

University of Wales Trinity Saint David

School of Engineering

Powertrain & Sustainability

M6X01206

Zhangwei Guo

1805078

04/01/2020

Contents

1	Introduction	1
2	Task One-Mixture of Isooctane and Methanol.....	2
2.1	Task One (a) – Mass Percentages.....	3
2.2	Task One (b) – Air: Fuel Mass Ratio	4
2.3	Task One (c) – Lower Heating Value	5
2.4	Task One (d) – Enthalpy of Formation	7
2.5	Task One (e) – Difference Between Higher and Lower Heating Value	8
2.6	Task One (f) – Mass of CO ₂ Produced.....	9
2.7	Task One (g) – Properties of ‘Ideal ‘ Fuel.....	10
3	Task Two – NO _x Model for Isooctane Running on the Lean Side of Stoichiometric	11
3.1	Task Two (a) - Graph of NO _x PPM	12
3.2	Task Two (b) – Effect of Adding EGR.....	17
4	Reference.....	20

1 Introduction

In order to deepen the understanding and mastery of the knowledge learned in the course, the author tried his best to finish this report. A huge of calculations through formula and excel have been done related to the combustion and emission of engine. Several analysis from the author has been included as well. All of the calculations have been divided into two main parts. (Williams, Assignment Specification, 2020). The other one asks the author demonstrates subject specific skills of the combustion and emissions mechanism for conventional and bio-fuels used in SI and CI automotive applications. (Williams, Assignment Specification, 2020)

For the first part, all the calculations are based on a blended mixture of isooctane and methanol which is 50% :50%. The analysis of mass percentages, AFR, lower heating value, enthalpy, mass of CO₂ have been included.

For the second part, a NO_x model for Isooctane running on the lean side of stoichiometric has to be established and the effects of the equivalence ratio (Φ) and E.G.R on the NO_x PPM have to be analysed.

All these calculations are carried out based on EXCEL, hence the excel data will also be submit to demonstrate author's work.

2 Task One-Mixture of Isooctane and Methanol

For this task, the author has to carry out a study of a blended mixture of isooctane and methanol— which has a molar composition as follows:

METHANOL - 50% ISOCTANE - 50%

2.1 Task One (a) – Mass Percentages

To calculate the mass percentages of methanol and isooctane in this blend, the mixture been assumed as 1mol. The methanol (CH_3OH) and isooctane (C_8H_{18}) are both 0.5mol as the rate of them is 50% : 50%.

CH_3OH	No.	Weight
H	1	1
C	6	12
O	8	16

$$0.5\text{mol} \times \text{methanol} (\text{CH}_3\text{OH}) = (4 \times 1 + 1 \times 12 + 1 \times 16) = 32\text{g}$$

C_8H_{18}	No.	Weight
H	1	1
C	6	12
O	8	16

$$0.5\text{mol} \times \text{isooctane} (\text{C}_8\text{H}_{18}) = (18 \times 1 + 8 \times 12) = 114\text{g}$$

The mass percentage are as follows:

$$\text{Mass Percentage of methanol} = 32 / (32 + 114) = 21.92\%$$

$$\text{Mass Percentage of isooctane} = 114 / (32 + 114) = 78.08\%$$

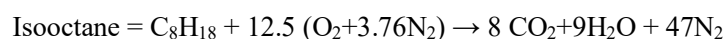
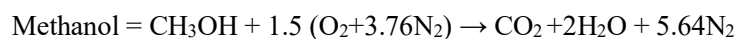
Mass Percentage (%)	
Methanol (CH_3OH)	21.92
Isooctane (C_8H_{18})	78.08

2.2 Task One (b) – Air: Fuel Mass Ratio

The Air/Fuel Ratio (AFR) by mass is the ratio of the air mass to the fuel mass (Williams, Combustion, 2020):

$$AFR = \frac{\text{Air Mass}}{\text{Fuel Mass}}$$

The stoichiometric burning of methanol and isooctane are as follows:



With the table as follows:

	No.	Weight
H	1	1
C	6	12
O	8	16
N	7	14

AFR could be obtained.

$$\text{AFR of methanol} = \frac{1.5 \times (16 \times 2 + 3.76 \times 14 \times 2)}{12 \times 1 + 1 \times 4 + 16 \times 1} = \frac{205.92}{32} = 6.435$$

$$\text{AFR of isooctane} = \frac{12.5 \times (16 + 3.76 \times 14 \times 2)}{12 \times 8 + 1 \times 18} = \frac{1716}{114} = 15.053$$

$$\text{AFR of blend} = \frac{205.92 + 1716(\text{mass of air})}{32 + 114(\text{mass of fuel})} = 13.1638$$

Otherwise the AFR of blend could also be achieved through the formula as follows since the mass percentages have been calculated.

$$\text{AFR of blend} = 6.435 \times 21.92\% + 15.053 \times 78.08\% = 13.1637$$

As been shown above, these two results are quite similar which means the calculations for both of the percentage and the AFR are correct.

2.3 Task One (c) – Lower Heating Value

As to the lower heating value, The ‘Lower Heating Value’ is the term used when H₂O is a gas (LHV) (Williams, Enthalpy and Fuels, 2020).

The enthalpy of pure elements when it in its standard state is zero and enthalpy of other substance could be found from the Properties of Fuels (Appendix, 2020) as follows.

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	Δh _f 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	-	-

^a Gas phase specific heat evaluated at 25°C

^b Heat of vaporization at 1 atm

^c Estimated equilibrium flame temperature

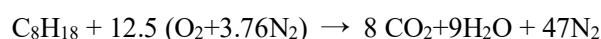
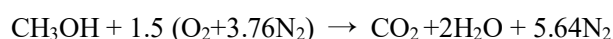
^d Research octane number

^e Motoring octane number

244

Appendix 1

	$\Delta \bar{h}_f^0$
CH ₃ OH	-201.5
C ₈ H ₁₈	-259.2
CO ₂	-393.5
H ₂ O(gas)	-241.8
O ₂	0
N ₂	0



Enthalpy needed:

$$\text{methanol} = 201.5 + 0 + 0 \text{ MJ} = 201.5 \text{ MJ}$$

$$\text{isooctane} = 259.2 + 0 + 0 \text{ MJ} = 259.2 \text{ MJ}$$

Enthalpy released:

$$\text{methanol} = 393.5 + 2 \times 241.8 + 5.64 \times 0 = 877.1 \text{ MJ}$$

$$\text{isooctane} = 8 \times 393.5 + 9 \times 241.8 + 47 \times 0 = 5324.2 \text{ MJ}$$

The net enthalpy:

$$\text{methanol} = 877.1 - 201.5 = 675.6 \text{ MJ}$$

$$\text{isooctane} = 5324.2 - 259.2 = 5065 \text{ MJ}$$

Enthalpy releases per kg:

$$\text{methanol} = \frac{675.6}{32} = 21.113 \text{ MJ / kg (LHV)}$$

$$\text{isooctane} = \frac{5065}{114} = 44.430 \text{ MJ / kg (LHV)}$$

For the blend of methanol and isooctane:

$$\text{LHV} = 21.92\% \times 21.113 + 78.08\% \times 44.430 = 39.319 \text{ MJ/kg}$$

2.4 Task One (d) – Enthalpy of Formation

First of all, Enthalpy of formation ($\Delta \bar{h}_f^0$) is the enthalpy change for the formation of 1 mol of a compound from its component elements. But the magnitude of ΔH for a reaction depends on the physical states of the reactants and the products (gas, liquid, solid, or solution), the pressure of any gases present, and the temperature at which the reaction is carried out. So another standard enthalpies of formation have been proposed which is the enthalpy change for the formation of 1 mol of a compound from its component elements when the component elements are each in their standard states and the standard conditions for which most thermochemical data are tabulated are a pressure of 1 atmosphere (atm) for all gases and a concentration of 1 M for all species in solution (1 mol/L). In addition, each pure substance must be in its standard state, which is usually its most stable form at a pressure of 1 atm at a specified temperature. We assume a temperature of 25°C (298 K) for all enthalpy changes given in this module, unless otherwise indicated. The standard enthalpy of formation of any element in its most stable form is zero by definition. (Williams, Enthalpy and Fuels, 2020).

However, most compounds cannot be prepared by the chemical equations that define their standard enthalpies of formation. Instead, values of are obtained using Hess's law and standard enthalpy changes that have been measured for other reactions, such as combustion reactions. (Williams, Enthalpy and Fuels, 2020)

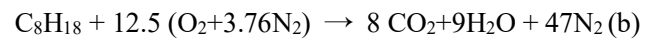
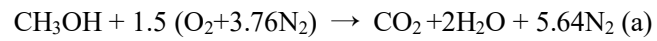
2.5 Task One (e) – Difference Between Higher and Lower Heating Value

First of all, whatever higher or lower heating value, they all indicate there is heat released in the process of combustion. But the $\Delta \bar{h}_f^0$ of H₂O is different, the higher value could be used when H₂O is liquid and the lower value only to be used when the H₂O is gas.



From the above, higher value is larger than lower value obviously so the lower heating value means all of the heat which could be released of a fuel.

2.6 Task One (f) – Mass of CO₂ Produced



From above, mass of CO₂ produced per kg:

$$\text{Methanol} = 44/32 = 1.375\text{kg}$$

$$\text{Isooctane} = 44 \times 8 / 114 = 3.088\text{kg}$$

Hence for the blend of methanol and isooctane:

$$\text{Blend} = 1.375 \times 21.92\% + 3.088 \times 78.08\% = 2.712\text{kg}$$

2.7 Task One (g) – Properties of ‘Ideal ‘ Fuel

First of all, the ideal fuel should have high heat efficiency so that the engine could keep working steadily. After that, AFR of the ideal fuel should be suitable and the molecule should be stable enough which could withstand higher compression and pressure.

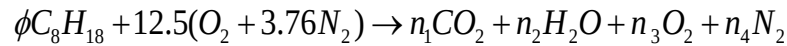
3 Task Two – NO_x Model for Isooctane Running on the Lean Side of Stochometric

For task two, three assumptions are the base of the whole task as follows:

1. The rise in pressure after start of combustion (S.O.C.) is linear and of a value 2 bar per degree from a cylinder pressure of 10 bar at S.O.C, to a peak value of 40 bar.
2. The engine is a 1600 cc four-cylinder, naturally aspirated.
3. The engine speed is 1800 RPM. (Williams, Assignment Specification, 2020)

3.1 Task Two (a) - Graph of NO_x PPM

The equation of combustion as follows:



$$\Delta H = -\phi 5065 MJ / kmol$$

The fuel equivalence ratio ranges from 0.6 to 1.0.

$$n_1 = 8\phi; n_2 = 9\phi; n_3 = (25 - 2n_1 - n_2) / 2; n_4 = 47$$

With all of these, $n_1 - n_4$ and ΔH can be obtained through Excel:

	A	B	C	D	E	F	G
		n1 CO2	n2H2O	n3O2	n4N2	ΔH	
2	0.6	4.8	5.4	5	47	3039	
3	0.65	5.2	5.85	4.375	47	3292.25	
4	0.7	5.6	6.3	3.75	47	3545.5	
5	0.75	6	6.75	3.125	47	3798.75	
6	0.8	6.4	7.2	2.5	47	4052	
7	0.85	6.8	7.65	1.875	47	4305.25	
8	0.9	7.2	8.1	1.25	47	4558.5	
9	0.95	7.6	8.55	0.625	47	4811.75	
10	0.96	7.68	8.64	0.5	47	4862.4	
11	0.97	7.76	8.73	0.375	47	4913.05	
12	0.98	7.84	8.82	0.25	47	4963.7	
13	0.99	7.92	8.91	0.125	47	5014.35	
14	1	8	9	0	47	5065	
15							
16							
17							

As we all know, the change in heat is equal to the change in energy when the pressure is constant and the net enthalpy released can be calculated from the 'enthalpy of formation' (Hf) at 298K. (Willimas, 2020) The temperature of the products raises from 298K to fuel flame front temperature on account of the enthalpy released, so the author chooses to find the approximate range of the temperature firstly.

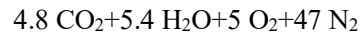
All the results come from Excel are as follows:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
		n1 CO2	n2 H2O	n3 O2	n4 N2	ΔH	1700K	1800K	1900K	2000K	2100K	2200K	2300K	2400K	Flame T	n1+n4	
1		0.6	4.8	5.4	5	47	3039	3038.964	3279.644	3521.94	3765.896	4010.896	4257.922	4505.416	4754.368	1700.015	62.2
2		0.65	5.2	5.85	4.375	47	3292.25	3064.379	3307.336	3551.945	3798.243	4045.612	4295.037	4544.938	4796.33	1793.791	62.425
3		0.7	5.6	6.3	3.75	47	3545.5	3089.793	3335.028	3581.95	3830.59	4080.327	4332.152	4584.46	4838.291	1885.238	62.65
4		0.75	6	6.75	3.125	47	3798.75	3115.208	3362.72	3611.955	3862.936	4115.043	4369.266	4623.981	4880.253	1974.426	62.875
5		0.8	6.4	7.2	2.5	47	4052	3140.622	3390.412	3641.96	3895.283	4149.758	4406.381	4663.503	4922.214	2061.584	63.1
6		0.85	6.8	7.65	1.875	47	4305.25	3166.037	3418.104	3671.965	3927.63	4184.474	4443.496	4703.025	4964.176	2146.628	63.325
7		0.9	7.2	8.1	1.25	47	4558.5	3191.451	3445.796	3701.97	3959.977	4219.189	4480.611	4742.547	5006.137	2229.736	63.55
8		0.95	7.6	8.55	0.625	47	4811.75	3216.866	3473.488	3731.975	3992.323	4253.905	4517.725	4782.068	5048.099	2311.157	63.775
9		0.96	7.68	8.64	0.5	47	4862.4	3221.948	3479.026	3737.976	3998.793	4260.848	4525.148	4789.973	5056.491	2327.175	63.82
10		0.97	7.76	8.73	0.375	47	4913.05	3227.031	3484.565	3743.977	4005.262	4267.791	4532.571	4797.877	5064.883	2343.135	63.865
11		0.98	7.84	8.82	0.25	47	4963.7	3232.114	3490.103	3749.978	4011.731	4274.734	4539.994	4805.781	5073.275	2359.036	63.91
12		0.99	7.92	8.91	0.125	47	5014.35	3237.197	3495.642	3755.979	4018.201	4281.677	4547.417	4813.686	5081.668	2374.88	63.955
13		1	8	9	0	47	5065	3242.28	3501.18	3761.98	4024.67	4288.62	4554.84	4821.59	5090.06	2390.666	64
14																	
15																	
16																	

For the process of calculation,

When $\phi=0.6$, $\Delta H = -3039\text{MJ/kmol}$

With the help of the fuel database, for:



When the temperature is 1700K, it needs $4.8 \times 73.44 + 5.4 \times 57.78 + 5 \times 47.94 + 47 \times 45.42 = 3038.964\text{MJ}$

When the temperature is 1800K, it needs $4.8 \times 79.4 + 5.4 \times 62.71 + 5 \times 51.66 + 47 \times 48.97 = 3279.644\text{MJ}$

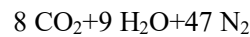
Hence the accurate temperature can be obtained as follows:

$$\frac{T - 1700}{1800 - 1700} = \frac{3039 - 3038.964}{3279.644 - 3038.964}$$

$$T = 1700.015$$

When $\phi=1.0$, $\Delta H = -5065\text{MJ/kmol}$

With the help of the fuel database, for:



When the temperature is 2300K, it needs $8 \times 109.66 + 9 \times 88.42 + 47 \times 66.99 = 4821.59\text{MJ}$

When the temperature is 2400K, it needs $8 \times 115.79 + 9 \times 93.74 + 47 \times 70.64 = 5090.06\text{MJ}$

Hence the accurate temperature can be obtained as follows:

$$\frac{T - 2300}{2400 - 2300} = \frac{5065 - 4821.59}{5090.06 - 4821.59}$$

$$T = 2390.666$$

Hence the rise in temperature of burned gas up to peak pressure is

$$T = 2390.666 - 1700.015 = 690.651$$

As for the burn zone temperature, it will rise when the pressure increases like the equation below.

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

Which comes from

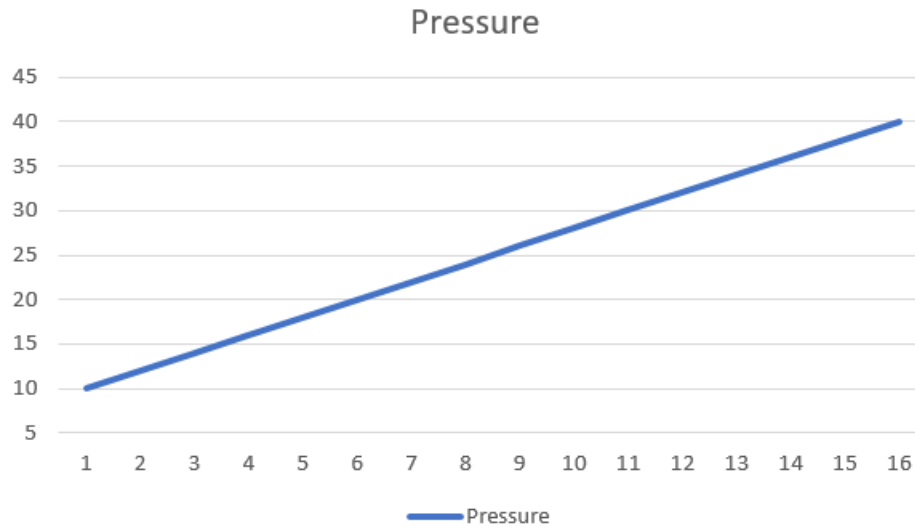
$$n = \frac{C_p}{C_v}$$

$$pv^n = \text{const } t.$$

The range of T can be obtained as follows with $n = 1.17$ which shows in the fuel database.

P/bar	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	0.96	0.97	0.98	0.99	1
10	1700.015	1793.791	1885.238	1974.426	2061.584	2146.628	2229.736	2311.157	2327.175	2343.135	2359.036	2374.88	2390.666
12	1745.652203	1841.945636	1935.847547	2027.429814	2116.927586	2204.255	2289.593656	2373.200417	2389.648424	2406.036873	2422.364738	2438.634073	2454.843851
14	1785.192411	1883.666956	1979.695809	2073.352478	2164.877435	2254.182	2341.454509	2426.95502	2443.775584	2460.535243	2477.232945	2493.870792	2510.447732
16	1820.1669	1920.570703	2018.480899	2113.972437	2207.290499	2298.345	2387.326972	2474.502561	2491.652665	2508.740669	2525.765504	2542.72931	2559.631016
18	1851.584899	1953.721778	2053.322007	2150.461829	2245.39066	2338.017	2428.534752	2517.215084	2534.661216	2552.044178	2569.362879	2586.619498	2603.812946
20	1880.148508	1983.861009	2084.997728	2183.639085	2280.029342	2374.085	2465.99872	2556.047085	2573.762352	2591.413473	2608.999342	2626.522171	2643.980855
22	1906.368845	2011.525598	2114.072651	2214.088502	2311.823946	2407.191	2500.386634	2591.690707	2609.65301	2627.550273	2645.381374	2663.148556	2680.850698
24	1930.621427	2037.118108	2140.96986	2242.256181	2341.237132	2437.817	2532.198891	2624.66462	2642.855456	2660.980425	2679.03839	2697.031623	2714.959888
26	1953.205894	2060.948376	2166.01499	2268.486161	2368.624994	2466.335	2561.820629	2655.368026	2673.771859	2692.108653	2710.377861	2728.581579	2746.718659
28	1974.351314	2083.260217	2189.464283	2293.044807	2394.267744	2493.036	2589.554917	2684.115058	2702.717929	2721.25344	2739.72043	2758.121222	2776.454654
30	1994.242943	2104.249105	2211.523179	2316.147279	2418.39004	2518.153	2615.644734	2711.157571	2729.947866	2748.670122	2767.323168	2785.909348	2804.42749
32	2013.031698	2124.074283	2232.359039	2337.968855	2441.174895	2541.878	2640.288024	2736.700735	2755.668063	2774.566711	2793.395496	2812.156786	2830.849397
34	2030.84223	2142.867278	2252.110096	2358.654307	2462.773475	2564.367	2663.64828	2760.914013	2780.049157	2799.115013	2818.110388	2837.037671	2855.895666
36	2047.778747	2160.738044	2270.891909	2378.324662	2483.312147	2585.753	2685.862179	2783.939074	2803.233798	2822.458657	2841.612447	2860.697576	2879.712841
38	2063.92929	2177.779482	2288.802115	2397.082175	2502.897682	2606.147	2707.045197	2805.895611	2825.34251	2844.718992	2864.023845	2883.259497	2902.424732
40	2079.368954	2194.070826	2305.923988	2415.01406	2521.621142	2625.642	2727.295827	2826.885712	2846.478088	2865.999521	2885.448788	2904.828335	2924.13694

The pressure of each crankshaft intervals can be seen as follows since the increase of the pressure is linear.



Each cylinder has a displacement of 400cc since the engine is a naturally-aspirated four-cylinder engine. The number of mixture get into each cylinder can be calculated from the ideal gas law when the volumetric efficiency is assumed as 50%.

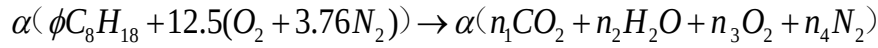
When $\phi=0.6$, the number of mixture get inside each cylinder can be obtained as the pressure is assumed as 1 Bar and at 20°C.

$$PV = nRT$$

$$\therefore n = \frac{1 \times 10^5 \times (400 \times 0.5) \times 10^{-6}}{8314 \times 293}$$

$$\therefore n = 8.21 \times 10^{-6} \text{ kmols}$$

For the calculation of the rate of NO_x production using the Zeldovich model, the author determines the concentrations of nitrogen and oxygen in combustion firstly. This requires a new variable, alpha (α), representing the actual number of kmols in the mixture. Multiplying the previous balanced chemical equation by alpha gives the correct number of kmols for one cycle of combustion. (Williams, Zeldovich Model, 2020)



$$\alpha(\phi C_8H_{18} + 12.5(O_2 + 3.76N_2)) = 8.21 \times 10^{-6} \text{ kmols}$$

$$\therefore \alpha(0.6 + 12.5(1 + 3.76)) = 8.21 \times 10^{-6} \text{ kmols}$$

$$\therefore \alpha = \frac{8.21 \times 10^{-6}}{0.6 + 12.5(1 + 3.76)} \text{ kmols}$$

$$\therefore \alpha = 1.37 \times 10^{-7} \text{ kmols}$$

It is obviously that alpha will change when the fuel equivalence ratio changes on account of the higher ratio means more fuel in the mixture and the concentrations of oxygen and nitrogen changes as well.

When the displacement is 400cc:

$$[O_2] = \frac{n_3 \times \alpha}{40 \times 10^{-6}} \quad [N_2] = \frac{n_4 \times \alpha}{40 \times 10^{-6}}$$

$$[O_2] = \frac{5 \times \alpha}{40 \times 10^{-6}} \quad [N_2] = \frac{47 \times \alpha}{40 \times 10^{-6}}$$

$$[O_2] = 0.017076 \quad \text{and} \quad [N_2] = 0.160515$$

After that, with the equation below,

$$\frac{d[NO]}{dt} = 4.17 \times 10^{13} [N_2][O_2]^{\frac{1}{2}} \exp\left(\frac{-67837}{T}\right)$$

$$1800 \times \frac{360}{60} = \text{° / sec}$$

The equation can be obtained as follows,

$$\frac{4.7 \times 10^{13} \times [N_2][O_2]^{\frac{1}{2}} \exp\left(\frac{-67837}{T}\right)}{1800 \times 6} \times 40 \times 10^{-6} = \frac{\text{kmols}}{\text{°}}$$

And the sum of NO_x over intervals can be achieved from:

$$\sum_{X_{soc}}^{X_{eoc}} \left(\frac{4.7 \times 10^{13} \times [N_2][O_2]^{\frac{1}{2}} \exp\left(\frac{-67837}{T}\right)}{1800 \times 6} \times 40 \times 10^{-6} \right) = \text{kmols / cycle}$$

X takes from 0° to 15°.

$$\text{NO}_x = 9.75 \times 10^{-11} \text{ kmols/cycle}$$

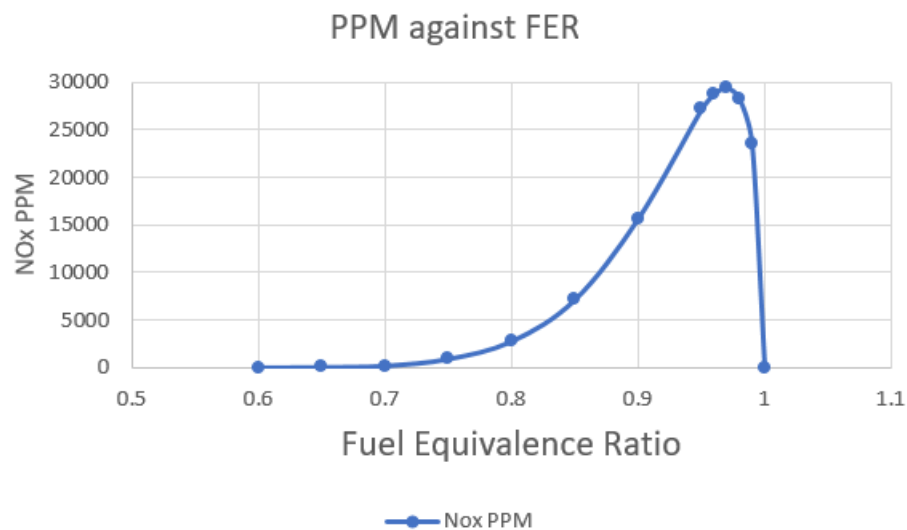
As to the PPM,

$$\begin{aligned} \text{PPM} &= \frac{\text{NO}_x \text{ kmols / cycle}}{\text{total exhaust kmols}} \times 10^6 \\ \text{and total exhaust} &= \alpha(n_1 + n_2 + n_3 + n_4) \\ \therefore \phi=0.6 \text{ total exhaust} &= 8.5 \times 10^{-6} \text{ kmols} \\ \therefore \text{PPM} &= \frac{9.75 \times 10^{-11}}{8.5 \times 10^{-6}} \times 10^6 = 11.4709 \end{aligned}$$

All the PPM have been calculated through Excel.

PPM	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	0.96	0.97	0.98	0.99	1
	11.4709003	61.07183872	199.422052	926.1789825	2787.363517	7176.511	15690.20934	27198.01066	28807.34913	29457.56214	28319.25489	23512.76672	0

And the graph is as follows:



From this graph, PPM increases as the FER rises before 0.97 on account of the temperature is becomes higher and higher to make it easier to split. The curve achieved highest of 29457.56 when $\phi=0.97$. After that PPM keeps going down on account of the N and O are not enough.

3.2 Task Two (b) – Effect of Adding EGR

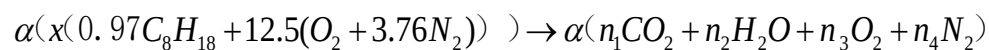
When $\phi=0.97$, using the Zeldovich model as follows:

$$\frac{\partial[NO]}{\partial t} = 4.7 \times 10^{13} \times [N_2][O_2]^{\frac{1}{2}} * \exp\left(\frac{-67837}{T}\right) \text{ kmols / m}^3 \text{ / sec}$$

There are several assumptions below as the base of the calculation:

1. Volumetric efficiency of 40%
2. EGR levels up to 20% of the air +fuel contents
3. The pressure in the cylinder at inlet valve closing is 1 bar (1 x 10⁵ N/m²) and that the temperature of the air fuel is 20°C.
4. Universal gas constant is 8314 J KMOL⁻¹ K⁻¹.
5. Polytopic index for burned zone up to peak pressure is 1.17.
6. The volume of the air/fuel during combustion is the head volume of 40 ccs and that [N₂] & [O₂] concentrations can be considered constant during combustion.

With the equation below, the influence of 0%, 5%, 10%, 15%, 20% EGR can be calculated and the results are as follows:



	100%	105%	110%	115%	120%
n1	7.76	8.148	8.536	8.924	9.312
n2	8.73	9.1665	9.603	10.0395	10.476
n3	0.375	0.39375	0.4125	0.43125	0.45
n4	47	49.35	51.7	54.05	56.4
xn	6.56814E-06	6.89655E-06	7.22495E-06	7.55336E-06	7.88177E-06

When compared with n without EGR which is 6.56814x10⁻⁶kmols, xn is also in the results on above which comes with x from 1 to 1.2.

But for α :

$$\alpha(x(0.97C_8H_{18} + 12.5(O_2 + 3.76N_2))) = x6.56814 \times 10^{-6} \text{ kmols}$$

$$\therefore \alpha(x(0.97 + 12.5(1 + 3.76))) = x6.56814 \times 10^{-6} \text{ kmols}$$

$$\therefore \alpha = \frac{6.56814 \times 10^{-6}}{(0.97 + 12.5(1 + 3.76))} \text{ kmols}$$

$$\therefore \alpha = 1.08618 \times 10^{-7}$$

It seems there is no difference from the α from the previous calculation which means x has no effect on α .

For $[O_2]$ and $[N_2]$:

$$[O_2] = \frac{n_3 \times \alpha}{40 \times 10^{-6}} \quad [N_2] = \frac{n_4 \times \alpha}{40 \times 10^{-6}}$$

Results of these two with x from 1 to 1.2 as follows:

O2	0.001018295	0.00106921	0.001120125	0.00117104	0.001221954
N2	0.127626335	0.134007652	0.140388969	0.146770286	0.153151602

Even the net enthalpy has not changed, the flame temperature drops with the EGR rises on account of the $n1$ - $n4$ has changed.

EGR	n1	n2	n3	n4												Flame T
1	7.76	8.73	0.375	47	4913.05	3227.031	3484.565	3743.977	4005.262	4267.791	4532.571	4797.877	5064.883	5318.127	5571.371	2343.135
1.05	8.148	9.1665	0.39375	49.35	4913.05	3388.383	3658.793	3931.176	4205.525	4481.18	4759.2	5037.771	5318.127	5571.371	5824.616	2255.228
1.1	8.536	9.603	0.4125	51.7	4913.05	3549.734	3833.021	4118.375	4405.788	4694.57	4985.828	5277.665	5571.371	5824.616	6077.86	2175.012
1.15	8.924	10.0395	0.43125	54.05	4913.05	3711.086	4007.25	4305.574	4606.051	4907.959	5212.457	5517.558	5824.616	6077.86	6333.881	2101.672
1.2	9.312	10.476	0.45	56.4	4913.05	3872.438	4181.478	4492.772	4806.314	5121.349	5439.085	5757.452	6077.86	6333.881	6600.000	2033.881

The temperature of burn zone should be calculated again as well and from the results below it is obviously that the temperature of burn zone drops because of the EGR.

ZoneT					
P/bar	1	1.05	1.1	1.15	1.2
10	2343.135	2255.228	2175.012	2101.672	2033.881
12	2406.036873	2315.769994	2233.400581	2158.091756	2088.480894
14	2460.535243	2368.223758	2283.988622	2206.974001	2135.786406
16	2508.740669	2414.62067	2328.735246	2250.211798	2177.629535
18	2552.044178	2456.299567	2368.931671	2289.052825	2215.217716
20	2591.413473	2494.191851	2405.476168	2324.365065	2249.390934
22	2627.550273	2528.972913	2439.020105	2356.777922	2280.75829
24	2660.980425	2561.148872	2470.0516	2386.763055	2309.77623
26	2692.108653	2591.109268	2498.946338	2414.683481	2336.796062
28	2721.25344	2619.160634	2525.999947	2440.82486	2362.094232
30	2748.670122	2645.54873	2551.449447	2465.41622	2385.892378
32	2774.566711	2670.47376	2575.487922	2488.644132	2408.371057
34	2799.115013	2694.101088	2598.274851	2510.662701	2429.679401
36	2822.458657	2716.568952	2619.943558	2531.600753	2449.94208
38	2844.718992	2737.994151	2640.606685	2551.567133	2469.26443
40	2865.999521	2758.476301	2660.360308	2570.654676	2487.73629

For the NO_x per cycle:

$$\frac{\partial[NO]}{\partial t} = 4.7 \times 10^{13} \times [N_2][O_2]^{\frac{1}{2}} \times \exp\left(\frac{-67837}{T}\right) \text{ kmols} / \text{m}^3 / \text{sec}$$

$$\sum_{x_{soc}}^{x_{eoc}} \left(\frac{4.7 \times 10^{13} \times [N_2][O_2]^{\frac{1}{2}} \exp\left(\frac{-67837}{T}\right)}{1800 \times 6} \times 40 \times 10^{-6} \right) = kmols / cycle$$

Results shown with the x from 1 to 1.2.

1	Nox/cycle	1.82771E-07	7.61637E-08	3.21691E-08	1.3796E-08	5.96674E-09
---	-----------	-------------	-------------	-------------	------------	-------------

For the NOx PPM:

$$PPM = \frac{NO_x \text{ kmols / cycle}}{\text{total exhaust kmols}} \times 10^6$$

and total exhaust = $\alpha(n_1 + n_2 + n_3 + n_4)$

The results of exhaust and PPM with x from 1 to 1.2 are as follows:

exhaust	6.9369E-06	7.28374E-06	7.63059E-06	7.97743E-06	8.32428E-06
---------	------------	-------------	-------------	-------------	-------------

EGR level	0%	5%	10%	15%	20%
PPM	26347.64182	10456.66317	4215.809967	1729.375148	716.7875169

As the results shows, PPM drops quickly with the EGR Level increases and nearly gone when the EGR achieved 20%. Since the EGR is a quite useful method to reduce the NOx, the EGR system should be applied on the car in order to achieve the Euro VI emission regulations.

4 Reference

Appendix. (2020 年 01 月 04 日). Properties of Fuels. 检索来源: MOODLE UWTSD:

[https://moodle.uwtsd.ac.uk/pluginfile.php/313892/mod_resource/content/1/Fuels%20Data
base.pdf](https://moodle.uwtsd.ac.uk/pluginfile.php/313892/mod_resource/content/1/Fuels%20Data%20base.pdf)

WilliamsOwen. (2020 年 01 月 04 日). Assignment Specification. 检索来源: MOODLE UWTSD:

<https://moodle.uwtsd.ac.uk/course/view.php?id=2566>

WilliamsOwen. (2020 年 01 月 04 日). Combustion. 检索来源: MOODLE UWTSD:

[https://moodle.uwtsd.ac.uk/pluginfile.php/310860/mod_resource/content/2/Week%20%20%
20-%20Combustion.pdf](https://moodle.uwtsd.ac.uk/pluginfile.php/310860/mod_resource/content/2/Week%20%20-%20Combustion.pdf)

WilliamsOwen. (2020 年 01 月 04 日). Enthalpy and Fuels. 检索来源: MOODLE UWTSD:

[https://moodle.uwtsd.ac.uk/pluginfile.php/313914/mod_resource/content/2/Week%20%20%
20-%20Enthalpy%20and%20Fuels.pdf](https://moodle.uwtsd.ac.uk/pluginfile.php/313914/mod_resource/content/2/Week%20%20-%20Enthalpy%20and%20Fuels.pdf)

WilliamsOwen. (2020 年 01 月 04 日). Zeldovich Model. 检索来源: MOODLE UWTSD:

[https://moodle.uwtsd.ac.uk/pluginfile.php/323838/mod_resource/content/2/6%20-%20Zel
dovich%20Model.pdf](https://moodle.uwtsd.ac.uk/pluginfile.php/323838/mod_resource/content/2/6%20-%20Zel%20dovich%20Model.pdf)

WillimasOwen. (2020 年 01 月 04 日). Flame Temperatures. 检索来源: MOODLE UWTSD:

[https://moodle.uwtsd.ac.uk/pluginfile.php/320472/mod_resource/content/4/Week%20%20%
20-%20Flame%20Temperatures.pdf](https://moodle.uwtsd.ac.uk/pluginfile.php/320472/mod_resource/content/4/Week%20%20-%20Flame%20Temperatures.pdf)