibrium, the blending of fuels is a simple process.



Figure 1 50:50 Blend of Iso-octane to Methanol fuel chemical equilibrium balance equation.

Starting with mass percentages of the fuels; given that the fuels consist of known elements with known mass properties, using them as if it were a one-to-one ratio (50:50), we can simply sum the atomic weights with respect to a single kilomole [kmol] and return a mass value for the individual fuels.

With this, we have a total mass for each fuel, which becomes the total fuel mass and it's a case of converting the mass of a fuel into a percentage of the total known mass. For example, with the 50:50 blend, using the basis of Iso-octane consisting of; eight carbon atoms and eighteen hydrogen, atomic mass of 12.0107 & 1.0079 (Kg/kmol) respectively. Total mass of one kmol being 114.2278 Kg/kmol and with methanol at; one carbon atom, four hydrogen atoms and an oxygen atom. So, with the addition of an oxygen atom at 31.9988 Kg/kmol, the mass of one kmol of methanol is 32 Kg/kmol, the total is 146.27 Kg/kmol with Iso-octane making up 78% of the mass and methanol at 22%.

To calculate the AFR, using the chemical equilibrium approach, we know the total of products on the right-hand side of the balance and these aid in understanding at stoichiometric combustion how much oxygen is to be required. With the correct amount of oxygen calculated from the right, with the oxygen and nitrogen being factorised on the left and in this case minus one for that within the methanol, the oxygen is to be put as one, same with nitrogen. Both to multiplied by the factor outside the brackets and this factor is the number of oxygen atoms required.

Then finally with the amount of nitrogen concerned, earths atmosphere is made up most of oxygen and nitrogen so with the percentage of oxygen as 20.75% and nitrogen at 78% a ratio of 3.76 is used to multiply the nitrogen inside the factor and this will then balance the equation fully.

With the known number of air atoms and they're atomic masses, calculating a total mass for the air percentage and then simply dividing the mass of air by the mass of fuel in the system and it'll return the equivalent air-to-fuel mass ratio and for this case it's 13.14 : 1.

Regarding the enthalpy of formation, the known basic products and reactants concerned have a given value. So, with the simplistic model, simply multiply the number of products/reactants by their respective enthalpy [MJ/kmol].

For a more accurate method of calculation, using a curve fitting tool within the appropriate software, in this case excel, to return an interpolation equation that can be used for finer results at certain temperatures that can then be used in the equation;

$$\frac{T_x - T_{below}}{T_{above} - T_{below}} = \frac{h_f - h_{f_{below}}}{h_{f_{above}} - h_{f_{below}}}$$

Equation 1 Interpolation equation.

So, with Carbon Dioxide being -393.5 MJ/kmol, having a total of nine kilomoles in the given fuel blend the total enthalpy of formation for CO_2 is -3541.5 MJ/kmol.

For the water products, this is what governs the LHV (net heating value) and HHV (gross heating value). The lower heating value is considered when the H_2O is in a gaseous state, meaning the higher heating value is when the water is in liquid form (Heywood, 1988). Hence the reason the LHV is usually referred to because the reality of combustion is it'll will result in the H_2O being gaseous. The same principle is used here, LHV enthalpy is -241.8 MJ/kmol, HHV is -285.8 totalling at -2659.8 and -3143.8 MJ/kmol respectively for the nine atoms of CO_2 and the eleven H_2O .

(Although there is oxygen (O_2) and nitrogen (N_2) molecules within the equation, they exist in their most stable form and therefore have an enthalpy of formation of zero (McAllister, Chen, & Fernandez-Pello, 2011).)

Total product enthalpy totalling at -6201.3 MJ/kmol (LHV) and -6685.3 MJ/kmol (HHV) leading the calculating the net enthalpy of the system with is defined as;

$$\text{Enthalpy of products} - \text{Enthalpy of reactants} = \text{Net Enthalpy}$$

Equation 2 Net Enthalpy.

During the combustion of a fuel in an ICE, energy is released in multiple forms, one of which is the energy that comes from the rearrangement of the chemical bonds of said reactants, into the products.

For the of enthalpy of formation, there are known enthalpies of formation for an abundance of molecules, however for this we need the primary known products; CO_2 , H_2O , CO and NO_x . Each of which have known values at standard conditions, being 25°C & 1 atm (McAllister, Chen, & Fernandez-Pello, 2011).

(Appendix 1)

Hence the enthalpy of formation at a new condition is shown as;

$$\tilde{h}_i(T) = \tilde{h}_{f,i}^\circ + \Delta \tilde{h}_i(T)$$

Equation 3 Enthalpy of formation (Merker, Schwarz, Stiesch, & Otto, 2006).

Showing that the total enthalpy is the standard enthalpy of formation with the addition of the temperature dependent term.

With this style of mathematical modelling, in terms of complete combustion, the amount of CO_2 produced from the fuel is known. With the known number of molecules, simply multiple this by the molar mass for a single kmol of carbon dioxide and this will return the mass of the product produced. For this study of the 50:50 blended fuel, the number of kilomoles is nine, singular mass of 44.0095 Kg/kmol, the total mass produced is 396.0855 Kg. (1150)

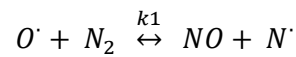
Regarding an “ideal fuel”;

- It's assumed that the fuel in question should be readily available, in terms of both how much refinement is required to obtain the fuel from the starting crude oil product. Along with, how easy it is to both transport and harness the fuel.
- The fuel should be “cheap”, which again is a derivative of the cost's involved with refining the fuel, the additives in the fuel for aiding RON and non-corrosive properties & of course the transportation of the fuel to place of sale.
- The fuel should have reliable combustibility, within the atmospheric air conditions, at a moderate rate. The idea being, the fuel doesn't take too much energy to ignite within the average operating conditions when mixed with the air, whilst still maintaining a quick enough burn that works within the operating limits of SI-ICE's across the Otto/Diesel cycle.
- There should be a considerable energy release from the fuel during combustion to make it worthwhile. For example, petroleum has an LHV of 44 MJ/Kg and considering they are, on average, operating at 30% efficiency the useful energy is only 13.2 MJ/Kg. However, this is considered adequate but if you were to use methanol, that has an LHV of 20 MJ/Kg it's clear that the 6 MJ/Kg of useable energy is not enough to be used as a standalone fuel (Heywood, 1988).
- An ideal fuel is also one that can be considered to not have an adverse effect on the environment because of combustion realising potentially destructive and toxic gases/particulates. Although it's known that burning petroleum can and will produce gases like; CO_2 , NO_x , CO and SO_3 they're produced at either an insignificant rate or are counteracted via a catalytic converter.

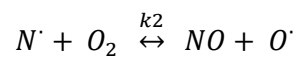
(BYJU'S, n.d.)

3. Nitric oxide modelling.

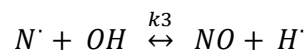
With the impending impact of new emissions regulations to come into action in 2021, understanding how to reduce the pollutants, that come as a product of combustion of fuels, has accelerated at an exponential rate in the past years. One of the most toxic of which is the nitric oxides, they come as a reaction between nitrogen, oxygen and hydroxide radicals when looking at thermal NO_x production. [equations; 4, 5, 6];



Equation 4 Thermal NOx Reaction one.



Equation 5 Thermal NOx Reaction two.



Equation 6 Thermal NOx Reaction three.

(Merker, Schwarz, Stiesch, & Otto, 2006)

Within the cylinder they have the potential to bond together, this happens more frequently at the higher temperatures, due to there being more initial energy within the system, which occurs around stoichiometric combustion. This can be seen in *figures 2 & 3*.

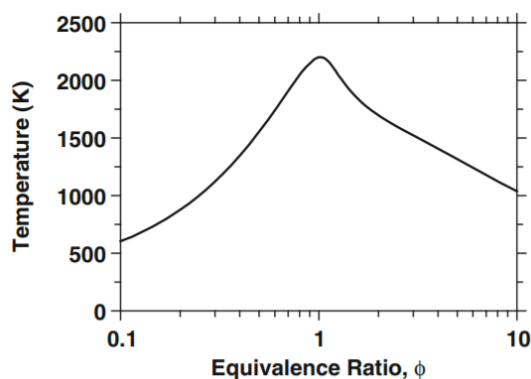


Figure 2 Flame temperatures against a range of Equivalence ratio (McAllister, Chen, & Fernandez-Pello, 2011).

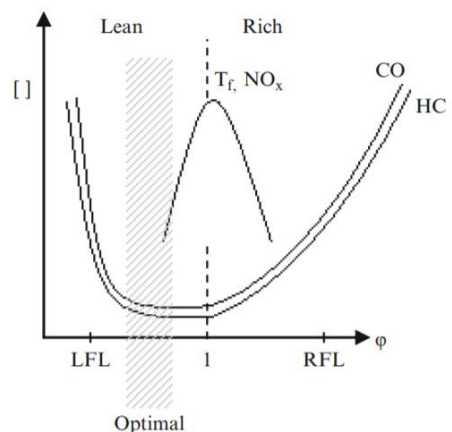


Figure 3 NOx Production against Equivalence ratio (McAllister, Chen, & Fernandez-Pello, 2011).

Which is unfortunate, because in terms of efficiency in an ICE, using the ideal gas law and the common practice of treating the situation as constant volume, the higher cylinder pressures come as product of the higher temperatures, with a fixed molar mass and gas constant. This will then lead to a larger BMEP and this is a known measure of engine performance, because it shows a more effective use of the available volume of the engine.

Looking at the simulation for production of nitric oxides, using the idea of complete combustion, a constant volume system and using the model equation for thermal NO_x proposed by Yakov Zeldovich and interpreted within the books; “Simulating combustion” (Merker, Schwarz, Stiesch, & Otto, 2006), “Fundamentals of Combustion Processes” (McAllister, Chen, & Fernandez-Pello, 2011) and “Internal Combustion Engine Fundamentals” (Heywood, 1988). Shown by the following equations respectively;

$$\frac{d[NO]}{dt} = 4.7 \cdot 10^{13} [N_2] [O_2]^{\frac{1}{2}} \exp \left\{ -\frac{67,837}{T} \right\}$$

Equation 7 NOx Formation rate equation 1 (Merker, Schwarz, Stiesch, & Otto, 2006).

$$\frac{d[NO]}{dt} \cong 1.476 \cdot 10^{15} [N_2] [O_2]^{\frac{1}{2}} \exp \left\{ -\frac{67,520}{T} \right\}$$

Equation 8 NOx Formation rate equation 2 (McAllister, Chen, & Fernandez-Pello, 2011).

$$\frac{d[NO]}{dt} = \frac{6 \cdot 10^{16}}{T^{\frac{1}{2}}} \cdot \exp \left\{ -\frac{69,090}{T} \right\} [O_2]^{\frac{1}{2}}_e [N_2]_e$$

Equation 9 NOx Formation rate equation 3 (Heywood, 1988).

As can be seen from these equations, the major component effecting the result is the temperature, because the oxygen and nitrogen concentration remain as a constant that's come from the indrawn air mixture.

This is the initial flame temperature that comes from the associated “enthalpy of formation”, along with the subsequent temperatures coming from a derivative of the polytropic relationship of $PV^n = \text{constant}$. As previously stated, using the tabulated values for enthalpies of formation and their corresponding temperatures, allows for the use of a graphical interpolation tool that can be used to refine the gaps in values between those that are tabulated. This aids “accuracy” regarding the initial flame temperature, which largely governs the rate of production due to the exponential function within the model equations. [Appendix 4]

The enthalpy of formation was the major “tool” in finding the predicted initial flame temperature, and because of the nature of decreasing the fuel equivalency ratio (Phi ϕ) to increase the air to fuel ratio (running lean combustion), which in this case was simplified as reducing the amount of fuel mass to the same air mass, the net enthalpy decreased every time, bringing down the starting flame temperature, as seen in *Figure 4*;

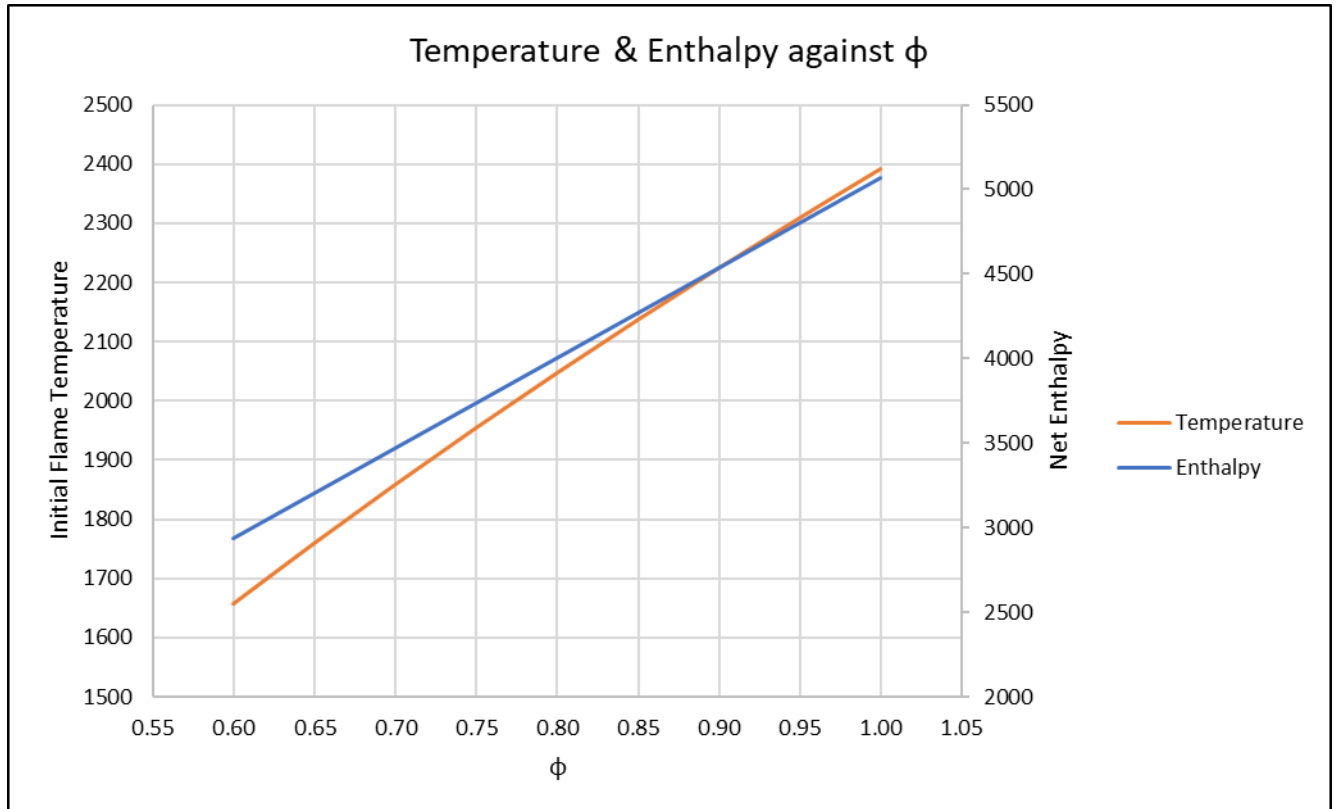


Figure 4 Temperature and Net Enthalpy changes against Fuel equivalency ratio.

So, with the initial flame temperature, using the polytropic relationship derived into the equation;

$$T_2 = T_1 \cdot \left(\frac{P_2}{P_1} \right)^{\frac{n-1}{n}}$$

Equation 10 Temperature propagation equation.

Then using the fixed linear increase of pressure as a 2 Bar step from 10 – 40 and the variable n as 1.17 the temperature increases through the combustion and Phi are shown in *figure 5*.

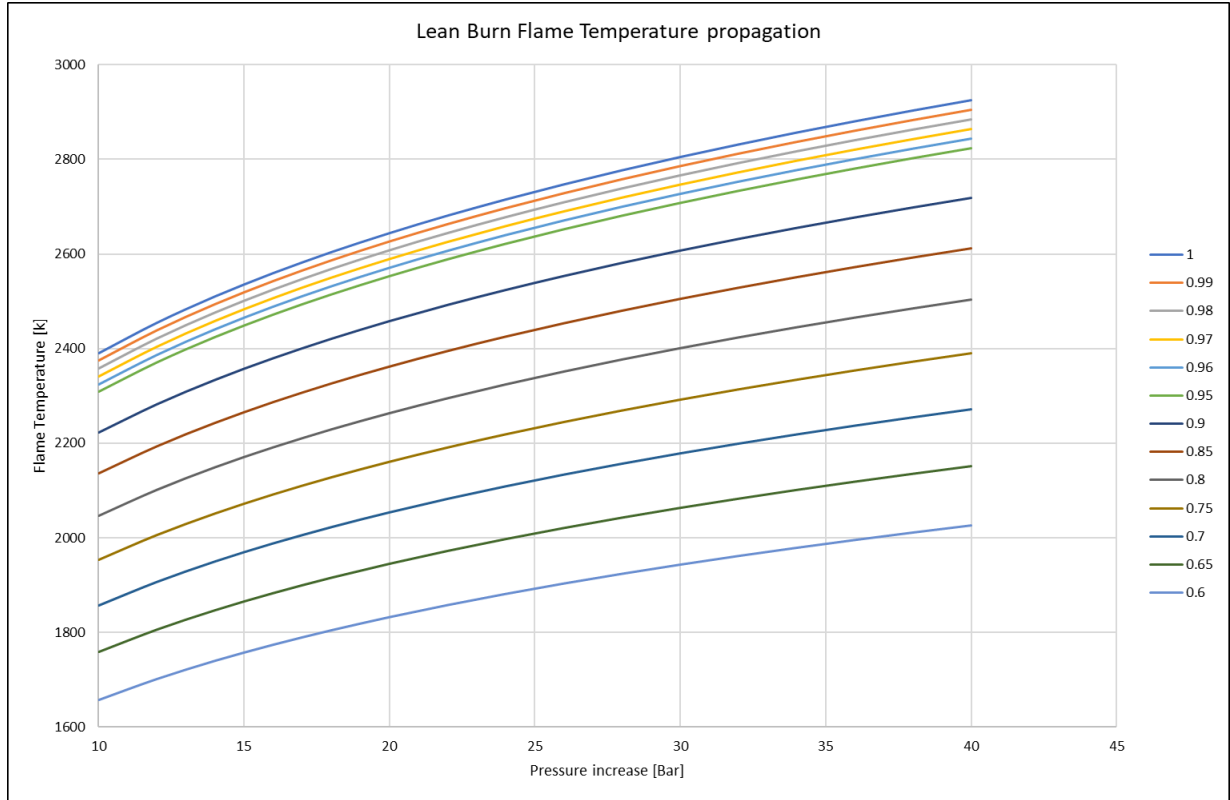


Figure 5 Flame propagation at each pressure step and corresponding Phi (0.6 – 1).

[Refer to appendix 5, to see the rich burn temperatures and the difference Phi makes to the starting temperatures & the subsequent final temperatures.]

As for the nitric oxide production, although the flame temperature is reducing with Phi, the correlation between that of temperature and NO_x production doesn't follow the same exact pattern, because of the increase in available oxygen, as will be discussed.

As shown in equations; 7, 8 and 9, the only other variables are that of the oxygen and nitrogen concentrations. These are found using the amounts of oxygen and nitrogen present due to full combustion equation as a percentage of the amount of air drawn in initially. For the initial air volume, using the following equation for α ;

$$\alpha = \frac{\left(\frac{PV}{R_u T} \right)}{\varphi + n(O_2 + 3.76(N_2))}$$

Where pressure is assumed atmospheric (Naturally aspirated engine), volume for this section was assumed as full cylinder volume of 400cc (100% VE), the universal gas constant was used as 8,314 J/Kmol · K and then temperature as ambient of 20°C (293 k).

Using this alpha value multiplied by the amount of kilomoles of each product, divided by the clearance volume, gives a concentration of oxygen and nitrogen just before assumed combustion, starting at TDC.

As stated, the development of nitric oxides through Phi doesn't follow the exact same trend as that of temperature and enthalpy, this can be seen in *figure 6*.

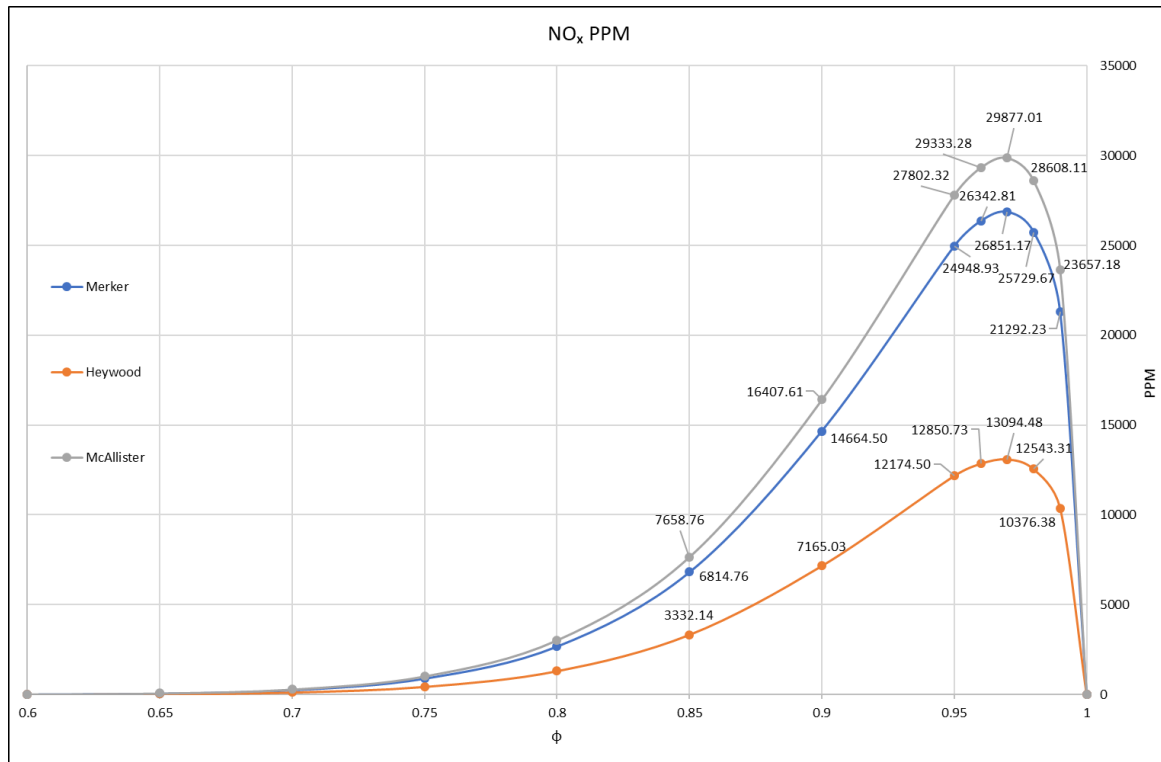


Figure 6 NOx produced in PPM.

As seen the PPM peaks at ϕ of 0.97, this is due to the reality of the concentrations of oxygen increasing as the mass of fuel decreases [appendix 6]. And although the temperature is consistently decreasing there is clearly still high enough temperatures for a slight increase than that of ϕ 0.98. After which the rate of production decreases in an exponential rate to a trivial amount of NO_x produced at ϕ of 0.6.

Although the production of nitric oxides is high when in these leaner conditions, as seen from *figure 2*, total pollutants is lower because of the lack in CO & HC (Hydrocarbons). This thermal NO_x modelling technique is good to show the trend of how varying fuel equivalency ratio effects the production, but it can “only be seen as a crude estimation, as it predicts an excessively high NO concentration” (Merker, Schwarz, Stiesch, & Otto, 2006).

4. Exhaust Gas Recirculation model.

There is multiple ways known to reduce the production of nitric oxides, all based on the idea of reducing the flame temperatures, because “When the flame temperature exceeds 1,800 K, a decrease of 30–70 K in peak flame temperature can decrease NO formation by half” (McAllister, Chen, & Fernandez-Pello, 2011).

Previous investigations have been carried out around; water/methanol injection in the unburnt mixture, studying the effect of spark timing and the use of exhaust gas recirculation [EGR], the latter of which was used in this study to show the positive effects it has on reducing NO_x production.

Exhaust gas recirculation is a very effective way to reduce the pollutants from combustion, because it's simply recycling otherwise wasted products, back into the fresh unburnt mixture to add more molar mass into the starting reactants. Recalling the ideal gas law; if the pressure, volume this time to be at 40% VE and with the gas constant remain the same as previous, then by adding more molar mass into this equation the temperature will have to reduce in order to remain balanced.

This is clearly demonstrated in *figure 7*, shown below.

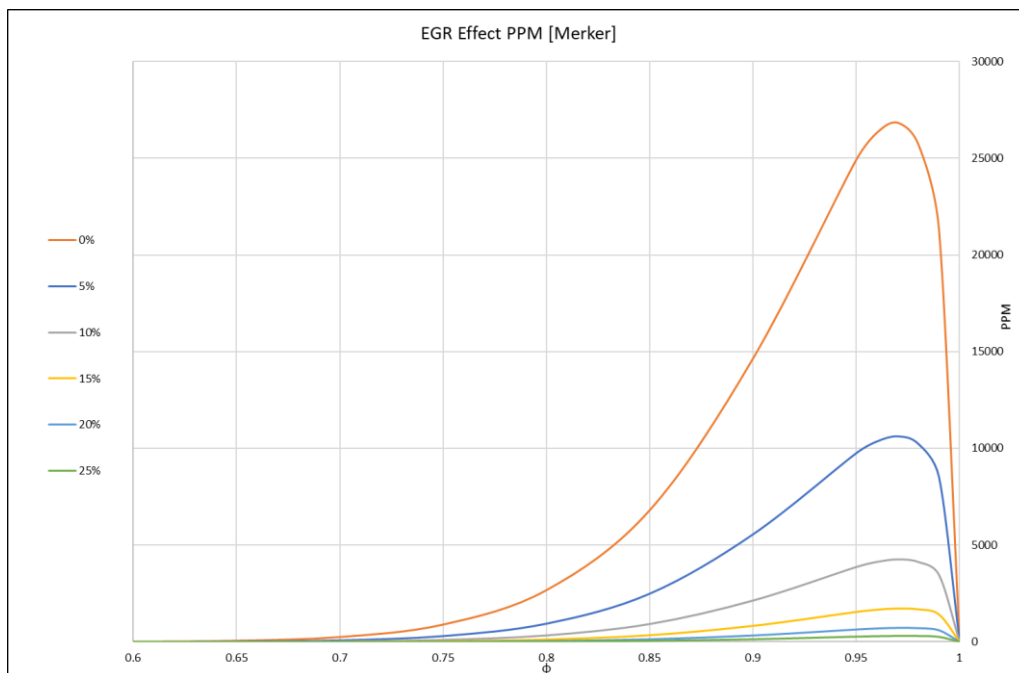


Figure 7 Effect of EGR% on the PPM production through Phi.

And as previously stated, the reduction in peak temperatures of around 30 – 70 kelvin is enough to have halved the production of NO_x as shown as 5% EGR was enough to drop PPM production by 61%.

To demonstrate this correlation, when looking at *figure 8* below, the 5% EGR added had reduced the initial temperature by around 90 kelvin and because of the modelling technique the increase in temperature is relatively linear, therefore confirming this statement and in turn the beneficial effects of using exhaust gas recirculation as a reduction in NO_x PPM production.

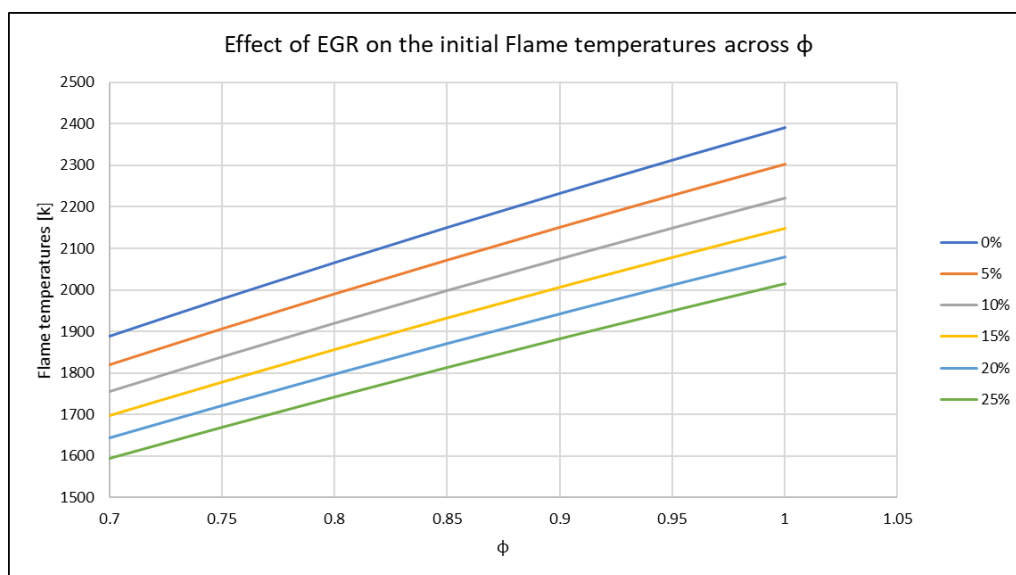


Figure 8 Effect of EGR on the initial flame temperatures across Φ .

5. Conclusion.

To conclude this report, there is most definitely an advantage to blending fuels; primarily from the fact of the abundance of alcohols in comparison to fuels like Iso-Octane, costs associated with the alcohols are far less and then the added bonus of being able to run most low alcohol blend fuels on a large amount of conventional SI - ICE's. Also, with the blending of the expensive fuels with the cheaper alcohols, it reduces the air mass required to burn the mixture, therefore reducing the amount of potential oxygen in the system. One concern with using blended fuels is that it will drop the net calorific value of the fuel, leading to less heat energy released, which could lead to issues in driveability.

When modelling the production of nitric oxides, there are many variables concerned that could lead to potentially drastic changes in final results. With this simple Zeldovich model technique, it ignores the realities of producing NO_x across both lean and rich conditions, it ignores the chemical kinetics involved and how much energy the systems components potentially have, it only assesses the oxides produced "behind" the flame front and therefore this model has ignored the prompt NO_x modelling also.

Although the model has grossly overpredicted the numbers associated with real operating conditions (because it has neglected a lot of variables), it shows the correct trends that correspond to that of real life, transient conditions and therefore is certainly still a valid mathematical tool to aid understanding.

As for the addition of EGR into the automotive world's ICE's, it was certainly a quick and effective way to reduce the production of NO_x , especially under low load situations, of which the governing testing procedures [NEDC & WLTP] frequently consist of. The main drawback of using EGR in engines is the potential for excess build up of HC/soot particulates throughout the intake air system which could cause faults. But using this alongside the multiple other technologies used in modern engines has helped reduce global pollution from both passenger vehicles and commercial vehicles.

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7. Appendices

1. Enthalpy of formation table.

TABLE 3.2
Standard enthalpies of formation

Species	State†	$\Delta\hat{h}_f^\circ$, MJ/kmol
O ₂	Gas	0
N ₂	Gas	0
H ₂	Gas	0
C	Gas	0
CO ₂	Gas	−393.52
H ₂ O	Gas	−241.83
H ₂ O	Liquid	−285.84
CO	Gas	−110.54
CH ₄	Gas	−74.87
C ₃ H ₈	Gas	−103.85
CH ₃ OH	Gas	−201.17
CH ₃ OH	Liquid	−238.58
C ₈ H ₁₈	Gas	−208.45
C ₈ H ₁₈	Liquid	−249.35

† At 298.15 K (25°C) and 1 atm.

Figure 9 Table of enthalpies of formation (Heywood, 1988).

2. Enthalpy of known fuel products.

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TABLE D.3
Enthalpy of C, CO, CO₂, H₂, H₂O, N₂, O₂

<i>T</i> (K)	$\hat{h}^o(T) - \hat{h}^o(298.15), \text{ kcal/mol}$						
	C	CO	CO ₂	H ₂	H ₂ O	N ₂	O ₂
298	0.000	0.000	0.000	0.000	0.000	0.000	0.000
300	0.004	0.013	0.016	0.013	0.015	0.013	0.013
400	0.250	0.711	0.958	0.707	0.825	0.710	0.724
500	0.569	1.417	1.987	1.406	1.654	1.413	1.455
600	0.947	2.137	3.087	2.106	2.509	2.125	2.210
700	1.372	2.873	4.245	2.808	3.390	2.853	2.988
800	1.831	3.627	5.453	3.514	4.300	3.596	3.786
900	2.318	4.397	6.702	4.226	5.240	4.355	4.600
1000	2.824	5.183	7.984	4.944	6.209	5.129	5.427
1100	3.347	5.983	9.296	5.670	7.210	5.917	6.266
1200	3.883	6.794	10.632	6.404	8.240	6.718	7.114
1300	4.432	7.616	11.988	7.148	9.298	7.529	7.971
1400	4.988	8.446	13.362	7.902	10.384	8.350	8.835
1500	5.552	9.285	14.750	8.668	11.495	9.179	9.706
1600	6.122	10.130	16.152	9.446	12.630	10.015	10.583
1700	6.696	10.980	17.565	10.233	13.787	10.858	11.465
1800	7.275	11.836	18.987	11.030	14.964	11.707	12.354
1900	7.857	12.697	20.418	11.836	16.160	12.560	13.249
2000	8.442	13.561	21.857	12.651	17.373	13.418	14.149
2100	9.029	14.430	23.303	13.475	18.602	14.280	15.054
2200	9.620	15.301	24.755	14.307	19.846	15.146	15.966
2300	10.212	16.175	26.212	15.146	21.103	16.015	16.882
2400	10.807	17.052	27.674	15.993	22.372	16.886	17.804
2500	11.403	17.931	29.141	16.848	23.653	17.761	18.732
2600	12.002	18.813	30.613	17.708	24.945	18.638	19.664
2700	12.602	19.696	32.088	18.575	26.246	19.517	20.602
2800	13.203	20.582	33.567	19.448	27.556	20.398	21.545
2900	13.807	21.469	35.049	20.326	28.875	21.280	22.493
3000	14.412	22.357	36.535	21.210	30.201	22.165	23.446

Source: *JANAF Thermochemical Tables*, National Bureau of Standards Publication NSRDS-NBS37, 1971.

Figure 10 Enthalpies of known combustion products. (Heywood, 1988)

3. Properties of Fuels.

Formula	Fuel	M (kg/kmol)	T_b (°C)	c_{pg}^a (kJ/kg·K)	T_{ig} (°C)	HHV (MJ/kg)	LHV (MJ/kg)	h_{fg}^b (kJ/kg)	AFRs	T_f (K) ^c	$\Delta \hat{h}^0$ (kJ/mol)	RON ^d	MON ^e
CH ₄	Methane	16.04	−161	2.21	537	55.536	50.048	510	17.2	2,226	−74.4	120	120
C ₂ H ₂	Acetylene	26.04	−84	1.60	305	49.923	48.225	—	13.2	2,540	8.7	50	50
C ₂ H ₄	Ethylene	28.05	−104	1.54	490	50.312	47.132	—	14.7	2,380	52.4	—	—
C ₂ H ₆	Ethane	30.07	−89	1.75	472	51.902	47.611	489	16.1	2,370	−83.8	115	99
C ₃ H ₈	Propane	44.10	−42	1.62	470	50.322	46.330	432	15.7	2,334	−104.7	112	97
C ₄ H ₁₀	n-Butane	58.12	−0.5	1.64	365	49.511	45.725	386	15.5	2,270	−146.6	94	90
C ₄ H ₁₀	iso-Butane	58.12	−12	1.62	460	49.363	45.577	366	15.5	2,310	−153.5	102	98
C ₅ H ₁₂	n-Pentane	72.15	36	1.62	284	49.003	45.343	357	15.3	2,270	−173.5	62	63
C ₅ H ₁₂	iso-Pentane	72.15	28	1.60	420	48.909	45.249	342	15.3	2,310	−178.5	93	90
C ₆ H ₁₄	n-Hexane	86.18	69	1.62	233	48.674	45.099	335	15.2	2,271	−198.7	25	26
C ₆ H ₁₄	iso-Hexane	86.18	50	1.58	421	48.454	44.879	305	15.2	2,300	−207.4	104	94
C ₇ H ₁₆	n-Heptane	100.20	99	1.61	215	48.438	44.925	317	15.2	2,273	−224.2	0	0
C ₈ H ₁₈	n-Octane	114.23	126	1.61	206	48.254	44.786	301	15.1	2,275	−250.1	20	17
C ₈ H ₁₈	iso-Octane	114.23	114	1.59	418	48.119	44.651	283	15.1	2,300	−259.2	100	100
C ₉ H ₂₀	n-Nonane	128.6	151	1.61	—	48.119	44.688	295	15.1	2,274	−274.7	—	—
C ₁₀ H ₂₂	n-Decane	142.28	174	1.61	210	48.002	44.599	277	15.1	2,278	−300.9	−41	−38
C ₁₀ H ₂₂	iso-Decane	142.28	171	1.61	—	48.565	44.413	—	15.1	2,340	—	113	92
C ₁₂ H ₂₆	n-Dodecane	170.33	216	1.61	204	47.838	44.574	256	15.0	2,276	−350.9	−88	−90
CH ₄ O	Methanol	32.04	65	1.37	385	22.663	19.915	1,099	6.5	2,183	−201.5	106	92
C ₂ H ₆ O	Ethanol	46.07	78	1.42	365	29.668	26.803	836	9.0	2,144	−235.1	107	89
H ₂	Hydrogen	2.02	−253	14.47	400	141.72	119.96	451	34.3	2,345	0	—	—

^aGas phase specific heat evaluated at 25°C

^bHeat of vaporization at 1 atm

^cEstimated equilibrium flame temperature

^dResearch octane number

^eMotoring octane number

Figure 11 Properties of fuels. (McAllister, Chen, & Fernandez-Pello, 2011)

4. Curve Fitting applications – Graphs and appropriate polynomial equations.

Using the polynomial curve fitting tool within Microsoft Excel, the sixth order is what achieved the most accurate fit for each and all applications. With the temperature being on the x-axis, it allows for ease of interpolation of enthalpy at the temperature required.

By simply using a row vector of increments of one kelvin, as opposed to the few hundred in the tabulated values provided primarily from JANAF, and then the equations from the curve fit with that temperature as the x component, it allows a slightly more accurate model to be produced because of the small decrease in margin of error.

Below are examples of the curve fitted trend lines and the corresponding line equations used, all to 15 decimal places, again to try aid in accuracy.

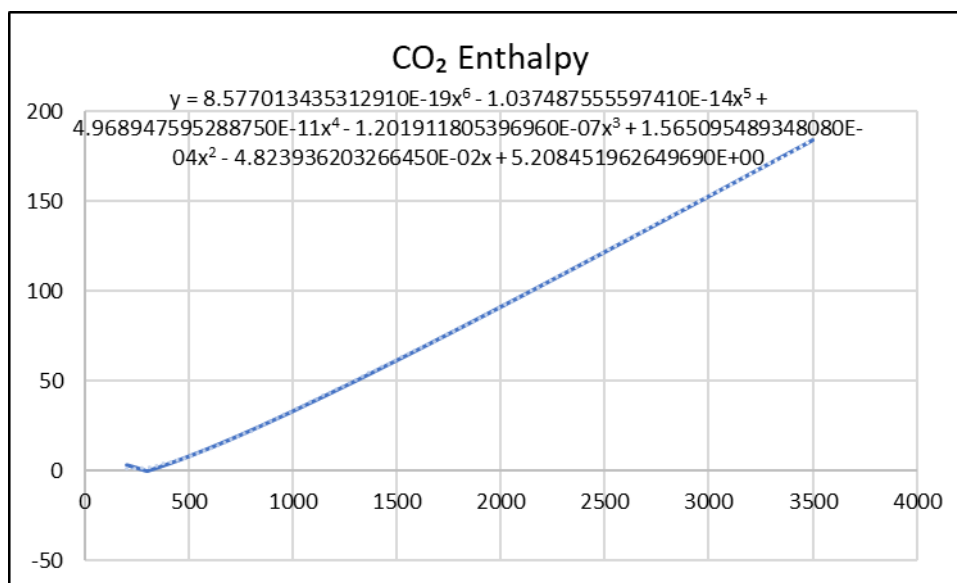


Figure 12 Carbon-Dioxide enthalpy temperature graph with polynomial curve fit.

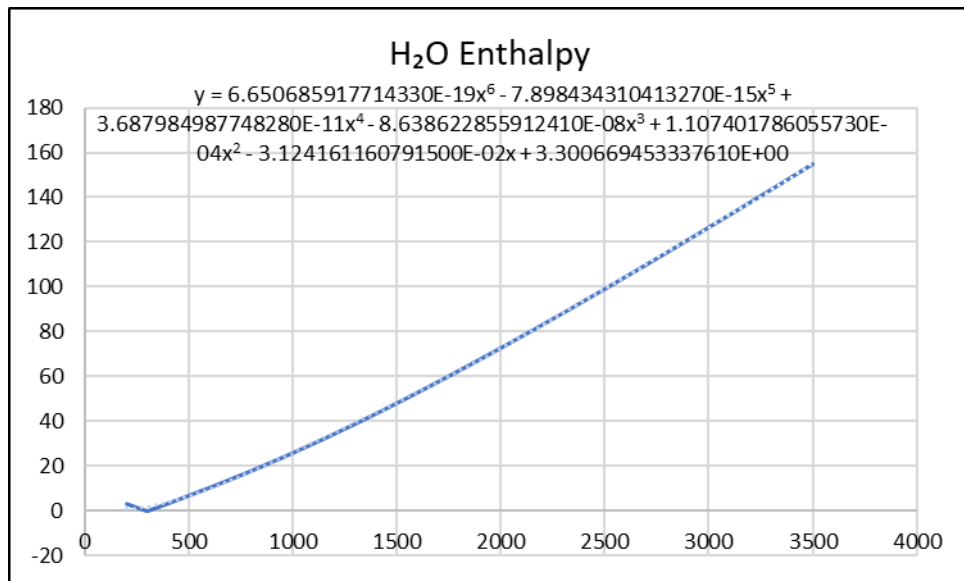


Figure 13 Dihydrogen monoxide enthalpy temperature graph with polynomial curve fit.

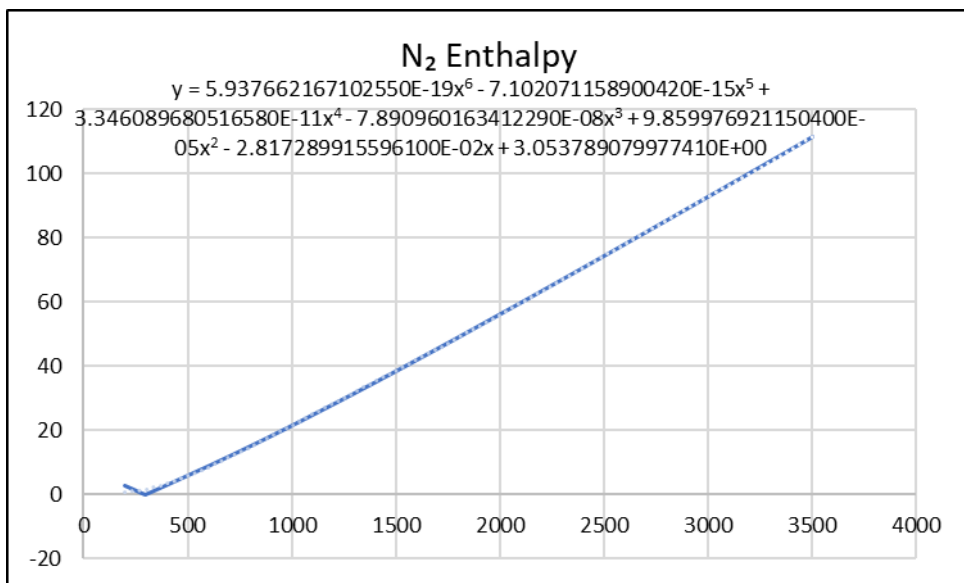


Figure 14 Nitrogen enthalpy temperature graph with polynomial curve fit.

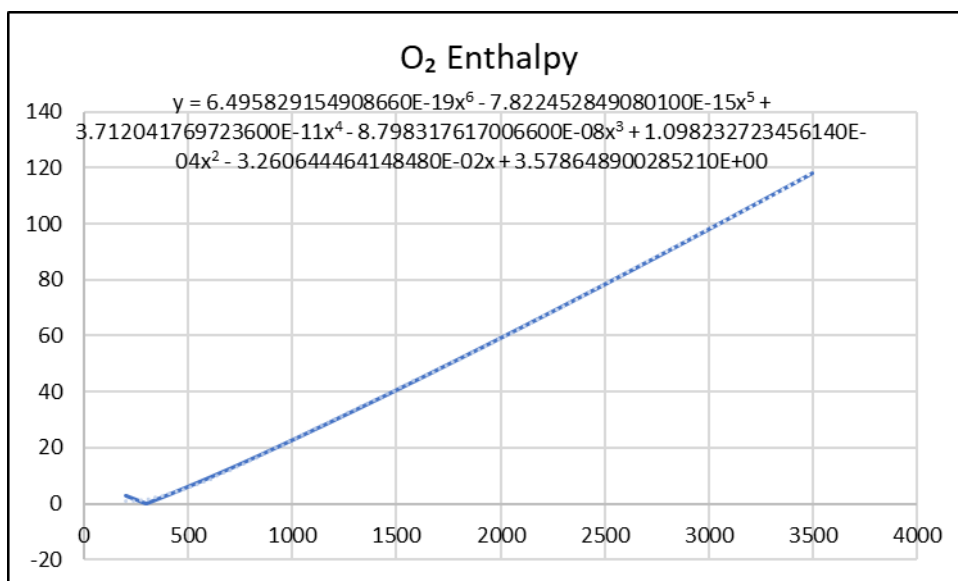


Figure 15 Oxygen enthalpy temperature graph with polynomial curve fit.

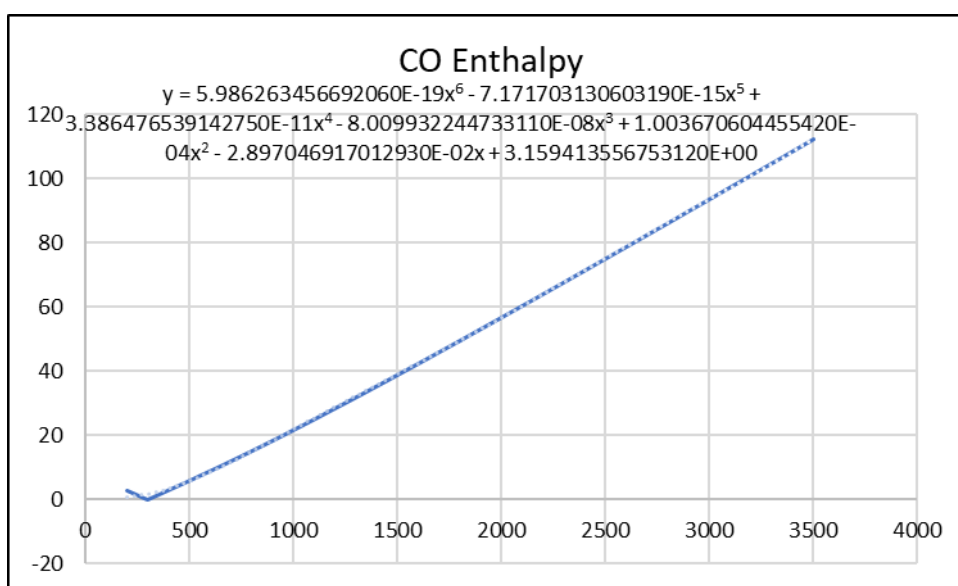


Figure 16 Carbon-Monoxide enthalpy temperature graph with polynomial curve fit.

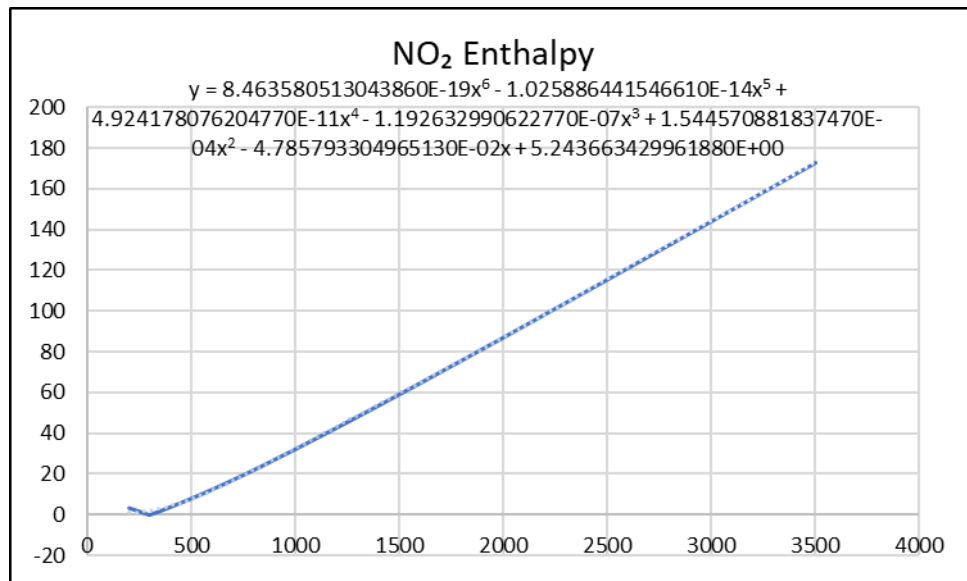


Figure 17 Nitrogen-Dioxide enthalpy temperature graph with polynomial curve fit.

5. Flame Temperatures.

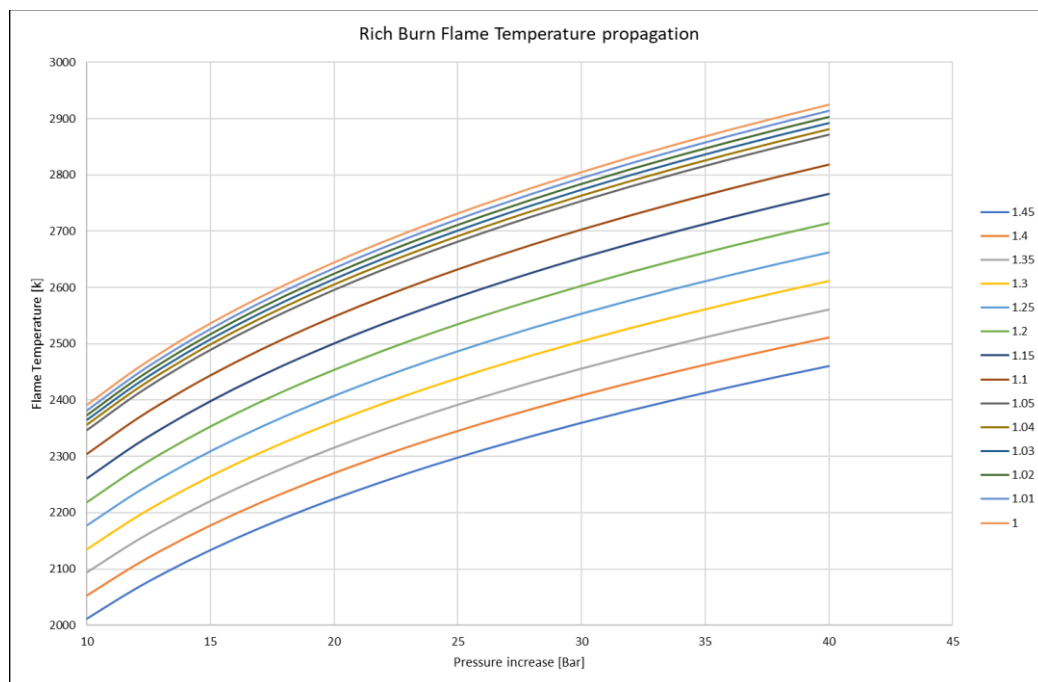


Figure 18 Rich Burn Flame propagation through pressure changes at each Φ .

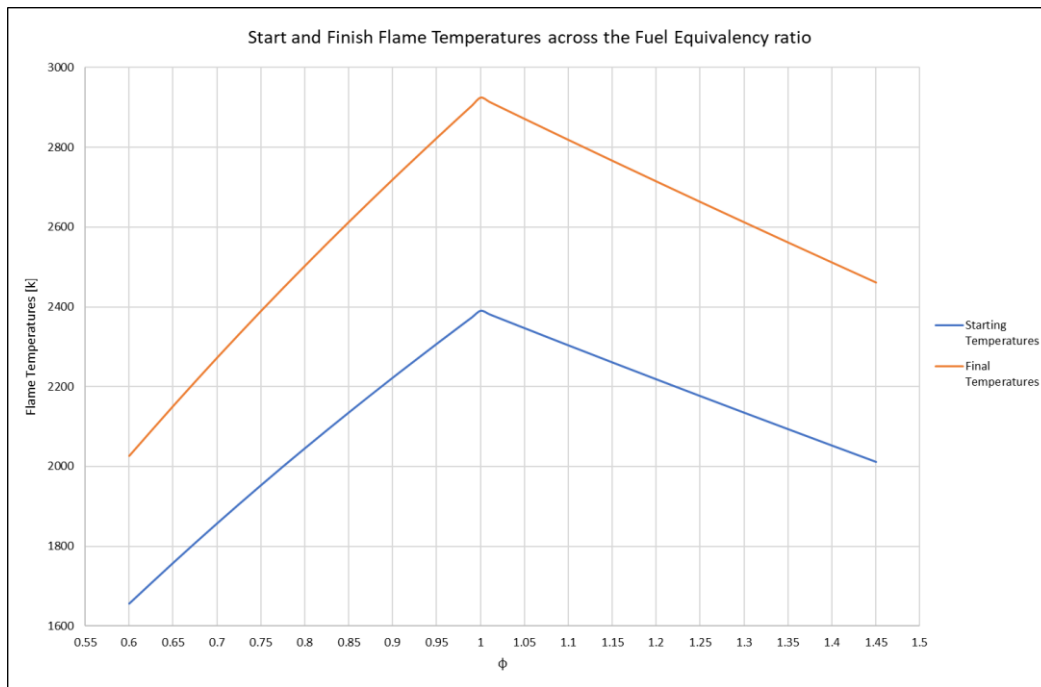


Figure 19 Initial and Final Flame temperatures across the Phi range.

6. Concentration of Oxygen available.

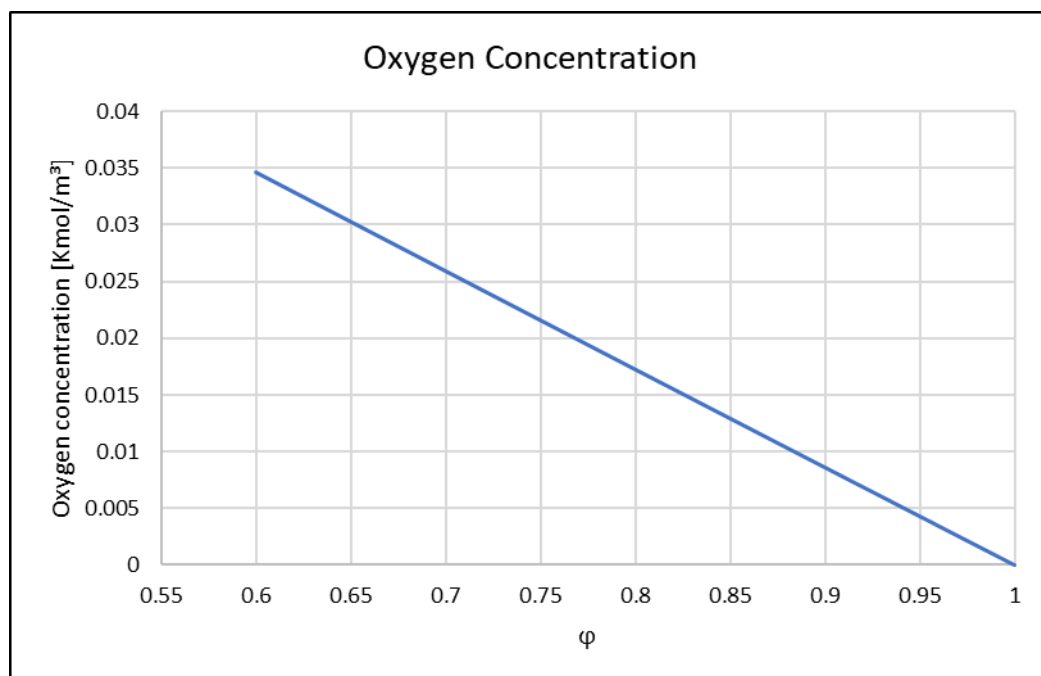


Figure 20 Oxygen concentration [Kmol/m³].

7. Percentage of decrease on NO_x production with EGR% changes.

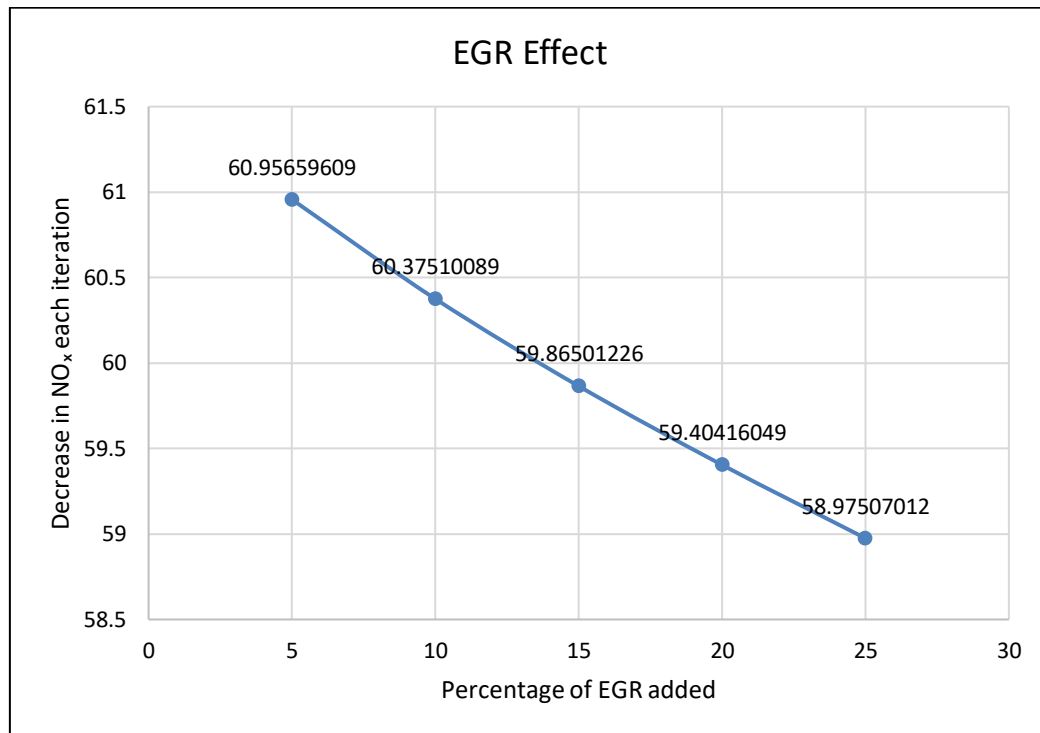


Figure 21 Percentage decrease of NO_x production as EGR% is added from 0 - 25%.

8. NO_x production change with EGR% using Heywood and McAllister's Zeldovich models.

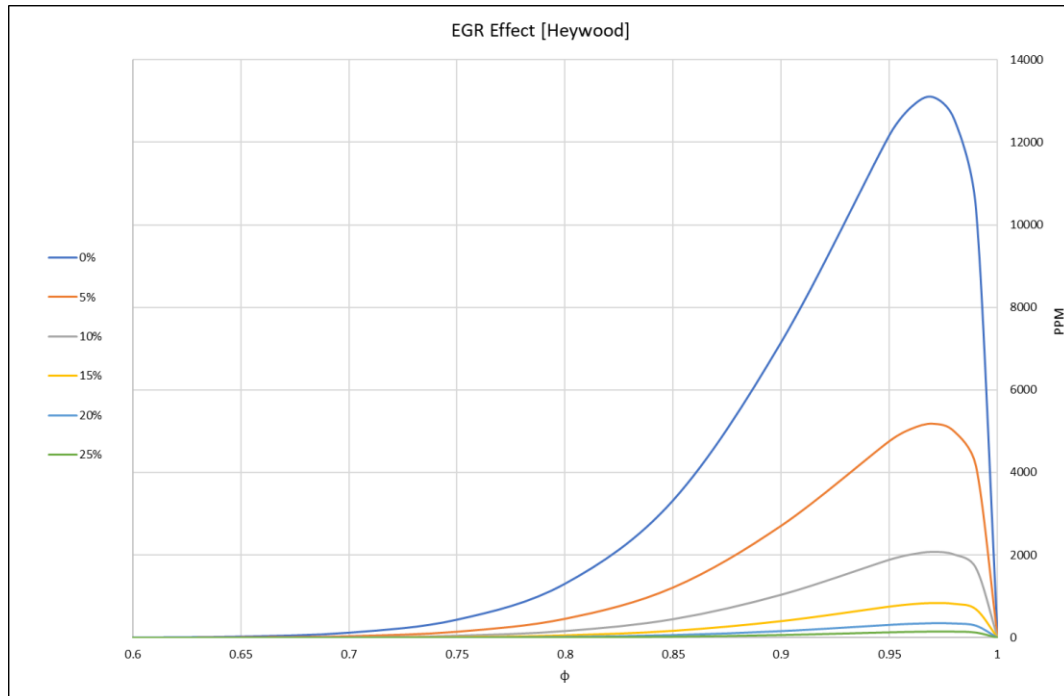


Figure 22 EGR% effect using Heywood's version of the Zeldovich model.

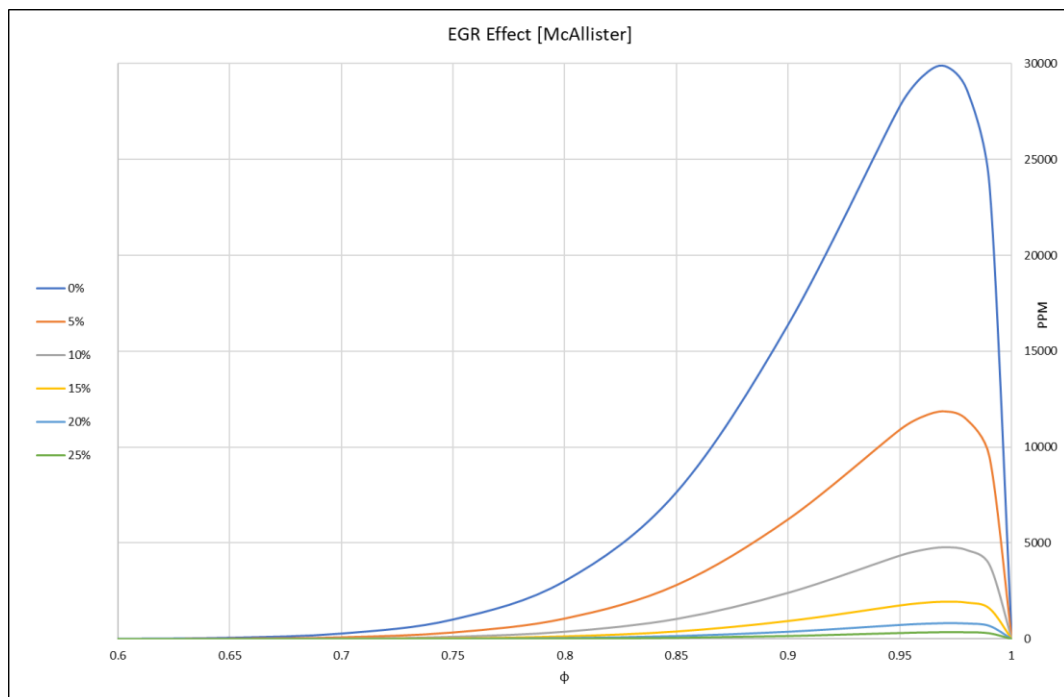


Figure 23 EGR% effect using McAllister's version of the Zeldovich model.