

COMBUSTION AND EMISSION STUDY: MODELLING FUELS AND NOX

POWERTRAIN and SUSTAINABILITY-M6X01206



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ABSTRACT

The aim of this assignment has been to create a carry out a study on fuels, producing a fuel calculator able to determine mass percentages of blend mixtures and AFR values moreover it'll explained how a NOX model was created using Microsoft Excel.

Exhaust gas recirculation (E.G.R.) is well known in the automotive industry as a system used to reduce emissions of vehicles, in this technical report it will be explained and demonstrated in a chemical and physical way how the emissions are reduced using this mechanical valve.

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1 TASK1: STUDY OF A BLENDED MIXTURE OF ISOOCTANE AND METHANOL

1.1 MASS PERCENTAGES CALCULATION THEORY

In order to determine the specific masses of air and fuel from a reaction is fundamental to start looking at the chemical formulas of the elements (air and fuel) which combined form the combustion process.

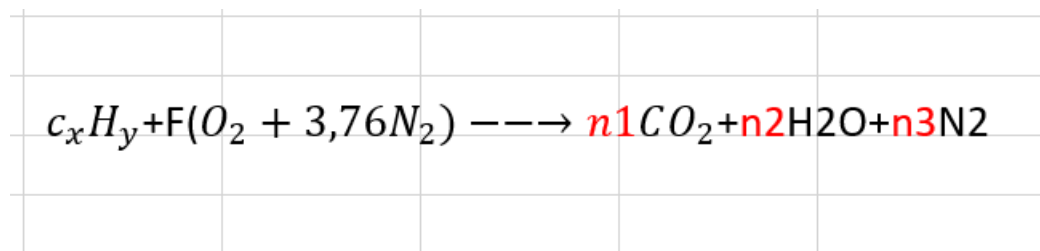


Figure 1 Generic hydrocarbon plus air formula

The above picture is a representation of a generic hydrocarbon combined with air on the left side, what's produced with after the reaction on the right side. The picture below represents the chemical formula of Isooctane which consist in 8 atoms of carbon and 18 atoms of hydrogen.

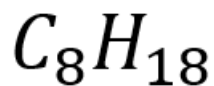


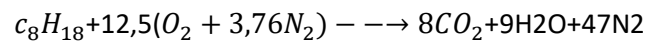
Figure 2 Isooctane's chemical formula

On the left-hand side there's the also the "air term" that represents the composition of air that is made up of 79% of Nitrogen and 21% of Oxygen. On the left right-hand side there are the substances produced with the reaction, Carbon Dioxide, water and Nitrogen. In front of each substance there are the specific coefficients that make the reaction correctly balanced.

1.2 MASS PERCENTAGES CALCULATION METHODOLOGY

Before the start of any calculation, the chemical reaction has to be in equilibrium to avoid numerical mistakes, one equation is balanced when the mass of the products (stuff produced with the reaction) is equal to the mass of the reactants (Caligaris, 2012).

Practically the number of atoms of each component on the left side of the equation has to be equal to the number of atoms, considering also the relative coefficients, which have to be multiplied by the number of atoms, (n1,n2...) to the right side of the reaction. Below the balanced equation for Isooctane.



In order to calculate the mass percentages of air and fuel it's necessary to use the periodic table which contains the average Atomic Mass of each chemical element in [Kg/Kmol] or [g/mol], once the Atomic Mass is found it has to be multiplied by the number of atoms of the respective chemical element. Here an example for Isooctane

C_8H_{18} Isooctane chemical formula.

		PERIODIC TABLE
Atomic No		Atomic weight
		Kg/kmol
Hydrogen	1	1.00797
Carbon	6	12.0107
Nitrogen	7	14.0067
Oxygen	8	15.9994

(Lenntech, 2019)

$$m(fuel) = (12.0107 * 8 + 1.00797 * 18) = 114.22 \text{ Kg}$$

$$m(air) = (12.5 * (2 * 15.994 + 3.76 * 2 * 14.0067)) = 1716.6148 \text{ Kg}$$

1.3 MASS PERCENTAGES CALCULATION WITH EXCEL

ISO-OCTANE	C_8H_{18}						
O2	21.00			Atmospheric	Ratio		
N2	79.00			Composition	3.76		
HC Fuel Balance		$C_xH_y + F(O_2 + 3,76N_2) \longrightarrow n1CO_2 + n2H_2O + n3N_2$					
		$C_8H_{18} + 12,5(O_2 + 3,76N_2) \longrightarrow 8CO_2 + 9H_2O + 47N_2$					
N. OF ATOMS	BALANCE	C_8H_{18}		F	12.5		
Carbon (x)	8			CO2 (n1)	8		
Hydrogen (y)	18			H2O (n2)	9		
Oxygen (2*F)	2			N2 (n3)	47		
m (air)	1716.615	Kg					
m (fuel)	114.2291	Kg					
AFR BY MASS	15.02783						
stoich ratio	14.7						
lambda λ	1.022301						
Equiv Ratio ϕ	0.978185						
1Kmol of	ISO-OCTANE	C_8H_{18}	114.229	Kg	CO2	352.076	Kg
					H2O	162.13806	Kg
					N2	1316.6298	Kg

Figure 3 Isooctane calculator

BLEND		(50% Iso-octane)+(50% Metahnol)			
CH3OH + C8H18 + F (O2 + 3.76 N2) ---→ n1 CO2 + n2 H2O + n3 N2					
				Atmospheric Composition	Ratio 3.76
N. OF ATOMS	BALANCE		F	14	
Carbon (x)	9		CO2 (n1)	9	
Hyrdrogen (y)	22		H2O (n2)	11	
Oxigen	1		N2 (n3)	52.64	
Tot oxigen balance	29		Tot oxigen balance	29	
Tot N2 balance	105.28		Tot N2 balance	105.28	
Tot Carbon balance	9		Tot Carbon balance	9	
Tot H balance	22		Tot H balance	22	
TOTAL m (air)	1922.609 Kg			%	
TOTAL m (fuel)	146.271 Kg		METHANOL m	21.9059	TOT check
AFR BY MASS	13.14415		Isococtne	78.0941	100
stoich ratio	14.7				
lambda λ	0.89416				
Equiv Ratio ϕ	1.118368				

Figure 5 Blend calculator

The blend mixture chemical equation was balanced, then an extra “Tot element balance” row was calculated to check and visualize that the number of atoms were correct in both sides.

The total mass of air and fuel were calculated as explained in the previous section, knowing the Isooctane (114Kg) and Methanol(32Kg) specific masses, it was possible to determine the mass percentage of the two fuels in the blend dividing the specific mass of one fuel by the total fuel mass (21.90% Methanol, 78%.09% Isooctane).

1.4 AIR: FUEL MASS RATIO FOR STOICHIOMETRIC COMBUSTION IN AIR

Once calculated the fuel masses involved, it was possible to see what value of AFR corresponds to this blend.

AFR by mass value represents the ratio between mass of air and mass of fuel, AFRs (stoichiometric) is the ratio for a complete combustion which means that all the Carbon atoms are burnt and transformed into Carbon Dioxide without producing any Carbon Monoxide

(CO), analysing from the “Oxygen” side, combustion is stoichiometric when there are the exact number of Oxygen atoms to burn all the fuel used. (Blair, 1999).

Each fuel has its own AFRs, the Isooctane and Methanol value were calculated and then compared to the official ones given from the Fuel tables.

FUEL AFRs	EXCEL CALCULATOR	OFFICIAL VALUE
ISOOCTANE	15.027	15.1
METHANOL	6.0428	6.5

(Williams, 2019)

The values calculated are quite close to the nominal values, which means that the process used is quite reliable. It's visible that Methanol has a lower AFRs than Isooctane, that's due to the fact that Methanol already contains one atom in its own formula so, it needs less Oxygen for a complete combustion (CH_4O).

Interesting fact is that the blended mixture has a AFR value of 13.14 which is a value between 6.5 and 15.1 which totally makes sense.

1.5 EXPLANATION OF ENTHALPY OF FORMATION

The Enthalpy of formation corresponds to the amount of heat created by the combustion, of one mole of substance with presence of Oxygen, at standard condition of pressure and temperature (1 atm and 298 K). This statement can be expressed mathematically as follows:

If we imagine an “Ideal Engine” where friction between piston rings and cylinder wall and any leakages are not taken in consideration the work done by the piston motion is (Blair, 1999):

$$\delta W = F \cdot dx = P \cdot A \cdot dx = P \cdot dV \quad (1)$$

According to the First law of Thermodynamics

$$dU = dQ - dW \quad (2)$$

thus

$$dQ = dU + P \cdot dV \quad (3)$$

Enthalpy can be Expressed as:

$$dH = dU + PdV$$

$$H = U + PV$$

$$dH = dU + P dV \quad (4)$$

So, at constant pressure it's possible to write:

$$\underline{dH = dU + P dV = dQ} \quad (5)$$

The value of Enthalpy of Formation of a reaction can be calculated using Hess's law.
(Halpern, 2016)

$$\Delta H = \sum \Delta H_{\text{of}}(\text{products}) - \sum \Delta H_{\text{of}}(\text{reactants}) \quad (6)$$

1.6 ENTHALPY OF FORMATION AND HEATING VALUES RESULTS

ENTHALPY OF FORMATION DATA				
		hf CO_2	-393.5	KJ/Kmol
		hf Liquid H_2O	-285.8	KJ/Kmol
		hf Gas	-241.8	KJ/Kmol
Assuming 1 Kmol of Methanol and Isoocatane have burnt		hf C_8H_{18}	-259.2	KJ/Kmol
ENTALPY OF FORMATION OF THE REACTIONS		hf CH_4O	-201.5	KJ/Kmol
$\text{CH}_3\text{OH} + \text{C}_8\text{H}_{18} + \text{F} (\text{O}_2 + 3.76 \text{ N}_2) \longrightarrow n_1 \text{ CO}_2 + n_2 \text{ H}_2\text{O}(\text{LIQUID}) + n_3 \text{ N}_2$				
H2O as liquid				
Δh	ENTALPHTY REACTANTS	-460.7	MJ/Kmol	
Δh	ENTALPHTY OF PRODUCTS	-6685.3	MJ/Kmol	
	HIGHER HHV	6224.6	MJ	HEAT PRODUCED
		42.55525	MJ/Kg	AT CONSTANT P
$\text{CH}_3\text{OH} + \text{C}_8\text{H}_{18} + \text{F} (\text{O}_2 + 3.76 \text{ N}_2) \longrightarrow n_1 \text{ CO}_2 + n_2 \text{ H}_2\text{O}(\text{GAS}) + n_3 \text{ N}_2$				
H2O as GAS				
Δh	ENTALPHTY REACTANTS	-460.7	MJ/Kmol	
Δh	ENTALPHTY OF PRODUCTS	-6201.3	MJ/Kmol	
	LOWER LHV	5740.6	MJ	HEAT PRODUCED
		39.24632	MJ/Kg	AT CONSTANT P

Figure 6 Enthalpy and heating values results

			HENTALPY OF FORMATION DATA		
hart Area			hf CO ₂	-393.5	KJ/Kmol
			hf Liquid H ₂ O	-285.8	KJ/Kmol
			hf Gas	-241.8	KJ/Kmol
Assuming 1 Kmol of Methanol and Isoocatane have burnt			hf c ₈ H ₁₈	-259.2	KJ/Kmol
ENTALPY OF FORMATION OF THE REACTIONS			hf CH ₄ o	-201.5	KJ/Kmol
CH3OH + C8H18 + F (O2 + 3.76 N2) ----> n1 CO2 + n2 H2O(LIQUID) + n3 N2					
H2O as liquid					
Δh	ENTALPHTY REACTANTS		=(\$V\$34)+(\$V\$33)		
Δh	ENTALPHTY OF PRODUCTS		-6685.3 MJ/Kmol		
HIGHER HHV					
			6224.6 MJ	HEAT PRODUCED	
			42.55525 MJ/Kg	AT CONSTANT P	

Figure 7 Enthalpy calculation explanation

Assuming 1 Kmol of Methanol and Isoocatane have burnt		hf c ₈ H ₁₈	-259.2 KJ/Kmol
ENTALPY OF FORMATION OF THE REACTIONS		hf CH ₄ o	-201.5 KJ/Kmol
CH3OH + C8H18 + F (O2 + 3.76 N2) ----> n1 CO2 + n2 H2O(LIQUID) + n3 N2			
Chart Area			
H2O as liquid			
Δh	ENTALPHTY REACTANTS	-460.7 MJ/Kmol	
Δh	ENTALPHTY OF PRODUCTS	-6685.3 MJ/Kmol	
	HIGHER HHV	=ABS(\$T\$40)-ABS(\$T\$39)	DUCTED
		ABS(number) kg	AT CONSTANT P

Figure 8 HHV calculation explanation

The Enthalpy values from the technical tables were copied in the Excel file and from Figure 7 and Figure 8 it's visible the process used.

1.6.1 DIFFERENCES BETWEEN HIGHER AND LOWER HEATING VALUES

For the Isooctane-Methanol fuel mixture analysed, two different values of Hf, (Enthalpy of formation) were used, the "liquid" and the "gas" value to determine Higher and Lower heating value respectively. The heating value of any substances represents the total quantity of heat (energy) generated by the complete combustion of that substance with O₂.

HHV (higher) is higher because it considers also the "unproduced" (latent) heat of the vaporization of water, it basically assumes that all the water produced is liquid at the end of combustion.

LHV (lower) value is lower as it assumes that the water produced by the combustion is a gas and the energy (heat) is not restored.

1.7 MASS OF CO₂, H₂O AND N₂ PRODUCED

1Kmol of FUEL	ISO-OCTANE	C_8H_{18}		CO ₂	396.086	Kg
	and (plus)			CO ₂	396.086	Kg
	METHANOL	CH_4O		H ₂ O	198.169	Kg
				N ₂	1395.63	Kg

Figure 9 Mass of CO₂ H₂O and N₂ produced

In order to calculate the mass of CO₂ produced by the burning of the fuel can be calculated in two ways, either calculate the mass of CO₂ of Isooctane and Methanol separately first then add them together or calculate it from the blend balance equation, to check coefficients the calculation was done in both ways, showing the exact same result.

Example:

$$\begin{aligned}
 m \text{ of } Co_2 &= n_1 * Carbon(molar \text{ wheight}) * 1 + n_1 * Oxygen(mol. \text{ wheight}) * 2 \\
 &= 9 * (12.0107) + 9 * (15.9994) * 2 = 396.086 \text{ Kg}
 \end{aligned}$$

1.8 PROPERTIES OF AN “IDEAL” FUEL

An ideal fuel should definitely have an hight calorific value which means that when it burns it produces a lot of heat releasing a lot of energy. Analysing the environmental point of view, it shouldn't produce any dangerous and toxic gasses, causing minimum air pollution.

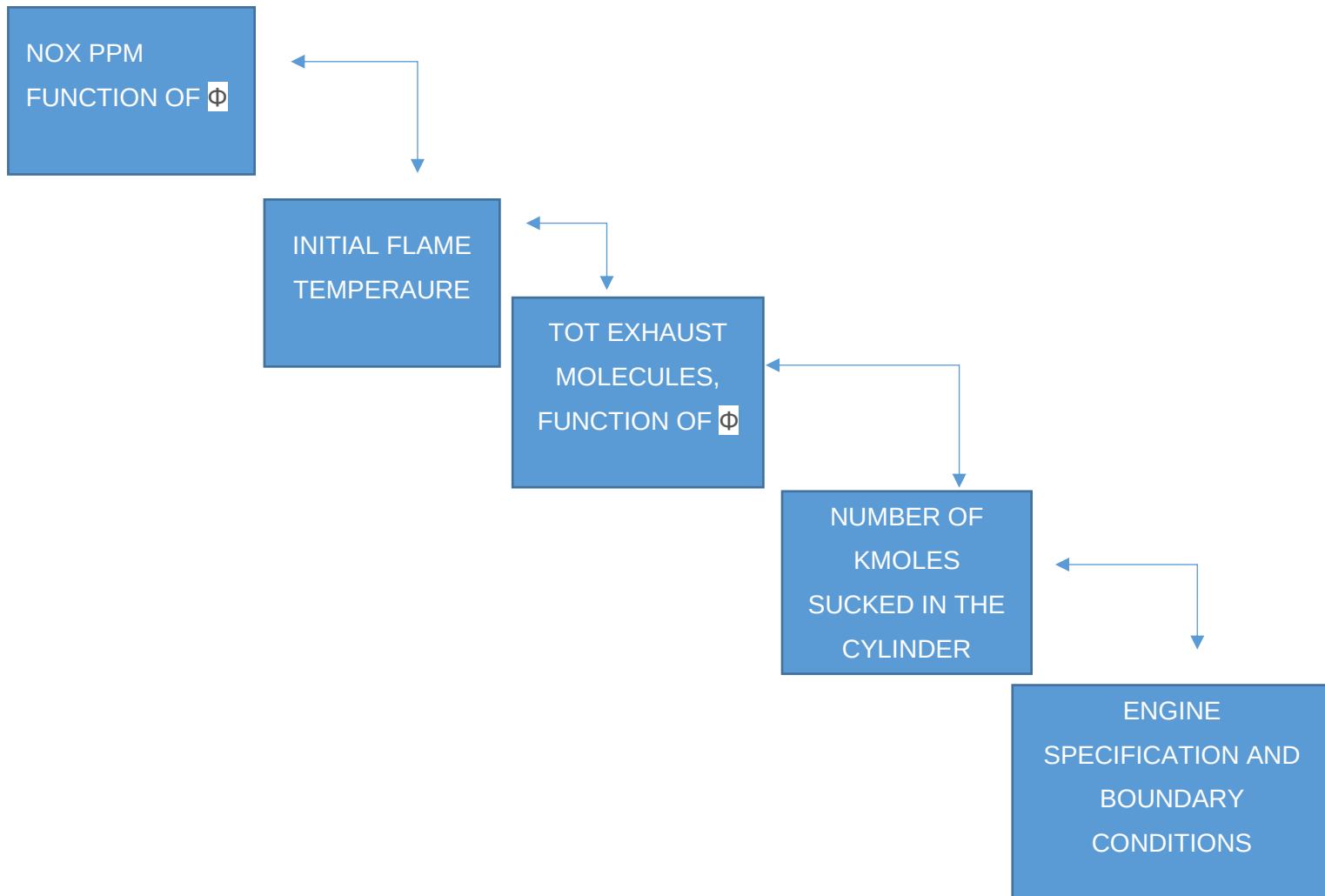
It should have an ideal ignition temperature, not low and not high. (Bishm, 2019)

The price of an Ideal fuel should be low it also should be easy to transport (R.K., 2018)

2 TASK2: ISOOCTANE NOX MODEL

2.1 WORK METHODOLOGY

Developing a NOX MODEL requires a very clear understanding of subject thus study and researches were done before start using Microsoft Excel, the following diagram was created to have a clear view of the correct process that has to be undertaken.



A first table containing all the engine characteristics and boundary conditions was created as follows:

2.2 ENGINE SPECIFICATIONS AND NUMBER OF KMOLS DRAWN IN

ENGINE Characteristics			
Displacement	1600	cm ³	
Clearance V.	40	cm ³	
N. Of cyl	4		
Vol eff	0.4		
P at inlet	1	Bar	
T at inlet	20	°C	
Gas Const. R	8314	J/(Kmol*K)	
Pol index	1.17		
RPM	1800	rpm	
	10800	°/sec	
n	6.57E-06	Kmols	
$P \cdot V = n \cdot R \cdot T$			
Alpha	1.09E-07	Kmols	
n	6.57E-06	Kmols	
number of Kmols sucked in the Cylinder			

Figure 10 Engine specifications and ambient conditions

Using the ideal gas Law, it was possible to achieve the second milestone of the process “Number of Kmoles sucked in the cylinder”. The “n” value is strictly directly proportional to the volumetric efficiency value, an increase of V.eff will determine and increase of the number of Kmoles drawn inside the cylinder. Here the mathematic relation:

$$n = \frac{P \cdot V \cdot \eta}{R \cdot T} \quad (7)$$

Where:

n: Number of Kmoles drawn inside the cylinder [Kmoles]

P: is the pressure at inlet section [Pa]

V: is the engine cylinder volume [m³]

η : Volumetric efficiency

R: Gas constant 8314 [J/(Kmol*K)]

T: Temperature at inlet section [K]

The second building step consisted on creating a table containing all the values of the coefficients (n1, n2..) and number of atoms related to PHI, representing 16 different balanced equations laid down horizontally as follows.

$\Phi(C_8H_{18}) + 12.5 (O_2 + 3.76 N_2) \rightarrow n_1 CO_2 + n_2 H_2O + n_3 O_2 + n_4 N_2$									
PHI DEPENDENT TABLE					n1	n2	n3	n4	
Carbon (x)	Hyrdrogen	Oxygen	F	Φ	CO2	H2O	O2	N2	
8	18	25	12.5	1		8	9	0	47
7.92	17.82	25	12.5	0.99		7.92	8.91	0.125	47
7.84	17.64	25	12.5	0.98		7.84	8.82	0.25	47
7.76	17.46	25	12.5	0.97		7.76	8.73	0.375	47
7.68	17.28	25	12.5	0.96		7.68	8.64	0.5	47
7.6	17.1	25	12.5	0.95		7.6	8.55	0.625	47
7.52	16.92	25	12.5	0.94		7.52	8.46	0.75	47
7.44	16.74	25	12.5	0.93		7.44	8.37	0.875	47
7.36	16.56	25	12.5	0.92		7.36	8.28	1	47
7.28	16.38	25	12.5	0.91		7.28	8.19	1.125	47
7.2	16.2	25	12.5	0.9		7.2	8.1	1.25	47
6.8	15.3	25	12.5	0.85		6.8	7.65	1.875	47
6.4	14.4	25	12.5	0.8		6.4	7.2	2.5	47
6	13.5	25	12.5	0.75		6	6.75	3.125	47
5.6	12.6	25	12.5	0.7		5.6	6.3	3.75	47
5.2	11.7	25	12.5	0.65		5.2	5.85	4.375	47
4.8	10.8	25	12.5	0.6		4.8	5.4	5	47

Figure 11 PHI dependent table

The Figure 11 table was then updated calculating actual number of Kmols (α), the concentration of N2 and O2 in the mixture and the total amount of exhaust Kmols.

$$\alpha = \frac{n}{\varphi + 12.5 * (1 + 3.76)} \quad (8)$$

$$[O_2] = \frac{n_3 * (\alpha)}{C. vol} \quad (9)$$

$$[N_2] = \frac{n_4 * (\alpha)}{C. vol} \quad (10)$$

$$TOT. Ex. (kmols) = \alpha * (n_1 + n_2 + n_3 + n_4) \quad (11)$$

Where:

n3, n4: balance coefficient relative to Oxygen and Nitrogen respectively.

C.Vol: Clearence volume [m³].

α : actual number of Kmoles drawn in.

n: theroretical number of Kmoles drawn in.

n1	n2	n3	n4				TOT EXH KMOLS
CO2	H2O	O2	N2	alpha	[N2] CONC	[O2] CONC	
8	9	0	47	1.08564E-07	0.127563	0	=S8*(O8+P8+Q8+R8)
7.92	8.91	0.125	47	1.08582E-07	0.1275841	0.000339319	6.94438E-06
7.84	8.82	0.25	47	1.086E-07	0.1276052	0.000678751	6.94064E-06
7.76	8.73	0.375	47	1.08618E-07	0.1276263	0.001018295	6.9369E-06
7.68	8.64	0.5	47	1.08636E-07	0.1276474	0.001357951	6.93316E-06
7.6	8.55	0.625	47	1.08654E-07	0.1276685	0.00169772	6.92941E-06
7.52	8.46	0.75	47	1.08672E-07	0.1276897	0.002037601	6.92567E-06
7.44	8.37	0.875	47	1.0869E-07	0.1277108	0.002377595	6.92193E-06
7.36	8.28	1	47	1.08708E-07	0.1277319	0.002717701	6.91818E-06
7.28	8.19	1.125	47	1.08726E-07	0.1277531	0.003057919	6.91443E-06
7.2	8.1	1.25	47	1.08744E-07	0.1277742	0.003398251	6.91068E-06
6.8	7.65	1.875	47	1.08834E-07	0.1278801	0.005101599	6.89192E-06
6.4	7.2	2.5	47	1.08924E-07	0.1279861	0.006807773	6.87313E-06
6	6.75	3.125	47	1.09015E-07	0.1280923	0.008516778	6.8543E-06
5.6	6.3	3.75	47	1.09105E-07	0.1281987	0.010228622	6.83545E-06
5.2	5.85	4.375	47	1.09196E-07	0.1283053	0.011943312	6.81656E-06
4.8	5.4	5	47	1.09287E-07	0.128412	0.013660855	6.79764E-06

Figure 12 Alpha, N2 and O2 concentration and Tot exhaust Kmols data

2.3 ENTHALPHY AND FLAME TEMPERATURE

The NO_x production is strictly dependent on the combustion temperature inside the combustion chamber, thus it was necessary to find a mathematical relation able to predict the flame temperature and heat produced with combustion, knowing that the Enthalpy released with the reaction is equal to the amount of Heat produced (equation 5, Page 9) it was able to calculate the exact value of enthalpy for all the PHIs value studied. The enthalpy calculation was done in the same way used for task 1 obeying equation 6 (Page 10) considering water as a gas, here an example of the calculation:

	n1	n2	n3	n4				TOT EXH KMOLS	ENTHALPY REFERENCE	
Φ	CO2	H2O	O2	N2	alpha	[N2] CONC	[O2] CONC			
12.5	1	8	9	0	47	1.08564E-07	0.127563	0	6.94811E-06	= (O8*(ABS(\$C\$31)))+(P8*ABS(\$C\$33))-ABS(\$C\$34*M8)
12.5	0.99	7.92	8.91	0.125	47	1.08582E-07	0.1275841	0.000339319	6.94438E-06	5014.3500 2375.452292 2375.436338
12.5	0.98	7.84	8.82	0.25	47	1.086E-07	0.1276052	0.000678751	6.94064E-06	4963.7000 2359.912729

hf CO ₂	-393.5	KJ/Kmol
hf Liquid H ₂ O	-285.8	KJ/Kmol
hf Gas	-241.8	KJ/Kmol
hf c ₈ H ₁₈	-259.2	KJ/Kmol
hf CH ₄ O	-201.5	KJ/Kmol

Once the enthalpy reference was found two different calculation ways were tried to find the correct value of flame temperature, both two methods are correct however just one was used at the end as it was quicker and more effective.

The first method tried consisted in copying in the Excel file the enthalpy tables values of CO₂, O₂, N₂ and H₂O then a table called “SUM OF ENTHALPIES OF ALL COMPONENTS” was created.

Figure 13 Sum enthalpies of all components table

Figure 14 Enthalpy range example

VALUE BELOW: 4952.93 MJ

ENTHALPY REFERENCE					Φ	1	2			
WJ		FLAME TEMP [K]	POLYNOMIAL EN	Temp T1 (FLAME		1 ENTHALPY RANGE	TEMP RANGE			
5065.0000	2390.913209	2390.903961	5065.000336	2390.913209						
5014.3500	2375.452292	2375.436338	5014.350002	2375.452292		=SMALL(Ent_tables!AE3:AE70;COUNTIF(Ent_tables!AE3:AE70;"<"&values_PHI_dependent!\$W\$8))+0.1				
4963.7000		2359.912729	4936.700025	2350.022655		=SMALL(array_k)	2400			

=SMALL(Ent tables!AE3:AE70;COUNTIF(Ent tables!AE3:AE70;"<"&values PHI dependent!W8)+1)

VALUE ABOVE:

=SMALL(Ent_tables!AE3:AE70;COUNTIF(Ent_tables!AE3:AE70;"<"&values_PHI_dependent!W8)+1)

With the enthalpy range automatized, using a VLOOKUP function also the temperature range, which is related to the enthalpies values range, was obtained.

	Φ	1	2					
Temp T1 (FLAME	1 ENTALP RANGE	TEMP RANGE						
=VLOOKUP(A9;Ent_tables!AE3:AF70;COLUMN(Ent_tables!AF3:AF70)-COLUMN(Ent_tables!AE3:AF70)+1;0)								
2350.022655	5089.922	COLUMN([reference])						

Using the following linear interpolation formula, it was possible determine the temperature related to the enthalpy reference (5065.0 MJ)

$$\frac{T - 2350}{2400 - 2350} = \frac{5065 - 4952.92}{5089.92 - 4952.92}$$

$$T = \frac{(5065 - 4952.92)}{(5089.92 - 4952.92)} * (2400 - 2350) + 2350 = 2390.903K$$

As the value of PHI changes even the enthalpy reference values change thus 13 “SUM OF ENTHALPIES OF ALL COMPONENTS” tables were needed, and many equations were required making the calculation too long. It was then necessary to find a quicker method.

SECOND METHOD:

Using the standard enthalpy tables of CO₂, O₂, N₂ and H₂O, the following graph for each element was plotted, it represents the relation between temperature and enthalpy.

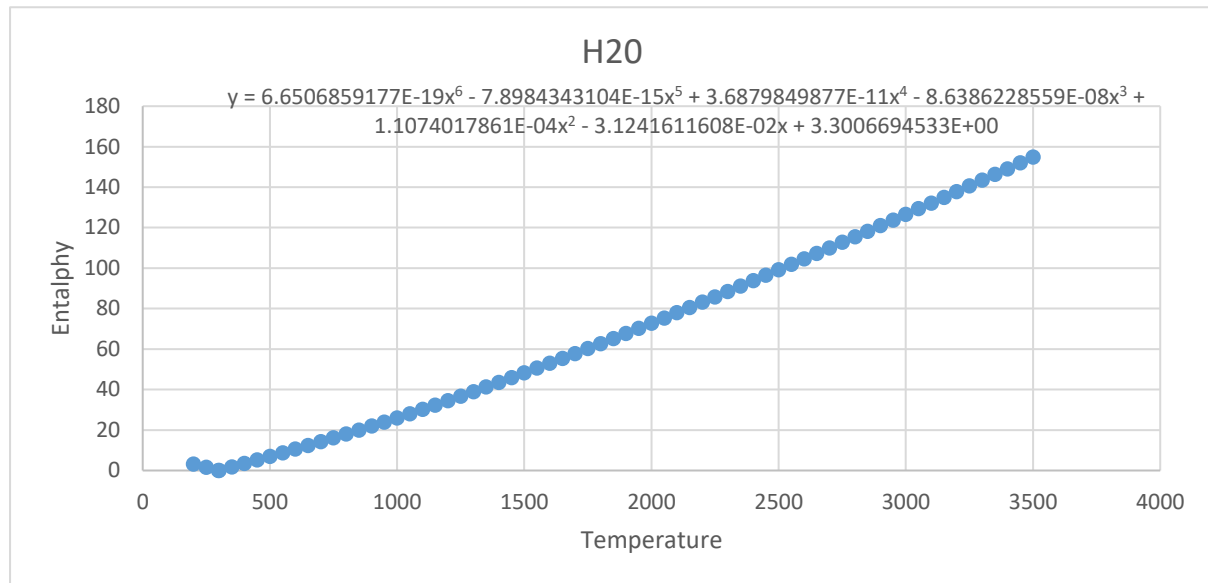


Figure 15 H₂O Temperature-Enthalpy graph

Using Excel, a 6th degree Polynomial function (*sextic equation*) was obtained for each element, knowing that the flame temperature is when the following relation happens,

$$= 8\phi * (\text{Polyeq. CO}_2) + 9\phi * (\text{Polyeq. H}_2\text{O}) + F(1 - \phi) * (\text{Polyeq. O}_2) + 47(\text{Polyeq. N}_2)$$

the relation was expressed in Excel as follows:

	2ND METHOD		1	2
	POLYNOMIAL ENT	Temp T1 (FLAME	1 ENTALP RANGE	TEMP RANGE
1	5065.000336	2390.913209	RANGE	
8	5014.350002	2375.452292	4952.928048	2350.00
9	$=8*M11*((((8.5770134353*10^{-19})*(AA11^6))-((1.0374875556*10^{-14})*(AA11^5))+((4.9689475953*10^{-11})*(AA11^4))-((1.2019118054*10^{-7})*(AA11^3))+((1.5650954893*10^{-4})*(AA11^2))-((4.8239362033*10^{-2})*(AA11))+5.2084519626))+9*M11*((((6.6506859177*10^{-19})*(AA11^6))-((7.8984343104*10^{-15})*(AA11^5))+((3.6879849877*10^{-11})*(AA11^4))-((8.6386228559*10^{-8})*(AA11^3))+((1.1074017861*10^{-4})*(AA11^2))-((3.1241611608*10^{-2})*(AA11))+3.3006694533))+L11*(1-M11)*(((6.4958291549*10^{-19})*(AA11^6))-((7.8224528491*10^{-15})*(AA11^5))+((3.7120417697*10^{-11})*(AA11^4))-((8.798317617*10^{-8})*(AA11^3))+((1.0982327235*10^{-4})*(AA11^2))-((3.2606444641*10^{-2})*(AA11))+3.5786489003))+47*(((5.9376621671*10^{-19})*(AA11^6))-((7.1020711589*10^{-15})*(AA11^5))+((3.3460896805*10^{-11})*(AA11^4))-((7.8909601634*10^{-8})*(AA11^3))+((9.8599769212*10^{-5})*(AA11^2))-((2.8172899156*10^{-2})*(AA11))+3.05378908))))))$			

Figure 16 Polynomial relation expressed in excel format

It was then necessary to assign the values of “X” of the polynomial to a specific cell (AA11 in the example above), this cell represents the flame temperature. Using the “Goal Seek

function” it was possible to assign the enthalpy reference value finding the exact value of temperature related to).

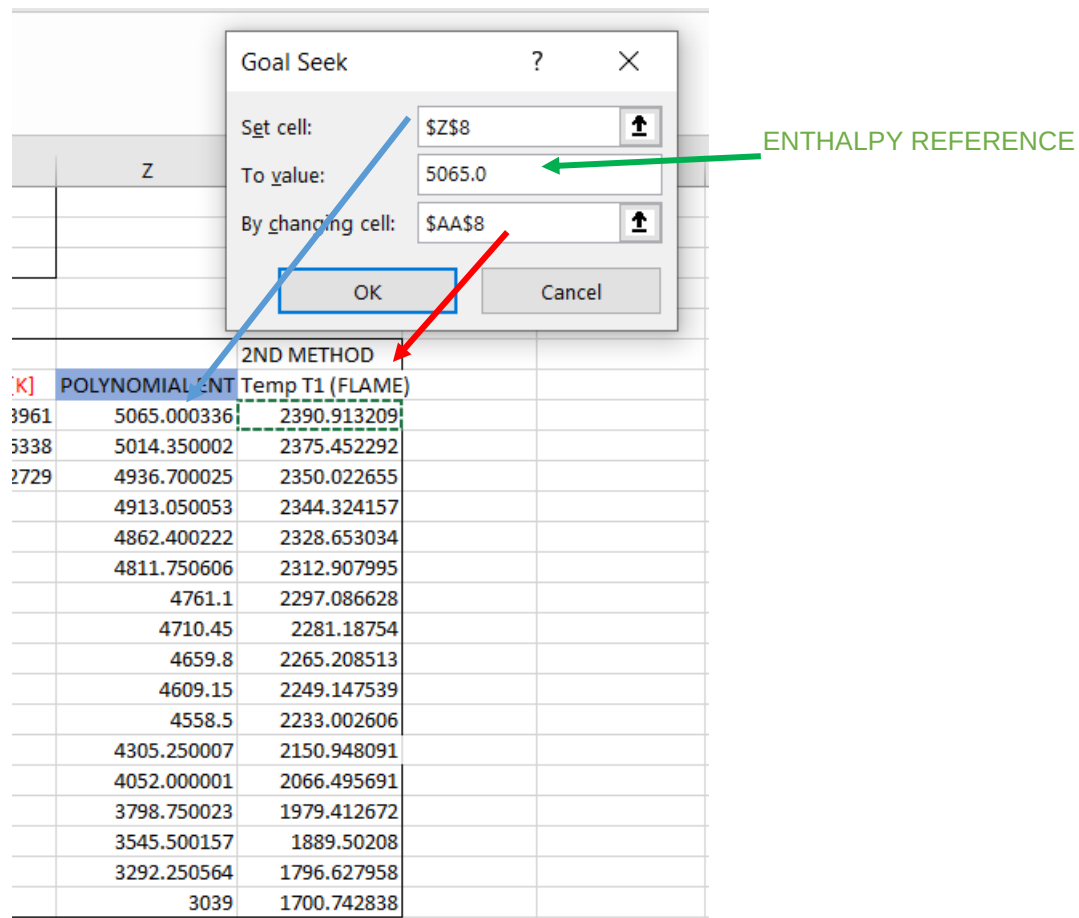


Figure 17 Goal seek method

2.4 FIRST METHOD VS 2ND METHOD RESULTS

1 METHOD		2ND METHOD
FLAME TEMP [K]	POLYNOMIAL ENT	FLAME TEMP [K]
2390.903961	5065.000336	2390.913209
2375.436338	5014.350002	2375.452292
2359.912729	4963.699996	2359.923274
	4913.050053	2344.324157
	4862.400222	2328.653034
	4811.750606	2312.907995
	4761.1	2297.086628
	4710.45	2281.18754
	4659.8	2265.208513
	4609.15	2249.147539
	4558.5	2233.002606
	4305.250007	2150.948091
	4052.000001	2066.495691
	3798.750023	1979.412672
	3545.500157	1889.50208
	3292.250564	1796.627958
	3039	1700.742838

Figure 18 First method vs second (goal seek) method

It's visible from Figure 18 that the two methods give almost the same result, however the Goal seek Method is the most effective one so it was used to calculate all the 13th temperatures.

2.5 BURN ZONE TEMPERATURE AND NOX ZELDOVICH MODEL

The 13th temperatures calculated represents the initial temperature of the combustion process, due to the increase of pressure the temperature rise it was calculated with the following relation:

$$T2 = T1 * \left(\frac{P2}{P1}\right)^{[(n-1)/n]} \quad (12)$$

Once calculated the burn zone temperatures the Zeldovich model was applied using the [N2] and [O2] concentration calculated previously.

Zeldovich Model Formula used:

$$\frac{d[NO]}{dt} = 4.17 * 10^{13} * [N2] * [O2]^{(1/2)} * e^{(-67837/T)} \quad (13)$$

POL INDEX	1.17							
INDICE AT	0.145299	phi 1		phi 0.99		phi 0.98		
deg	PRESSURE	TEMP [K]	NOX [Kmol/°]	TEMP [K]	NOX [Kmol/°]	TEMP [K]	NOX [Kmol/°]	TEMP [K]
0	10			2375.452292	1.43716E-10	2359.923274	1.685E-10	
1	12	$=0.29 \cdot (N_{30}/N_{29})^{0.27}$		2439.221728	3.03211E-10	2423.275831	3.572E-10	
2	14	2510.707328	0	2494.471758	5.61387E-10	2478.164676	6.64E-10	
3	16	2559.895698	0	2543.34205	9.4668E-10	2526.715488	1.124E-09	
4	18	2604.082195	0	2587.242814	1.48853E-09	2570.329261	1.772E-09	
5	20	2644.254259	0	2627.155104	2.21693E-09	2609.980632	2.646E-09	
6	22	2681.127914	0	2663.790314	3.16214E-09	2646.376348	3.783E-09	
7	24	2715.239731	0	2697.681546	4.35439E-09	2680.046023	5.22E-09	
8	26	2747.002687	0	2729.239106	5.82376E-09	2711.397281	6.995E-09	
9	28	2776.741756	0	2758.785867	7.60003E-09	2740.750886	9.145E-09	
10	30	2804.717485	0	2786.580689	9.71256E-09	2768.364006	1.171E-08	
11	32	2831.142123	0	2812.834452	1.21903E-08	2794.446141	1.471E-08	
12	34	2856.190983	0	2837.721333	1.50615E-08	2819.170329	1.82E-08	
13	36	2880.010621	0	2861.386939	1.83542E-08	2842.681226	2.221E-08	
14	38	2902.72486	0	2883.954297	2.20955E-08	2865.101055	2.677E-08	
16	40	2924.439314	0	2905.528333	2.63122E-08	2886.534055	3.192E-08	

Figure 19 Burn zone temperature and NOX values in relation to PHI

NOX prediction results were calculated for all the 13th cases analysed, producing then final results in PPM (part per million) and the following graph.

PHI	NOX SUM	TOT EXH MOL [Kmol]	PPM
	[Kmol/cycle]	[Kmol]	Parts per million
1	0	6.94811E-06	0
0.99	1.30327E-07	6.94438E-06	18767.26909
0.98	1.57403E-07	6.94064E-06	22678.48453
0.97	1.64176E-07	6.9369E-06	23666.99634
0.96	1.60981E-07	6.93316E-06	23218.93843
0.95	1.5238E-07	6.92941E-06	21990.38755
0.94	1.40891E-07	6.92567E-06	20343.23634
0.93	1.28037E-07	6.92193E-06	18497.34548
0.92	1.14785E-07	6.91818E-06	16591.80259
0.91	1.01751E-07	6.91443E-06	14715.74168
0.9	8.9324E-08	6.91068E-06	12925.49734
0.85	4.13972E-08	6.89192E-06	6006.623566
0.8	1.62335E-08	6.87313E-06	2361.875985
0.75	2.85456E-09	6.8543E-06	416.4624766
0.7	1.51653E-09	6.83545E-06	221.8622728
0.65	3.47273E-10	6.81656E-06	50.94547721
0.6	6.27673E-11	6.79764E-06	9.233687957

Figure 20 NOX results in PPM at each phi

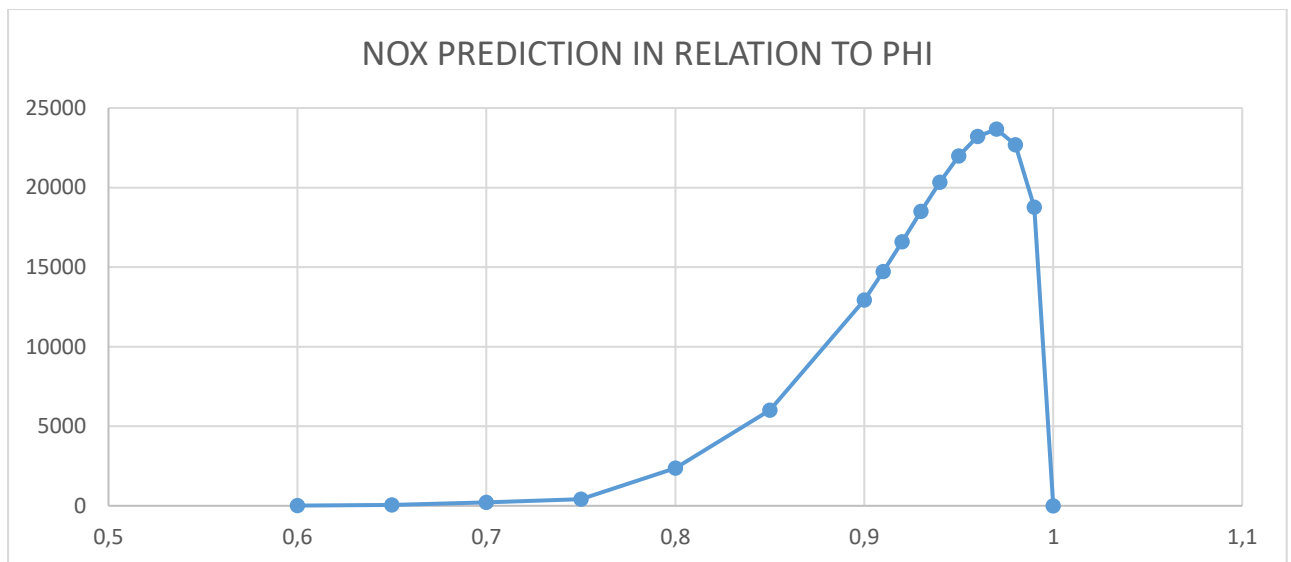


Figure 21 NOX PPM as a function to PHI

2.6 ANALYSIS

In order to fully understand the results obtained from Figure 21, further analysis was carried out, plotting the following graphs:

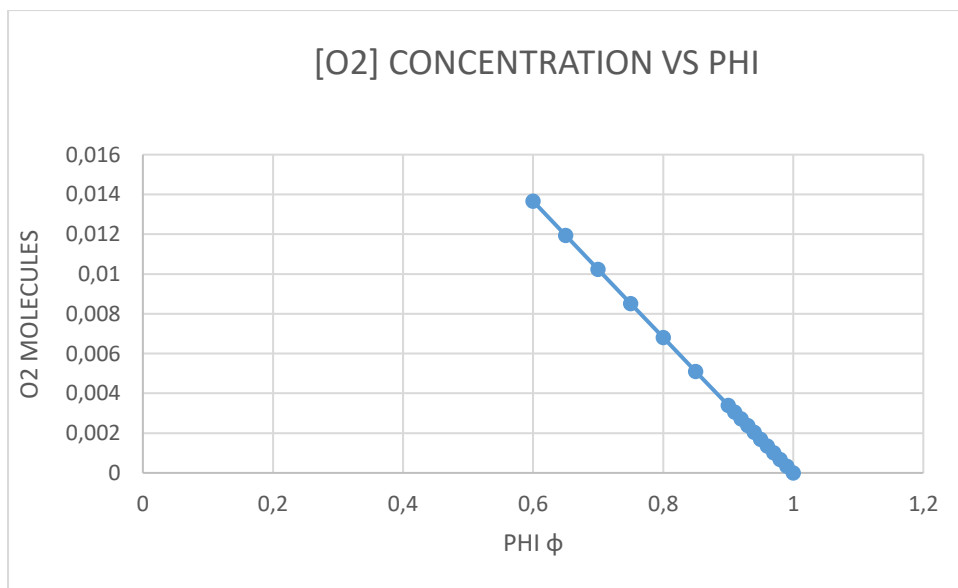


Figure 22 O2 concentration molecules

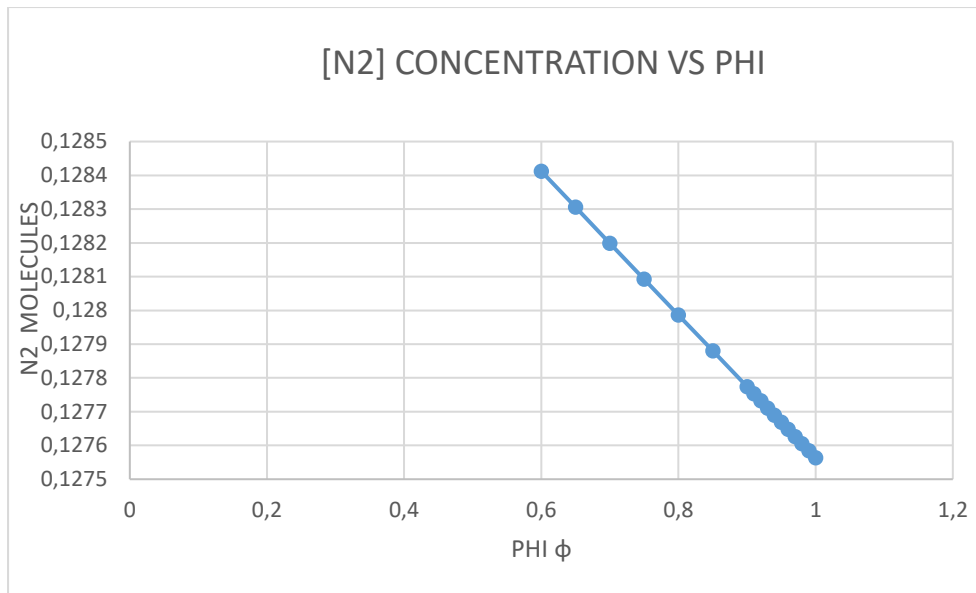


Figure 23 N2 concentration molecules

Figure 22 and Figure 23 show that the concentrations of Oxygen and Nitrogen increase as the fuel equivalence ratio ϕ decreases, which means that leaner is the mixture used (less fuel more air), bigger will be the O₂ and N₂ concentrations.

An important analysis was done also on the trend of the burn zone temperatures in relation to ϕ and the pressure increase.

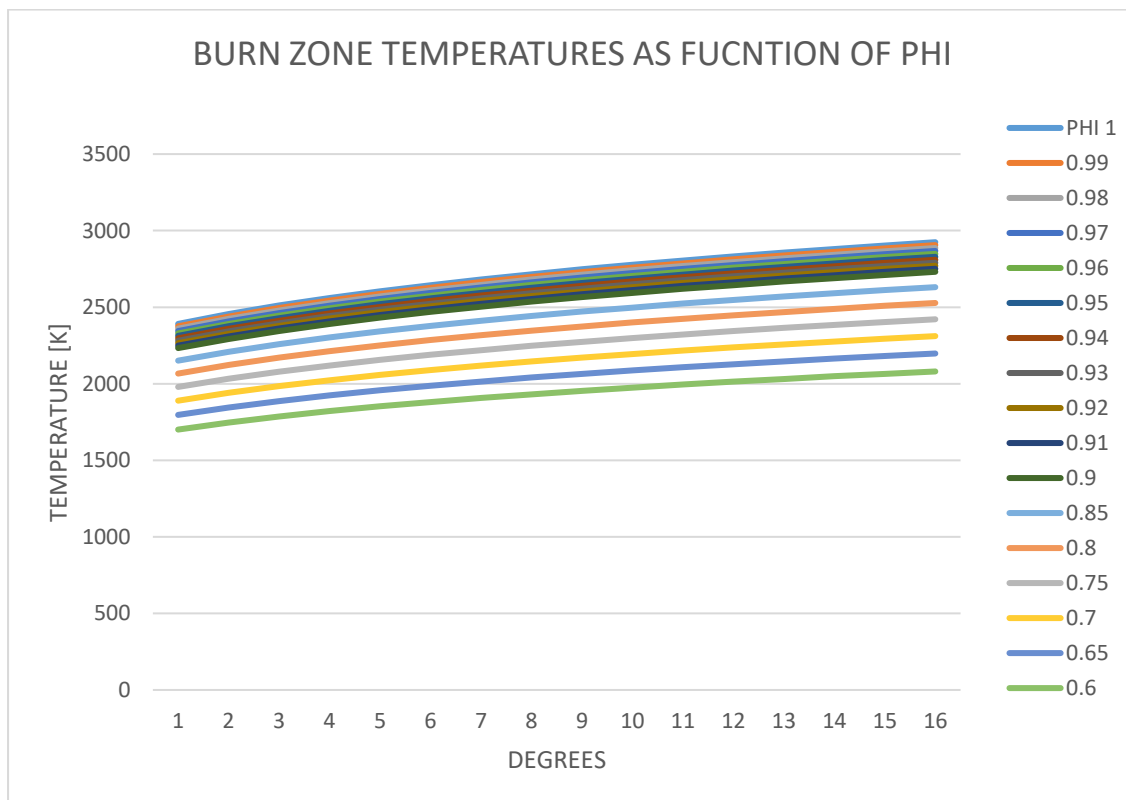


Figure 24 Burn zone temperatures as function of phi and δP

It's clearly visible from the above graph that leaner is the mixture lower is be the burn zone temperature, this due to the fact that there is less heat produced by the combustion process (less enthalpy released) also the biggest burn zone temperatures verifies in stoichiometric conditions.

Although there is a different starting temperature for each PHI all temperatures rise with the same gradient as they follow the same "law" explained previously (section 2.5 Pag 21).

2.7 ZELDOVICH MATHEMATICAL ANALYSIS

Looking to the Zeldovich model formula is visible that the rate of NOx produced is dependent on [N2] and [O2] concentrations but it's also depends on the exponent of the " $e^{(-67837/T)}$ " term. A mathematical analysis was carried out to see how the burn zone temperature value affects the term and obviously the value of NOx.

Bigger the burn zone temperature, bigger will be the result of the term, smaller the temperature smaller will be the value of the term and lower the relative NOx result. This is due to the fact that being the numerator negative a bigger denominator will determine a bigger elevation number.

Here an example:

$\phi:0.6$ Temperature= 2080.259 [K] @ P=40 [Bar]

$\phi:0.97$ Temperature= 2867.45 [K] @ P=40 [Bar]

$$e^{(-67837/2080.259)} = e^{(-32.61)} = 1.266 * 10^{-14}$$

$$e^{(-67837/2867.45)} = e^{(-23.65)} = 1.02 * 10^{-10}$$

At PHI 0.97 the burn zone temperature is not the highest as explained with Figure 24 but it's still high with the combination of nitrogen an oxygen values it leads to the highest NOx production rate.

3.2 RESULTS AND ANALYSIS

		POLYNOMIAL
Temp T1 (FLAME)	FOR GOAL SEEK	
2258.050738	4913.05	5% EGR
	0	
2179.016998	4913.05	10% EGR
	0	
2106.212909	4913.05	15% EGR
	0	
2038.845528	4913.05	20% EGR

Figure 26 Flame temperatures table

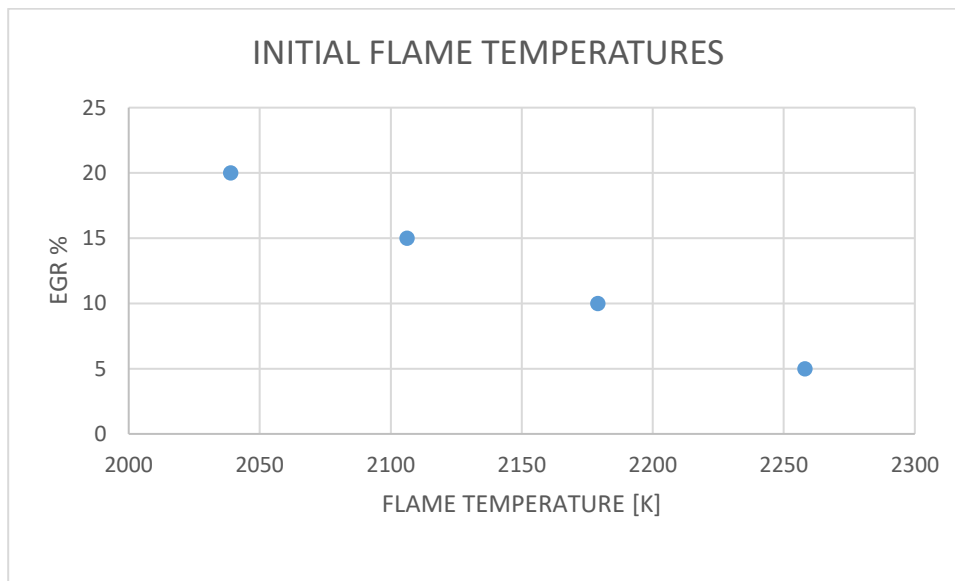


Figure 27 Flame temperature trend with EGR%

POL INDEX	1.17				POL INDEX	1.17			
INDICE AT POW	0.145299145	phi0.97 (5%EGR)			INDICE AT	0.145299145	phi0.97 (10%EGR)		
deg	PRESSURE[bar]	TEMP [K]	NOX [Kmol/°]		deg	PRESSURE[bar]	TEMP [K]	NOX [Kmol/°]	
0	10	2258.050738	6.07065E-11		0	10	2179.016998	2.04178E-11	
1	12	2318.668509	1.33147E-10		1	12	2237.513094	4.60763E-11	
2	14	2371.187926	2.54542E-10		2	14	2288.194286	9.01805E-11	
3	16	2417.64291	4.41063E-10		3	16	2333.023305	1.59409E-10	
4	18	2459.373975	7.10024E-10		4	18	2373.293746	2.61087E-10	
5	20	2497.313687	1.0796E-09		5	20	2409.905535	4.03065E-10	
6	22	2532.138282	1.56859E-09		6	22	2443.511239	5.93618E-10	
7	24	2564.354513	2.19624E-09		7	24	2474.599874	8.41355E-10	
8	26	2594.352409	2.9821E-09		8	26	2503.547818	1.15515E-09	
9	28	2622.438886	3.94589E-09		9	28	2530.651243	1.54409E-09	
10	30	2648.86001	5.10742E-09		10	30	2556.147605	2.01741E-09	
11	32	2673.816238	6.48652E-09		11	32	2580.230343	2.58446E-09	
12	34	2697.473138	8.10296E-09		12	34	2603.059232	3.25466E-09	
13	36	2719.969124	9.9764E-09		13	36	2624.767839	4.0375E-09	
14	38	2741.421139	1.21264E-08		14	38	2645.469014	4.94248E-09	
16	40	2761.928926	1.45723E-08		16	40	2665.25901	5.97909E-09	

Figure 28 burn zone temperatures at 5%-10% EGR

POL INDEX	1.17				POL INDEX	1.17			
INDICE AT POW	0.145299145	phi0.97 (15%EGR)			INDICE AT	0.145299145	phi0.97 (20%EGR)		
deg	PRESSURE[bar]	TEMP [K]	NOX [Kmol/°]		deg	PRESSURE[bar]	TEMP [K]	NOX [Kmol/°]	
0	10	2106.212909	6.96077E-12		0	10	2038.845528	2.40145E-12	
1	12	2162.754566	1.61564E-11		1	12	2093.578696	5.73119E-12	
2	14	2211.742427	3.23638E-11		2	14	2140.999676	1.17471E-11	
3	16	2255.073644	5.8346E-11		3	16	2182.944941	2.15942E-11	
4	18	2293.998592	9.72053E-11		4	18	2220.624871	3.65882E-11	
5	20	2329.387128	1.52335E-10		5	20	2254.881502	5.81966E-11	
6	22	2361.870018	2.27375E-10		6	22	2286.325424	8.80214E-11	
7	24	2391.919937	3.26175E-10		7	24	2315.414194	1.27783E-10	
8	26	2419.900688	4.52762E-10		8	26	2342.499979	1.79308E-10	
9	28	2446.098549	6.11308E-10		9	28	2367.859899	2.4451E-10	
10	30	2470.743041	8.06111E-10		10	30	2391.716135	3.25388E-10	
11	32	2494.02114	1.04157E-09		11	32	2414.249683	4.24007E-10	
12	34	2516.087283	1.32217E-09		12	34	2435.610038	5.42493E-10	
13	36	2537.070574	1.65245E-09		13	36	2455.922177	6.83025E-10	
14	38	2557.080093	2.03703E-09		14	38	2475.291691	8.47826E-10	
16	40	2576.208877	2.48054E-09		16	40	2493.808639	1.03916E-09	

Figure 29 figure 22 burn zone temperatures at 15%-20% EGR

EGR RESULTS				
PHI 0.97	NOX TOTAL	TOT-EXH MOL	PPM	% DROP
0% EGR	1.6418E-07	6.9369E-06	23666.99634	0
5% EGR	6.9744E-08	7.28374E-06	9575.28295	59.5416
10% EGR	2.793E-08	7.63059E-06	3660.276967	84.5343
15% EGR	1.1321E-08	7.97743E-06	1419.110567	94.0038
20% EGR	4.6378E-09	8.32428E-06	557.1390144	97.6459

Figure 30 EGR effect results

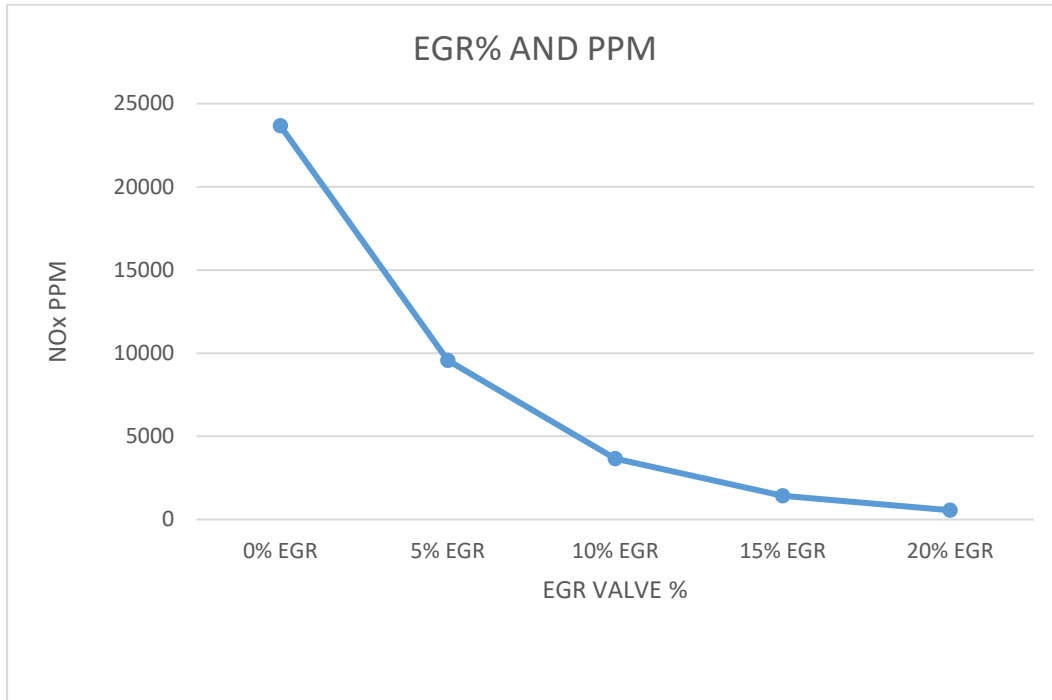


Figure 31 EGR effect on NOx PPM

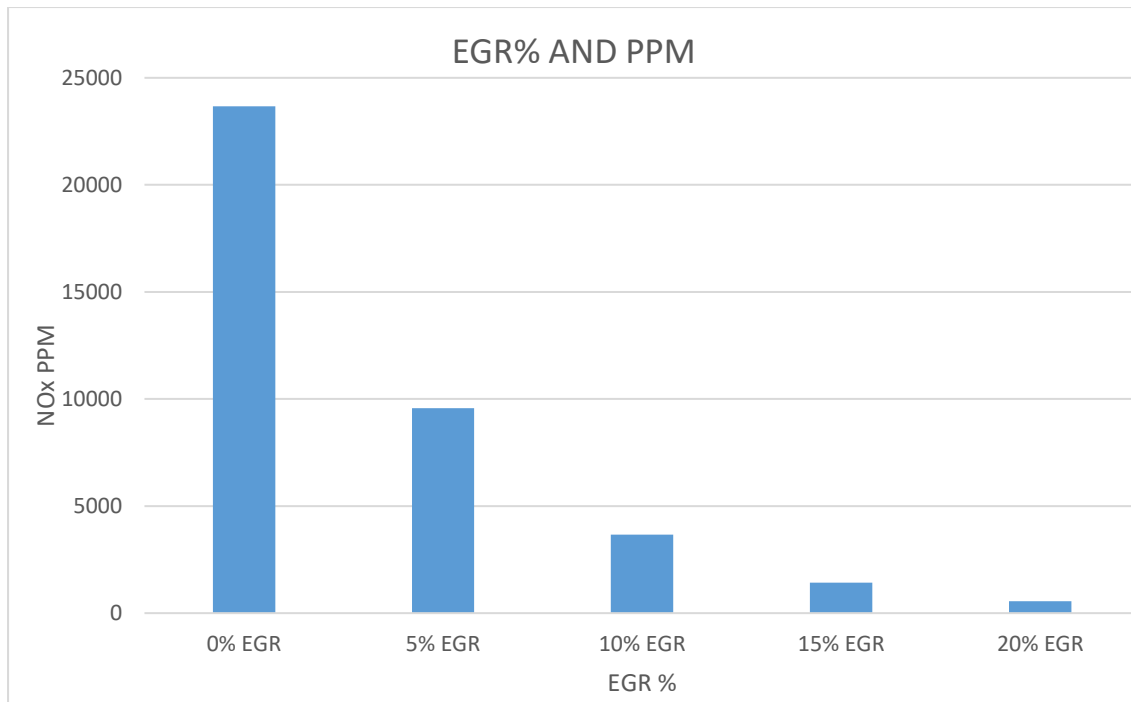


Figure 32 EGR effect on NOx PPM

2 + 3.76 N2)+EGR%*(n1co2+n2H2O+n3O2+n4N2) → (1+EGR%)*(n1 CO2 + n2 H2O + n3 O2 + n4 N2)										
n1 CO2	n2 H2O	n3 O2	n4 N2	alpha	[N2] CONC	[O2] CONC	ENTHALPY REFERENCE	TOT EX MOLECU	Temp T1 (FLAM	POLYNOMIAL
8.15	9.17	0.39	49.35	1.09E-07	0.1340076	0.0010692	4913.0500	7.28374E-06	2258.050738	=(H9*SR\$17)+(I9*SR\$18)+(J9*SR\$19)+(K9*SR\$20)
8.54	9.60	0.41	51.70	1.09E-07	0.1403889	0.0011201	4913.0500	7.63059E-06	2179.016998	4913.05 10% EGR
8.92	10.04	0.43	54.05	1.09E-07	0.1467703	0.001171	4913.0500	7.97743E-06	2106.212909	4913.05 15% EGR
9.31	10.48	0.45	56.40	1.09E-07	0.1531516	0.001222	4913.0500	8.32428E-06	2038.845528	4913.05 20% EGR
CONSTANT								POLY CO2	106.9482356	5% EGR
								POLY H2O	86.08314748	
								POLY O2	68.87985801	
								POLY N2	65.35832127	
IE)	1.17									
AT	0.145299145	phi0.97 (10%EGR)								

Figure 33 Polynomial formula example

It's visible from Figure 33 how the polynomial equation was applied to the model, as the balance coefficients (n1, n2, n3, n4) varies with different EGR working percentage also the polynomial equation changes.

From Figure 27 is visible that as EGR percentage increases the initial flame temperature decreases, this drop obviously affect the burn zone temperatures and the NOx PPM which decreases drastically.

EGR RESULTS					
PHI 0.97	NOX TOTAL	TOT-EXH MOL	PPM	% DROP	EGR MAGNITUDE EFFECT
0% EGR	1.6418E-07	6.9369E-06	23666.99634	0	0
5% EGR	6.9744E-08	7.28374E-06	9575.28295	59.5416	59.54162154
10% EGR	2.793E-08	7.63059E-06	3660.276967	84.5343	24.99263488
15% EGR	1.1321E-08	7.97743E-06	1419.110567	94.0038	9.469585273
20% EGR	4.6378E-09	8.32428E-06	557.1390144	97.6459	3.642082586

Figure 34 EGR results summary

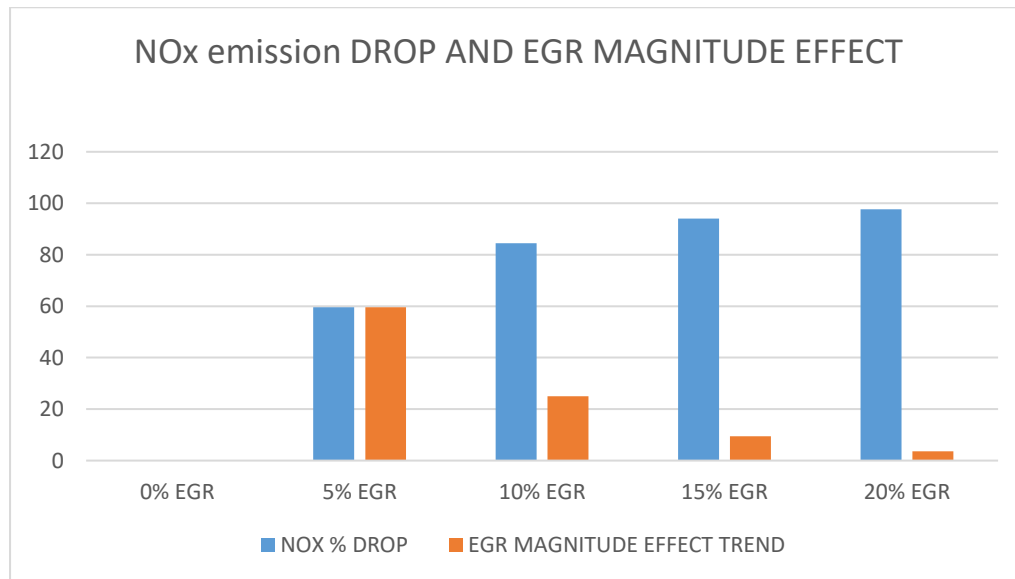


Figure 35 EGR effect analysis

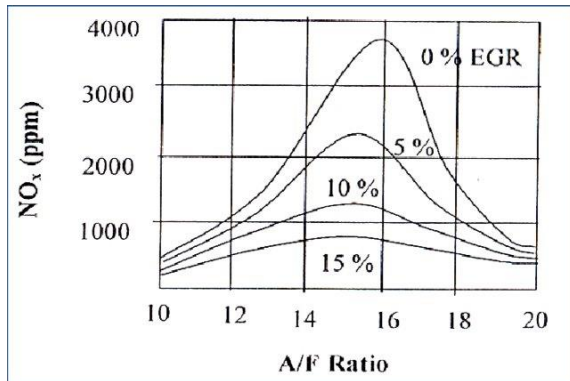
Analysing more in depth the results obtained using the above table and graph, it's understandable that the NOx PPM, (emission) drops heavily(59.5%) from "NO EGR" to 5% EGR, the decrease continues until 20% but the EGR EFFECT has a lighter impact on the NOx PPM (look at the EGR MAGNITUDE EFFECT).

4 EXTRA RESEARCH

Once the analysis was done further research on EGR effect on NOx production rate in order to see if the results obtained from the model created were similar to someone else job.

The following picture represents a study carried out by the Institute of Engineering & Technology, Tumkur- Karnataka on the EGR EFFECT on NOX formation.

Even if the engine studied has different specifications and working load it's visible that even in this study EGR valve has a stronger effect from 0% EGR TO 5% EGR, the effect continues at 10% and 15% decreasing NOx PPM but with a lighter effect.



(Srinath, 2013)

Figure 36 EGR effect study by the Institute of Engineering & Technology, Tumkur- Karnataka

5 FURTHER WORK AND CONCLUSION

Once finished the analysis several research was done to see how reliable and valid was the emission calculator done with Excel, few interesting NOx data data were found, the problem was that the simulation created is very far from simulating a real engine, all the information found are related on a "real engine cycle" in order to compere the data calculated it would be necessary to convert the model adapting the model to cylinder pressure and temperature, however it has been demonstrated that adding an EGR can effective reduce chamber temperature and the NOX emission.

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