

GDI Combustion Modelling for NO_x Prediction and Analysis

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Abstract

In this report cylinder pressure data from the Ford Motor Company for a 1l Ford Fox and 1.5l Ford Sigma will be utilised to develop a two-zone combustion model developed from first principles. This combustion model will then be developed into a NO_x prediction model encompassing the use of a dissociation model allowing the use of the Zeldovich mechanism. The model will be put through various sensitivity analyses to give an understanding on how engine operating conditions can affect NO_x formation in the engine. Finally, the inclusion of water injection will be studied with a simple water injection model used to determine the effectiveness of the charge cooling effect brought by its inclusion.

Acknowledgements

I would like to thank my family for their continued support throughout the course. This report and the knowledge and understanding behind the theory would not have been possible without the help and support of my project supervisor, Malcolm McDonald. He has not only kept me motivated throughout the year but has also ignited a passion, a passion that now actively gets me to debate in theoretical discussion and one that I hope will stay with me wherever I go. For this, I am grateful.

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Symbols

$\tilde{R}$ - Universal Gas Constant

A- Gas Kinetic Collision Frequency

C- Carbon Atoms

CO- Carbon Monoxide

CO₂- Carbon Dioxide

c_p- Specific Heat at a Constant Pressure

c_v- Specific Heat at a Constant Volume

E_A- Activation Energy

H- Enthalpy

H- Hydrogen

H₂O- Water

HC- Hydrocarbons

J- Joule

k- Constant Relating RPM to Turbulent Air Velocity

K- Kelvin

k'- Rate Constant

K_p- Partial Pressure Equilibrium

K'_c- Concentration Equilibrium

k_{AF}- Arrhenius Equation Rate Constant

K_f- Forward Reaction Rate Constant

Kg- Kilogram

K_r- Reverse Reaction Rate Constant

m- Mass

n- Number of Atoms

n₁- Number of Carbon Dioxide Molecules

N₂- Nitrogen Atoms

n₂- Number of Water Molecules

n₃- Number of Carbon Monoxide Molecules

n₄- Number of Hydrogen Molecules

n₅- Number of Oxygen Molecules

NO- Nitric Oxide

NO₂- Nitrogen Dioxide

NO_x- Nitrous Oxides

n_t- Total Number of Atoms

O- Oxygen Atoms

O₂- Oxygen

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p- Pressure

P_x - Partial Pressure

Q- Heat Release

Q - Heating Value

Q_{HV} - Higher Heating Value

Q_{LV} - Lower Heating Value

R- Gas Constant

S_L - Laminar Flame Speed

S_T - Turbulent Flame Velocity

T- Temperature

T_b - Temperature of the Burnt Zone

T_{un} - Temperature of the Unburnt Zone.

U- Internal Energy

V- Volume

α - Kmols in the Cylinder

γ - Specific Heat Ratio

ΔG^0 - Gibbs Free Energy

θ - Crank Angle

λ - Lambda

ρ - Density

Φ - Fuel Equivalence Ratio

Abbreviations

A/F- Air/Fuel

ABDC- After Bottom Dead Centre

ATDC- After Top Dead Centre

Atm= Atmosphere

BDC- Bottom Dead Centre

BMEP- Brake Mean Effective Pressure

BSFC- Brake Specific Fuel Consumption

EGR- Exhaust Gas Recirculation

EOC- End of Combustion

EZM- Extended Zeldovich Mechanism

FER- Fuel Equivalence Ratio

FL- Full Load

GDI- Gasoline Direct Injection

GDI- Gasoline Direct Injection

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HC- Hydro Carbons

ICE- Internal Combustion Engine

IMEP- Indicated Mean Effective Pressure

m_{air} - Air Mass

MBT- Maximum Brake Torque

MFB- Mass Fraction Burned

m_{fuel} - Fuel Mass

NA- Naturally Aspirated

NEDC- New European Drive Cycle

PL- Part Load

ppm- Parts per Million

PV- Pressure versus Volume

RG- Residual Gas

RGF- Residual Gas Fraction

SOC- Start of Combustion

TDC- Top Dead Centre

V.E- Volumetric Efficiency

WLTP- Worldwide Harmonised Light Vehicle Test Procedure

W/F- Water/ Fuel Ratio

1. Introduction

Vehicles are becoming increasingly scrutinised in terms of their emissions, with ever increasing legislation and test procedures such as the incoming WLTP replacing the NEDC manufacturers are looking towards engine simulation to help save time and cost compared to traditional testing. With recent practices coming to light in the automotive industry a lot of attention has been focused on the production of NO_x which has been shown to have a negative impact on people's health and the environment. (Chossiere, et al., 2017)

The model used in this report will be a two-zone combustion model which will then be used to predict the NO_x being produced by the engine. The two-zone model assumes that there are only two zones present in the engine, the burnt and un-burnt zone which assumes homogeneity throughout both zones which is a model limitation in itself which will be discussed in the report. This kind of engine out emissions simulation is useful as it allows the manufacturer to combat the problem directly which saves the need of adding after treatment devices which can add to the cost and weight of the vehicle.

The model will work from first principles based around pressure and volume data provided by the Ford Motor Company for their 1 litre Fox engine and 1.5 litre Sigma engine. Each are turbocharged but have drastically different operating parameters in terms of their A/F ratio which will hopefully give an interesting contrast which will should give an interesting contrast in the functionality and limitations of the model used.

A dissociation model will then be used, using the temperature of the burn zone calculated by the two-zone model and from this the Zeldovich mechanism will be employed to predict the NO_x being produced by the engine. Furthering on from this the effect of the inclusion of water injection into the cylinder will be studied which will reduce the temperature through multiple means.

'This thesis is the result of the author's original research. It has been composed by the author and has not been previously submitted for examination which has lead to the award of a degree.'

Signed:

Date:

2. Combustion Thermochemistry

2.1 Ideal Gas Law

The Products and reactants within the ICE will be treated as an ideal gas throughout the entire combustion process therefore the ideal gas law can be used:

$$pV = mRT = n\tilde{R}T$$

Equation 2-1 Ideal Gas Law

Where p is the pressure, V is the volume, m is the mass of the gas, R is the gas constant, $\tilde{R}$ is the universal gas constant of 8314 J/kmols at 1 atm. K and T is the temperature.

2.2 Specific Heat

For a mixture there are two specific heat values, specific heat at a constant volume (c_v) and specific heat at a constant pressure (c_p) both of which are influenced by the temperature of the gas. This is because three systems store a molecules internal energy; rotational, vibration and translational energy. In a cold state, molecules move slowly and have minimal vibrational and rotational energy, because of this energy transfer between molecules is low. As the temperature increases the rotational and vibrational energy increases due to the increased likelihood of molecular collision and energy transfer between molecules, raising the specific heat. From the first law of thermodynamics we know that:

$$Q = U + pV$$

$$dQ = dU + pdV$$

Equation 2-2 Heat Release

Where Q is the heat released and U is the internal energy and since we know that for a constant volume:

$$dV = 0 \therefore pdV = 0$$

$$\therefore dQ = dU$$

As energy increase is only due to energy transfer in the form of heat:

$$c_v = \frac{dU}{dT}$$

Equation 2-3 Specific Heat at a Constant Volume (Greitzer, et al., 2007)

We can see the specific heat at a constant pressure as:

$$c_p = \frac{dU}{dT} + \frac{pdV}{dT}$$

$$\therefore c_p = c_v + \frac{pdV}{dT}$$

Rearranging *equation 2-1*:

$$\frac{V}{T} = \frac{mR}{p}$$

However, because it is a constant pressure:

$$\frac{dV}{dT} = \frac{mR}{p}$$

$$\therefore c_p = c_v + mR$$

However, if the mixture is being heated by 1K and is 1Kg of mass then:

$$c_p = c_v + R$$

Equation 2-4 Specific Heat for a Constant Pressure

2.3 Stoichiometric Combustion

For perfect combustion in which all the fuel & air in the cylinder has been burnt is called stoichiometric. (The Engineering Toolbox, n.d.) This is typically found with an A/F ratio of around 14.7:1 depending on which fuel is used and is denoted as $\lambda=1$. Lambda is the A/F measured in the exhaust gases as seen in *figure 2-1* and works by measuring the oxygen content in the gases.

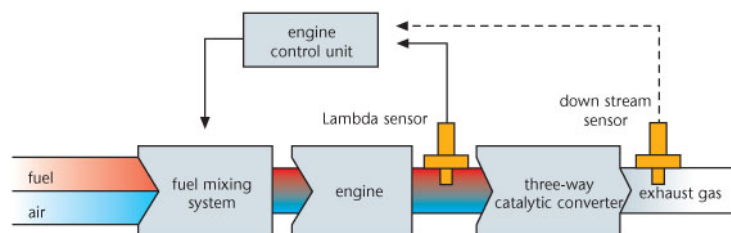


Figure 2-1 Lambda Sensor (NGK, 2010)

A stoichiometric combustion is important because at this A/F ratio HC should theoretically be negligible due to complete combustion, CO should be minimal as formation is more prevalent in rich mixtures and NOx whilst high at $\lambda=1$ will be lower than that of a slightly lean mixture and is usually only high at this point due to the temperature.

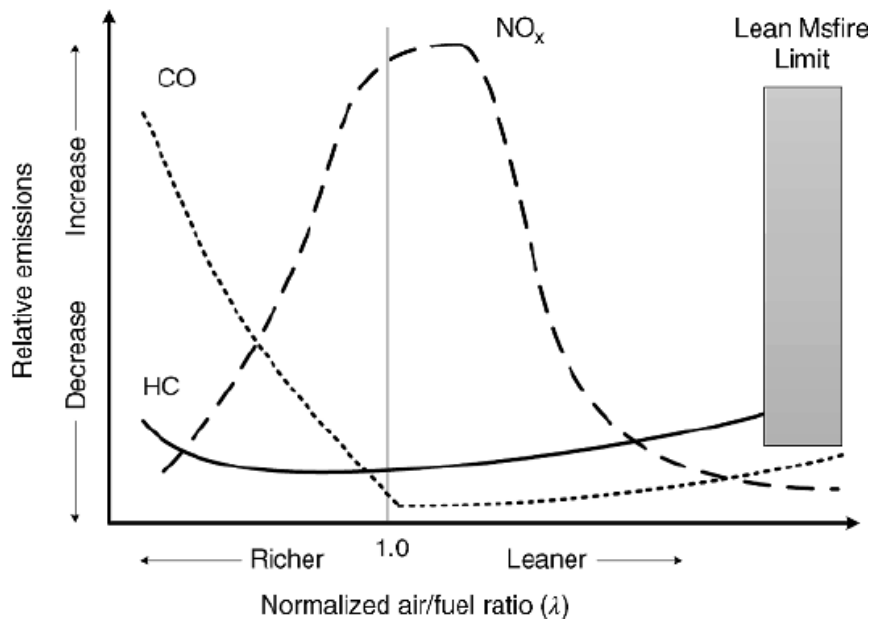
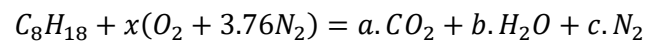


Figure 2-2 Effect of A/F Ratio on Emissions (Fallah, et al., 2014)

In a completely stoichiometric homogeneous engine if sufficient oxygen is available, a hydrocarbon fuel can be completely oxidized converting it to CO_2 and H_2O . (Heywood, 1988, p. 69) The chemical equation for isooctane which is the fuel used in the engines can then be seen as:



Equation 2-5 Stoichiometric Equation

Air is composed of about 20.95% oxygen and 78.08% nitrogen and 0.97% other elements. (Engineering Toolbox, 2003) Therefore, nitrogen should be considered in the chemical balance equation meaning there is approximately 3.76 times more nitrogen present compared to oxygen. If we balance the equation to find the unknowns:

$$\text{C} = 8$$

$$a = \text{C} = 8$$

$$\text{H} = 18$$

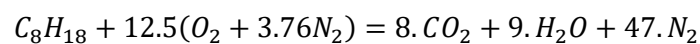
$$2b = \text{H} = 18 \therefore b = 9$$

$$\text{O} = 2a + b = 25$$

$$\therefore x = 12.5$$

$$\text{N} = 12.5 \times 3.76 = 47$$

Therefore:



Equation 2-6 Balanced Stoichiometric Equation

2.4 Air/Fuel Ratio

In practice an engine is hardly running stoichiometric and is instead running lean or rich leading to products other than CO₂ and H₂O such as CO and O₂. Using the molecular masses found in *appendix 11.1* we can determine the stoichiometric A/F ratio:

$$\lambda = \frac{m_{air}}{m_{fuel}}$$

$$\frac{12.5[(2 \times 15.999) + (3.76 \times 2 \times 14.007)]}{(8 \times 12.011) + (18 \times 1.008)} = \frac{1716.633}{114.84} = 14.95:1$$

Equation 2-7 Isooctane Stoichiometric A/F Ratio

Whilst λ gives us an idea if the mixture is rich or lean for calculations we need to use the FER which is the inverse of λ :

$$FER(\phi) = \frac{1}{\lambda}$$

Equation 2-8 FER

It can then be seen that lean mixtures:

$$\phi < 1, \lambda > 1$$

Stoichiometric mixtures:

$$\phi = \lambda = 1$$

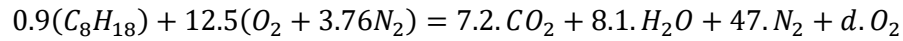
Rich mixtures:

$$\phi > 1, \lambda < 1$$

(Heywood, 1988, p. 72)

Rich operation is desirable as maximum engine output can be found around $\lambda=0.85$ to $\lambda=0.95$ depending on the fuel used. (BOSCH, 2014) A rich mixture can also be used to bring down combustion temperatures as seen in one of the engines analysed in this report. Lean operation is desirable for reduced fuel consumption and for reducing HC emission issues as the fuel is more likely to completely burn during combustion. However, due to the increased free O₂ molecules NO_x emissions tend to increase during lean operation before decreasing due to reduced temperature as there is less fuel to burn.

Examples of the chemical equation showing the different combustion products for a lean and rich mixture respectively:

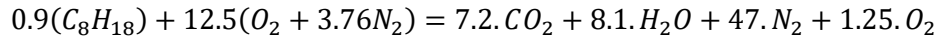


$$(12.5 \times 2) O \text{ atoms} = (7.2 \times 2) + 8.1 O \text{ atoms}$$

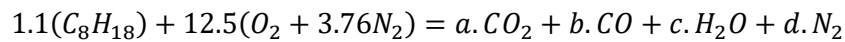
$$25 = 22.5 + 2d$$

$$2d = 2.5$$

$$d = 1.25$$



Equation 2-9 Lean Chemical Balancing



$$C_{atoms} = 8.8 = a + b$$

$$H_{atoms} = 19.8 = 2c$$

$$\therefore c = 9.9$$

$$O_{atoms} = 25 = 2a + b + c$$

$$O_{atoms} = 25 = 2a + b + 9.9$$

$$25 - 9.9 = 2a + b$$

$$15.1 = 2a + b$$

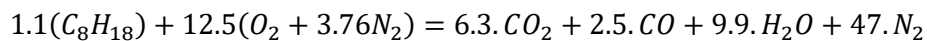
$$15.1 - 8.8 = a$$

$$6.3 = a$$

$$8.8 = 6.3 + b$$

$$8.8 - 6.3 = b$$

$$b = 2.5$$



Equation 2-10 Rich Chemical Balancing

2.5 Heating Values

The heating value of a fuel is the energy released from the complete combustion of one-unit mass of fuel under standard conditions at around a temperature of 298 K. (Heywood, 1988, p. 78) Therefore it can be seen that:

$$Q_{HV_p} = -(\Delta H)_{p,T_0}$$

$$Q_{HV_p} = -(\Delta H)_{p,T_0}$$

Equation 2-11 Heating Value

Two heating values can be used, the lower heating value and higher heating value. The lower heating value is used when it is for example assumed that the water stays in a gaseous state after combustion while the higher heating value is used if the water condenses recovering the heat energy. The higher heating value tends to be 11% higher than the lower heating value because of this energy recovery. (Turns, 2006, p. 136) This is an important process for rich running engines for cooling purposes, as the fuel is being injected directly into the engine it will be assumed that it will be in a liquid phase, heat energy will then be required to change it to a gaseous state, this heat energy will be removed from the system and with this reduction in heat energy there will be a reduction in temperature.

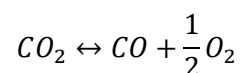
2.6 Gibbs Free Energy

To predict chemical changes, it is necessary to know the available free energy of a species. Looking at the standard state free energy which is generally taken at 298.15 K 1 atm, the free energy when a compound is formed from its elements, or the difference between the energy available of a substance compared to its base elements can be given as:

$$\Delta G^0 = \sum \Delta G_{f_{products}}^0 - \sum \Delta G_{f_{reactants}}^0$$

Equation 2-12 Gibbs Free Energy

Therefore, if we look at the free energy of carbon dioxide:



Equation 2-13 Carbon Dioxide Chemical Equilibrium (Heywood, 1988, p. 86)

At 3000 K:

$$\Delta G^0 CO_2 = -395.461 \text{ MJ/Kmol}$$

$$\Delta G^0 CO = -367.816 \text{ MJ/kmol}$$

$$\Delta G^0 O_2 = 0 \text{ MJ/Kmol}$$

Equation 2-14 Gibbs Values at 3000 K

Oxygen is 0 MJ/Kmol because free energy is based on the enthalpy of formation, which is the enthalpy required to form 1 mole of a compound from its base elements at the standard state. (Heywood, 1988, p. 76) Oxygen consists of its elements which are already in their standard state therefore there is no change in enthalpy. Therefore, the free energy available for CO₂ is:

$$\Delta G_{overall}^0 = -395.461 - (-367.816)$$

$$\Delta G_{overall}^0 = -27.645 \text{ MJ/Kmol}$$

$$\Delta G_{overall}^0 = -27645000 \text{ J/Kmol}$$

Equation 2-15 Overall Gibbs Free Energy for Carbon Dioxide

3. One-Zone Model

In a simple one-zone combustion model the entire volume is seen as an ideally mixed volume termed homogenous and that the volume changes with crank angle but not the mass. (Merker, et al., 2006) The one-zone model will be used to calculate an average combustion temperature to aid the development of a two-zone model.

3.1 Pressure versus Volume

The first step to analysing the combustion process in the engine is to look at how the change in pressure relates to the change in volume.

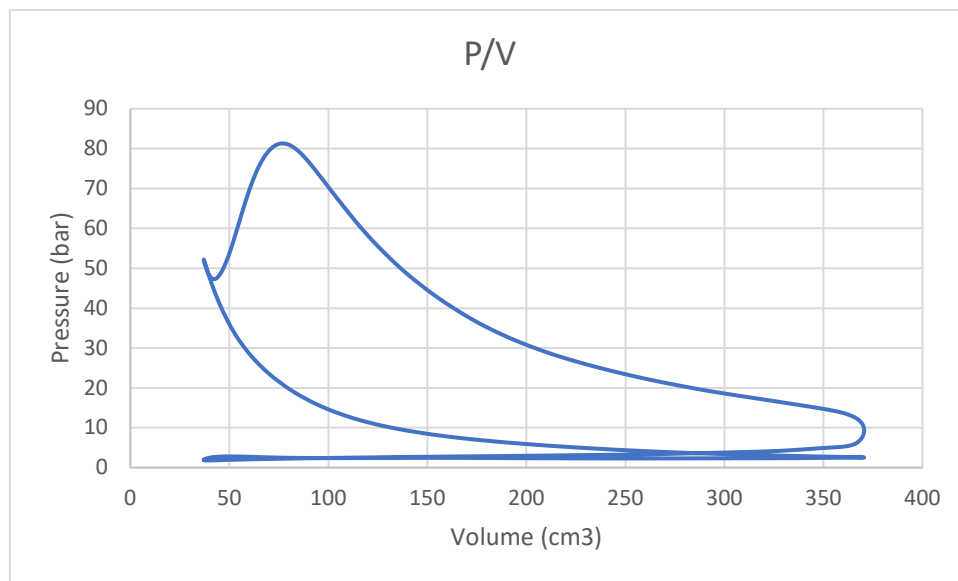


Figure 3-1 PV Diagram of the Ford Fox at 3000 RPM at FL

Looking at *figure 3-1* there is a spike in pressure followed by a drop and then a rapid increase in pressure with declining volume. The first spike is due to the piston reaching TDC causing maximum pressure from compression alone, as the piston begins to travel back down pressure drops with volume increasing and then combustion occurs, rapidly increasing the pressure. This is due to the ignition being heavily retarded to help prevent auto-ignition occurring and is common in most turbo engines and sometimes NA engines.

Comparing *figures 3-1, 3-2 and 3-3* this initial spike then dip gradually disappears as the ignition is advanced as the RPM increases as the chance of auto-ignition decreases. This is due to the flame speed at higher RPM is faster thus there is less time for heat transfer to occur as turbulent flame velocity can be seen as:

$$S_T = S_L + k \times RPM$$

Equation 3-1 Turbulent Flame Velocity (McDonald, 2018)

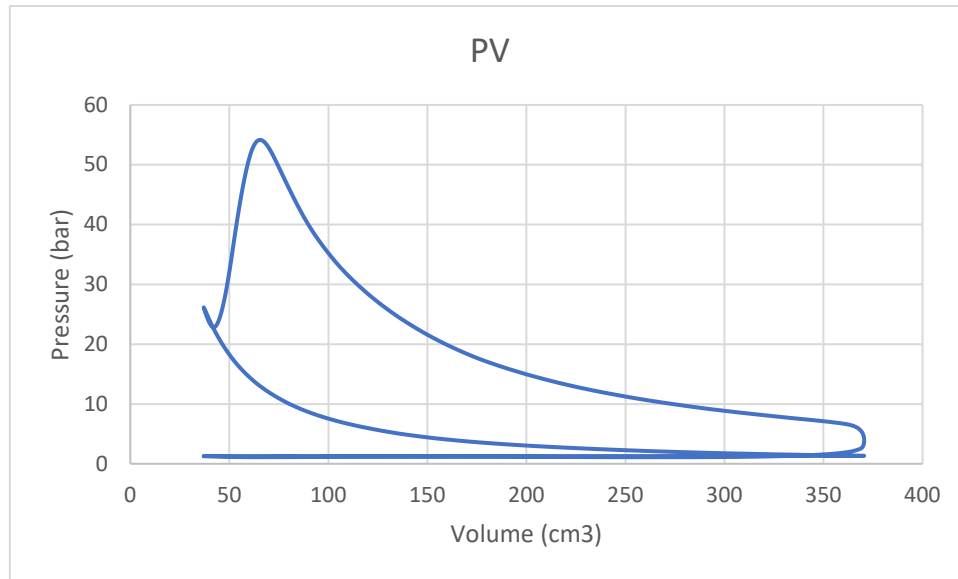


Figure 3-2 PV Diagram of the Ford Fox at 1000 RPM at FL

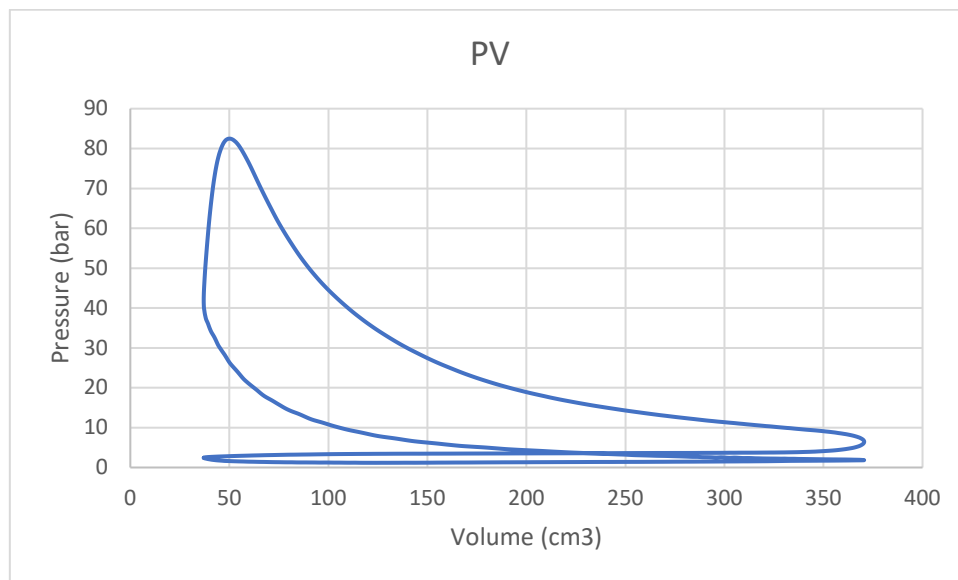


Figure 3-3 PV Diagram of the Ford Fox at 6500 RPM at FL

Looking at *figure 3-3* the pumping loop has increased, this indicates that the engine could be choking as the piston work has now increased to try and draw air into the cylinder but also because at a high RPM there is insufficient time for all the exhaust gas to escape increasing the residual gas in the cylinder which increases the residual cylinder pressure increasing the pumping work. (Baechtel, 2015)

3.2 Polytropic Index

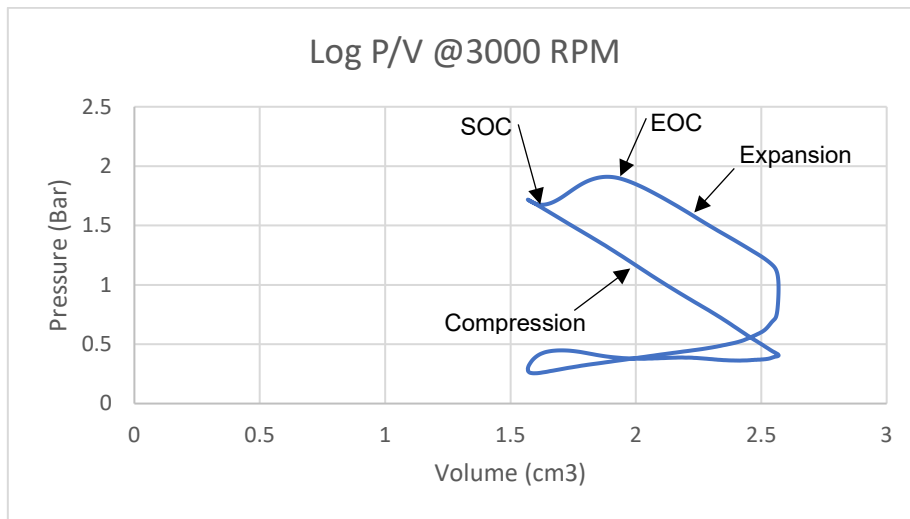


Figure 3-4 Log P/V Diagram for Ford Fox at 3000 RPM

By taking the logarithms of the provided pressure and volume, graphs similar to that of *figure 3-4* can be obtained. SOC occurs after the volume begins to increase again, this can be explained by *figure 3-5* in that due to the timing ignition occurs after TDC when the piston is travelling back down, this is done to reduce in-cylinder temperatures to help prevent pre-ignition of the un-burnt mixture. (Walker, 2001, p. 23)

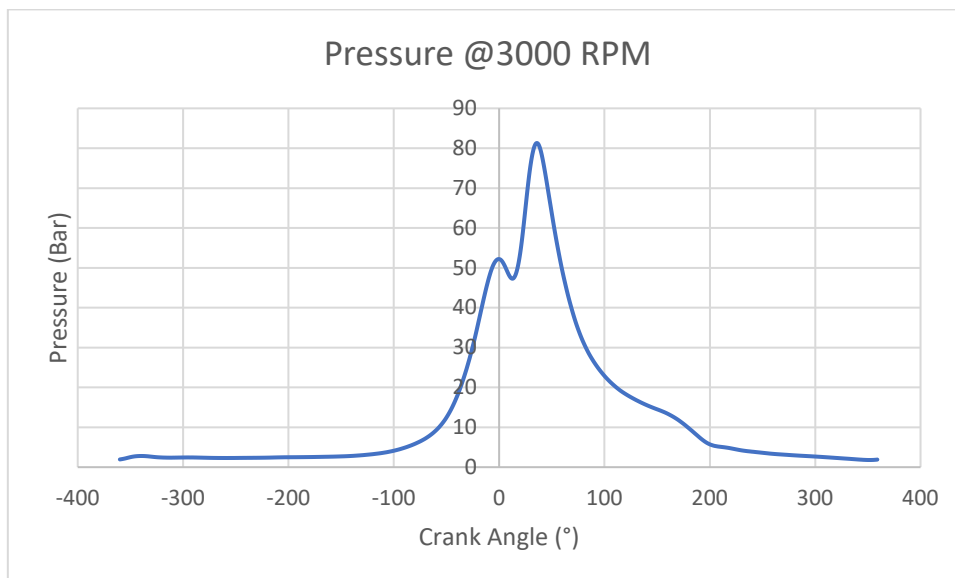


Figure 3-5 Ford Fox P/V Diagram at 3000 RPM

The compression of the unburnt mixture and the expansion of the burnt mixture are close to an adiabatic isentropic process pV^γ . (Heywood, 1988, p. 385) However, in-depth studies have shown that the processes fit closer to a polytropic relation $pV^n = \text{constant}$. (Lancaster, et al., 1975) (Caris & Nelson, 1959) Meaning that if:

$$pV^n = C$$

$$\begin{aligned} \ln p_1 V_1^n &= \ln p_2 V_2^n \\ \ln p_1 + n \ln V_1 &= \ln p_2 + n \ln V_2 \\ n &= \frac{-(\ln p_2 - \ln p_1)}{(\ln V_2 - \ln V_1)} \end{aligned}$$

Equation 3-2 Polytropic Index

Using equation 3-2 gives:

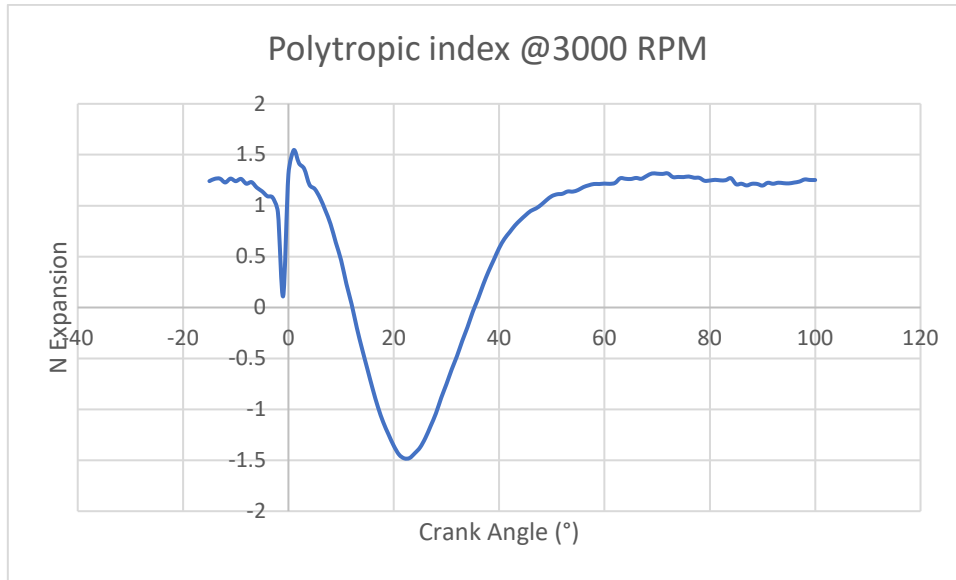


Figure 3-6 Expansion Polytropic Index for Ford Fox at 3000 RPM

Another method to calculate the polytropic index is to calculate the gradient of the compression and expansion slopes on the log P/V diagram (Rassweiler & Withrow, 1938) it is also suggested that an average across the middle regions of both slopes should yield the greatest accuracy. (Asgari, et al., 2012) Gradient can be defined as:

$$\text{Gradient} = \frac{\Delta y}{\Delta x}$$

Equation 3-3 Log P/V Gradient

An issue found was that no matter where the gradient was taken from the slopes a different polytropic index was produced. This indicates that although the slopes look straight they are in fact fluctuating. This could be down to measurement errors as the piezoelectric sensors used to measure the cylinder pressure can be thrown off due to several factors such as:

- Inaccurate calibration.
- Sensitivity to temperature causing thermal shock.
- Sensor mounting.
- Mechanical vibration noise.
- Electrical noise.

(Brunt & Pond, 1997)

As these errors would be present in both methods it was decided to use the second method and to keep the calculated polytropic index as a constant throughout calculation, the values of which can be found in *appendix 11.2*.

3.3 Pressure Gained from Combustion

The mechanical compression of the mixture from the piston increases the pressure in the cylinder however, the heat release of the mixture during combustion can also add to the increase in pressure in the system. Using the polytropic relation:

$$p_1 V_1^n = p_{2n} V_2^n$$

$$p_{2n} = p_1 \left(\frac{V_1}{V_2} \right)^n$$

Equation 3-4 Pressure Without Combustion

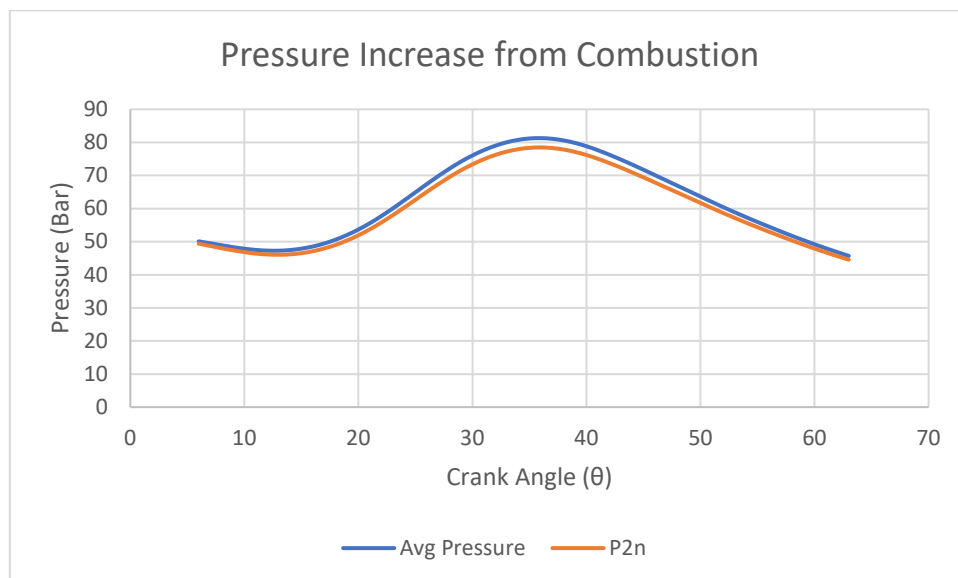


Figure 3-7 Pressure Gained from Combustion on the Ford Fox at 3000 RPM

3.4 Mass Fraction Burned

Calculating the MFB allows us to see the percentage of the mixture that has been burnt at each degree of crank angle.

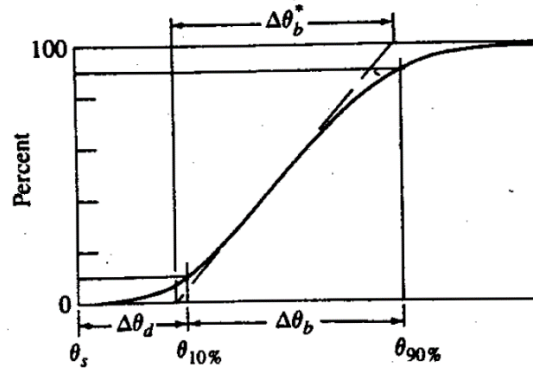


Figure 3-8 Phases of Combustion (Heywood, 1988, p. 390)

Combustion can be split into three sections as seen in *figure 3-8* where:

- $\Delta\theta_d$ = Flame development.
- $\Delta\theta_b$ = Rapid burning.

Flame development begins after spark discharge and usually occurs between 0-10% MFB, although this is dependent by the mixture state and proximity to the spark, this stage only a small fraction of the mixture has burnt meaning that the energy release and as such pressure rise is small. The next stage is rapid burning as the flame front is now propagating across the cylinder and is the crank angle interval required to burn the bulk of the mixture. (Heywood, 1988, p. 389) This stage usually occurs between 10-90% MFB, after 90% MFB there is only a small amount of mixture left to burn as such the combustion process begins to tail off.

Two methods will be used to estimate the MFB; the Rassweiler and Withrow method and the Wiebe function. The R&W method can be defined as:

$$MFB_{\theta} = \frac{\sum_{i=ign}^{i=\theta} \Delta p}{\sum_{i=ign}^{i=EOC} \Delta p}$$

Equation 3-5 Rassweiler and Withrow MFB (Brunt & Emtage, 1997)

Where:

- MFB_{θ} = MFB at crank angle θ .
- Δp = Change in pressure.
- i = integer crank angle location.
- ign = Ignition crank angle location.
- EOC = End of combustion.

Change in pressure can be given as:

$$\Delta p = p_2 - p_1 \left(\frac{V_1}{V_2} \right)^n$$

Equation 3-6 Change in Pressure

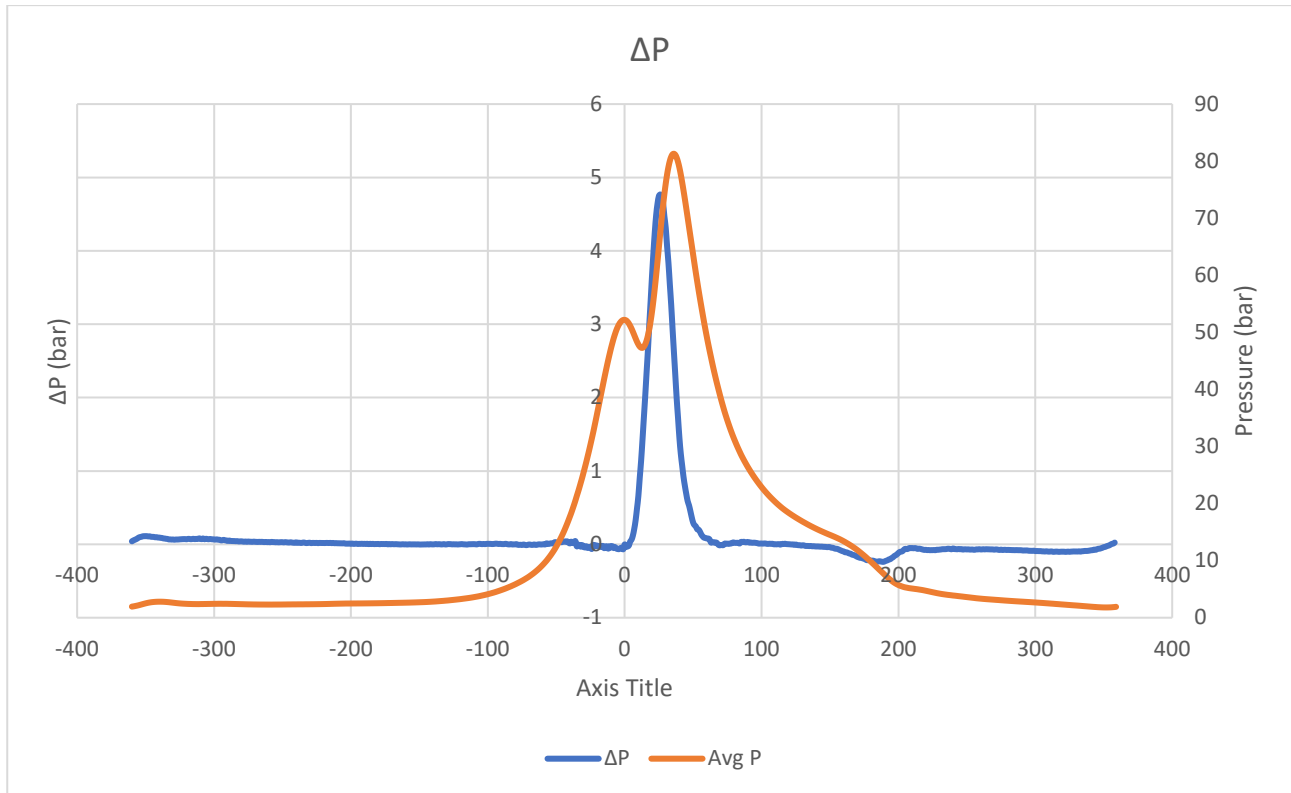


Figure 3-9 Change in Pressure

Using *equation 3-6* allows the SOC and EOC to be estimated as seen in *figure 3-10*, where the value of n used depends on SOC, if SOC begins BTDC then n_{comp} is used, if SOC begins ATDC then n_{exp} is used, a p/v diagram such as *figure 3-1* can be used to determine this, in this case n_{exp} is used. Once the change in pressure stops fluctuating and begins to rise this is seen as the SOC, the accumulation of this pressure is then carried out and then the MFB can be estimated by dividing the Δp accumulation by the final value before Δp becomes negligible or begins to fluctuate again.

-0.03197		
-0.0313		
-0.01222		
0.01841		
0.07564	0.07564	0.00131
0.18387	0.25951	0.00449
0.34236	0.60188	0.01042
0.5698	1.17168	0.02028
0.86224	2.03392	0.03521
1.21591	3.24983	0.05626
1.5963	4.84613	0.08389
1.9851	6.83123	0.11825
2.40002	9.23125	0.1598
2.88722	12.1185	0.20978
3.37553	15.494	0.26821
3.84658	19.3406	0.33479
4.15756	23.4981	0.40676
4.3043	27.8024	0.48127
4.336	32.1384	0.55633
4.28296	36.4214	0.63047
4.10802	40.5294	0.70158
3.81895	44.3484	0.76769
3.36944	47.7178	0.82601
2.78924	50.507	0.8743
2.18741	52.6944	0.91216
1.63962	54.3341	0.94054
1.15862	55.4927	0.9606
0.79633	56.289	0.97439
0.5221	56.8111	0.98342
0.34764	57.1587	0.98944
0.25659	57.4153	0.99388
0.16524	57.5806	0.99674
0.11707	57.6976	0.99877
0.07109	57.7687	1
0.04752		
0.03367		
0.0625		

Figure 3-10 From Left to Right; Δp , Δp Accumulation, MFB.

The second method using the Wiebe function can be defined as:

$$MFB = 1 - \exp \left[-a \left(\frac{\theta - \theta_0}{\Delta\theta} \right)^{m+1} \right]$$

Equation 3-7 Wiebe Function (Heywood, 1988, p. 390)

Where:

- θ_0 = SOC.
- θ = Crank Angle.
- $\Delta\theta$ = Combustion duration.
- a & m = Adjustable parameters.

Both adjustable parameters can be determined using the curve fitting tool in Matlab as seen in *appendix 11.3* however, doing it this way requires method one to be carried out initially but gives the results seen in *figure 3-11*. However, if values suggested by Heywood of $a = 5$ & $m = 2$ (Heywood, 1988, p. 390) (Heywood, et al., 1979) we can see that the MFB curve is drastically different from previous calculations. Lotus recommends values of $a = 10$ & $m = 2$ for gasoline engines (Dresler & Richtar, 2011) which can be seen to be a closer fit to the Rassweiler and Withrow method.

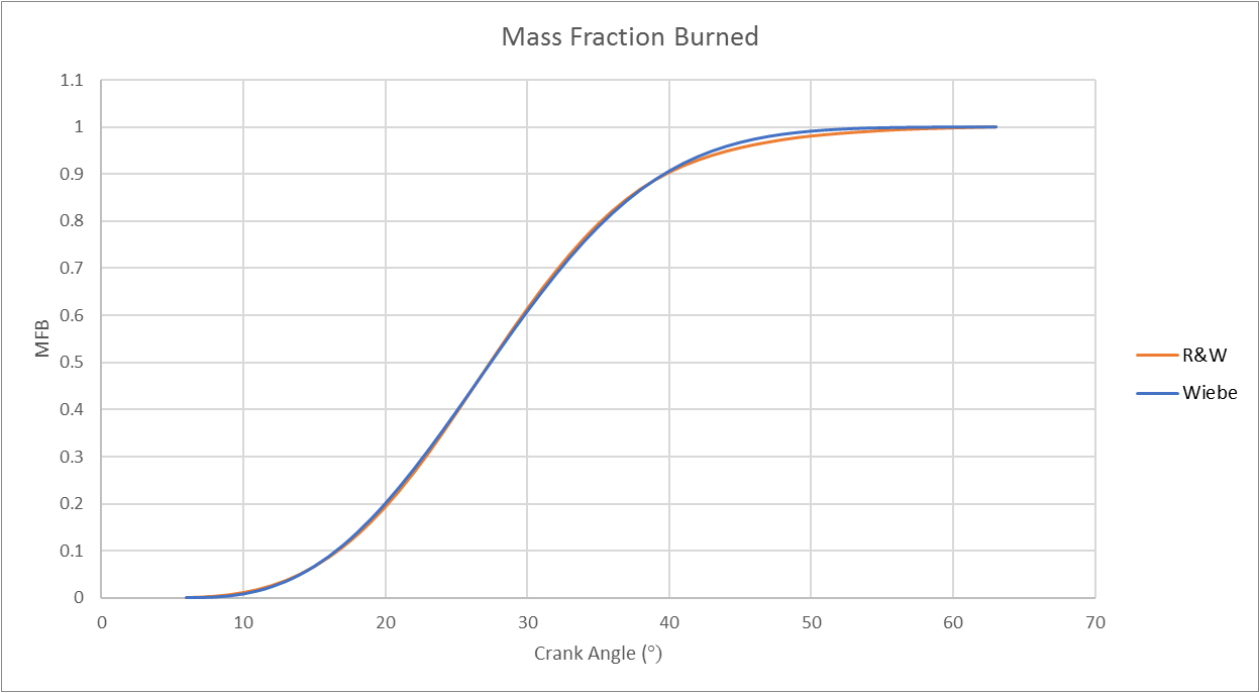


Figure 3-11 MFB with Both Calculated Methods for the Ford Fox at 3000 RPM

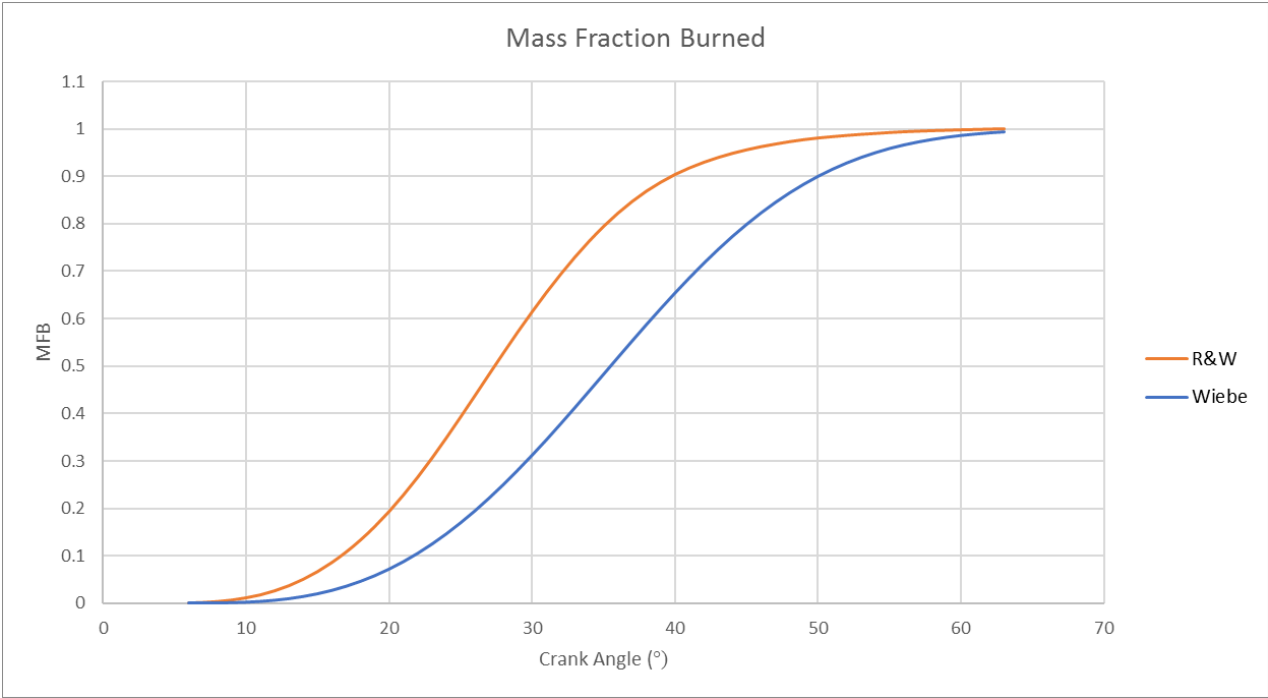


Figure 3-12 MFB Wiebe Function with Suggested a & m Values for the Ford Fox at 3000 RPM

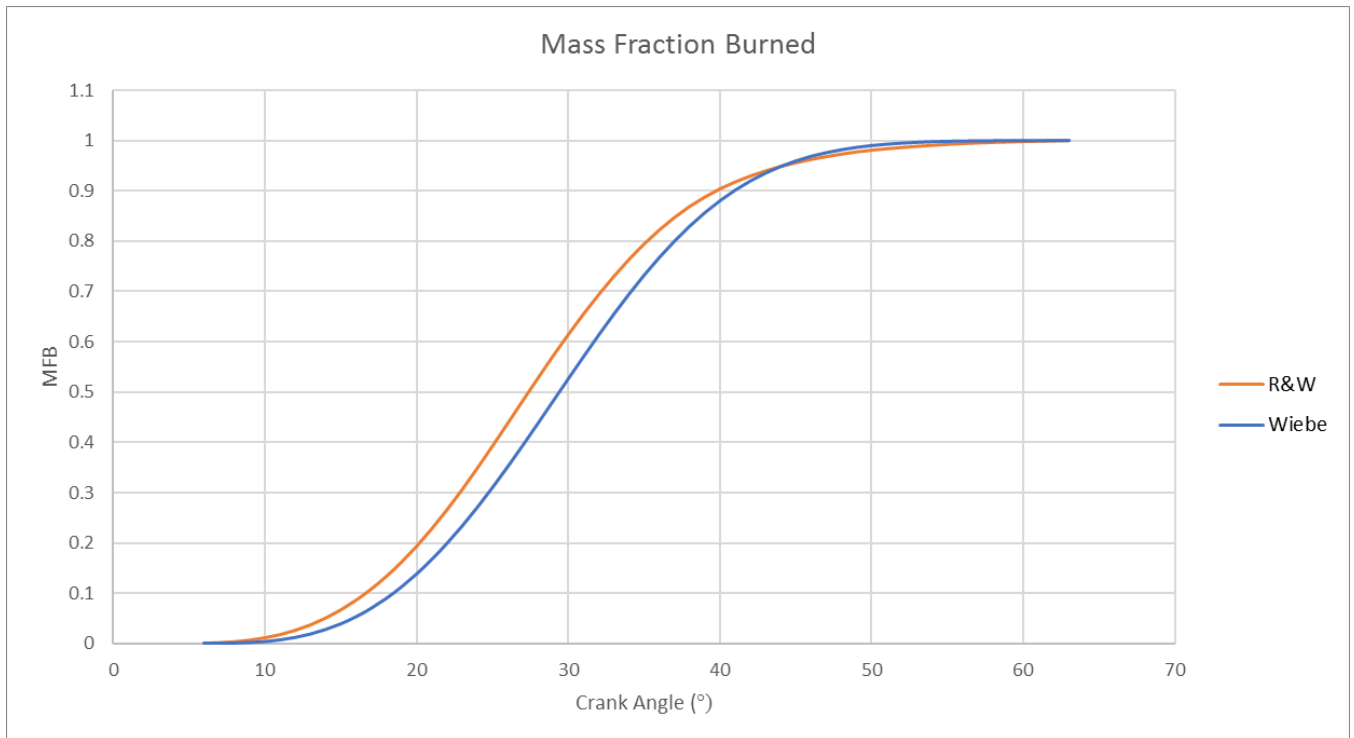


Figure 3-13 MFB Wiebe Function with Lotus Suggested a & m Values for the Ford Fox at 3000 RPM

However, it was observed that by using the R & W method that MFB concluded to 1 equalling to 100% burnt whilst any iteration of the Wiebe method never reached 100% burnt. In practice however, the mixture will rarely reach 100% MFB. This is due to some of the mixture reaching places that the flame will not reach, it has been observed that 6% of the mixture escapes into piston ring gap of which 2% will flow back out towards EOC. (Merker, et al., 2006, p. 120) Unburnt HC will also reduce the % MFB due to the fuel not completely oxidising which will mainly occur in rich patches within the cylinder. (Li, et al., 2012) In this model however, it will be assumed that all of the homogenous mixture will be burnt.

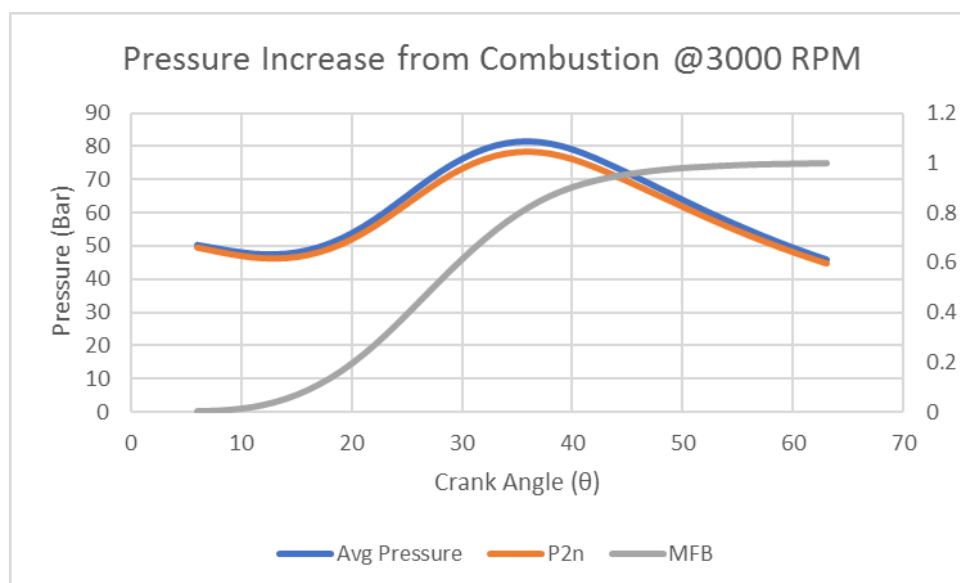


Figure 3-14 MFB with Pressure

Figure 3-14 shows a clear relationship between the pressure in the cylinder and the MFB in that peak pressure occurs when most of the mixture has been burnt and rapidly increases as MFB rapidly increases.

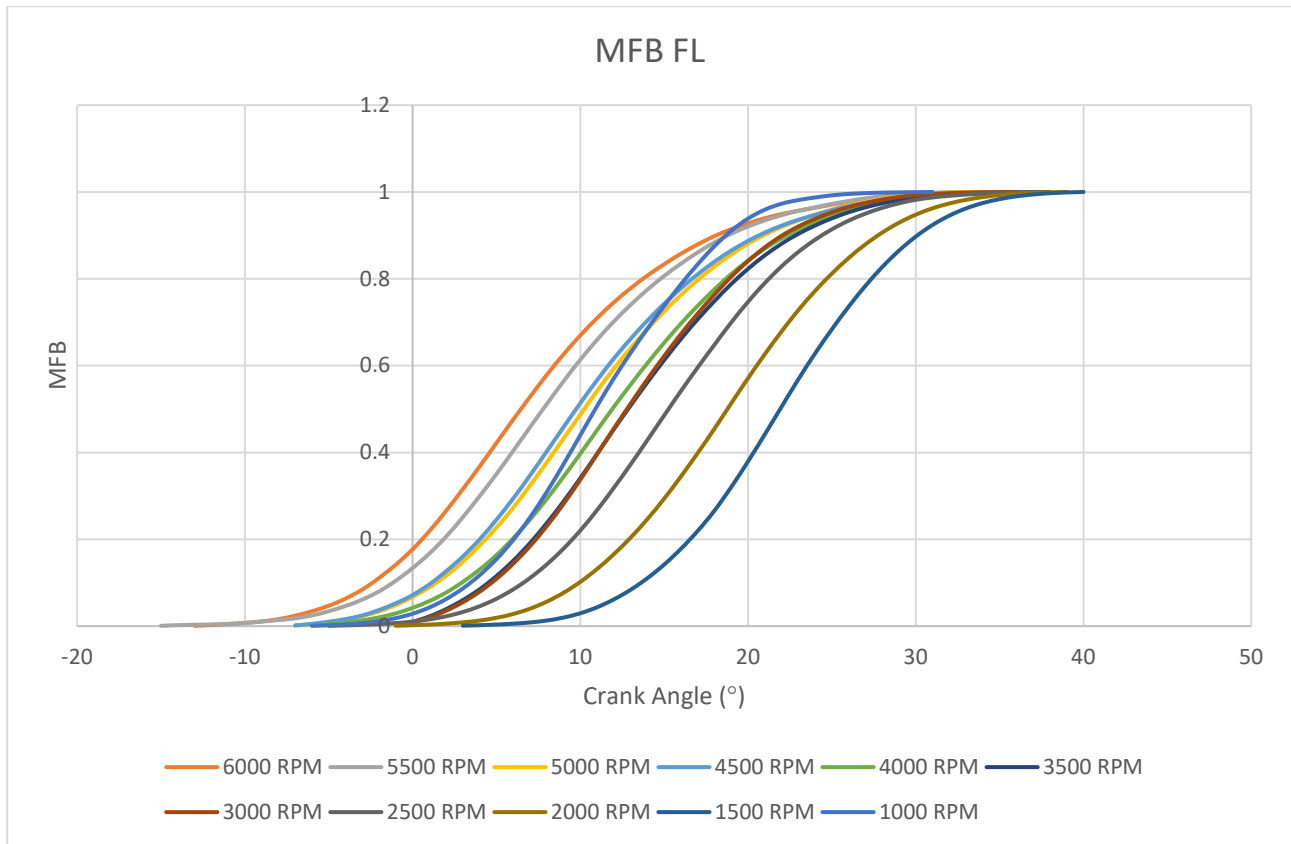


Figure 3-15 MFB FL RPM Range for Ford Sigma

Figure 3-15 gives a good overview of the combustion characteristics over the RPM range. At low RPM, ignition has been heavily retarded as everything is moving much slower meaning that there is more time for heat transfer to occur increasing the likelihood of pre-ignition. This means that combustion must occur in a shorter duration increasing the curve steepness. As RPM increasing this likelihood decreases meaning that the timing can be advanced but also the burn duration increases because the piston is now moving faster therefore more time is needed to burn the mixture completely.

3.5 In-Cylinder Mass

Using the data provided by the Ford data sheets for both engines found in *appendix 11.7 & 11.8*, the mass of the mixture entering the cylinder can be determined. Both sheets provide the air mass into the cylinder (Kg/h) and the fuel mass (Kg/h) both of which need to be converted into Kg/rev:

$$\text{Air mass per cylinder (Kg /rev)} = \frac{\text{Air mass (Kg /h)}}{60 \times \text{RPM} \times \frac{\text{No. of Cylinders}}{2}}$$

$$\text{Fuel mass per cylinder (Kg /rev)} = \frac{\text{Fuel mass (Kg /h)}}{60 \times \text{RPM} \times \frac{\text{No. of Cylinders}}{2}}$$

Equation 3-8 Fuel and Air Mass into the Cylinder per Revolution

There the total mass in the cylinder is:

$$m_{total} (Kg) = \text{Fuel mass} + \text{Air mass}$$

Equation 3-9 Total In-Cylinder Mass

However, both data sheets have information that can change this mass. The Fox data has information regarding the residual gas fraction present in the engine, at full load the RG present is not EGR as such but part of the combustion product that remains in the cylinder which then mixes with the fresh charge (Liu & Karim, 1996) increasing the total mass. Including the residual gas, we get:

$$M_{total.RG} (Kg) = (RGF \times M_{total}) + M_{total}$$

Equation 3-10 Total In-Cylinder Mass with Residual Gas

The Sigma data contains the amount of blowby occurring at each RPM & load which is when the mixture in the combustion chamber makes its way into the crankcase reducing the total in-cylinder mass, the data gives blowby in litres/minute, we can obtain the % of mixture lost by:

$$\text{Blowby (l /sec)} = \frac{\text{Blowby (l /min)}}{60}$$

$$\text{Air entering the cylinder (l /rev)} = \frac{\frac{\text{Engine Displacement (l)}}{2}}{\text{Revs/s}}$$

$$\text{Blowby \% lost} = \frac{\text{Blowby}}{\text{Air entering the cylinder}} \times 100$$

Equation 3-11 Percentage Mass Loss through Blowby

The total mass can then be reduced by the % lost caused by blowby.

3.6 Gas Constant

Using the ideal gas law, if:

$$pV = mRT$$

Is relating the pressure and volume to the mass of the mixture in kg and:

$$pV = n\tilde{R}T$$

Relates it to the number of moles in the mixture. If the number of moles is 1 then:

$$mRT = \tilde{R}T$$

In which case the relation between the gas constant and the universal gas constant is:

$$R = \frac{\tilde{R}}{m}$$

Equation 3-12 Gas Constant

As the universal gas constant is known to be 8314 J/Kmol K, it means that the molecular mass of both the unburnt reactants and burnt products must be calculated. The mass of isooctane C_8H_{18} , can be determined through the equation:

$$m_{fuel} = \phi[(8 \times m_c) + (18 \times m_H)]$$

Equation 3-13 Isooctane Mass

The mass of the air entering the cylinder can be equated as:

$$m_{air} = x(n \cdot m_{O_2} + 3.76 \cdot m_{N_2})$$

Equation 3-14 Air Mass

The molecular mass of the reactants (Kg/mol) then can be seen as:

$$m_{reactant} = \frac{m_{fuel} + m_{air}}{\phi + [x(1 + 3.76)]}$$

Equation 3-15 Reactant Molecular Weight

Similarly, for the molecular weight of the product (Kg/mol):

$$m_{product} = \frac{(n \cdot CO_2 \times m_{CO_2}) + (n \cdot H_2O \times m_{H_2O}) + (n \cdot O_2 \times m_{O_2}) + (n \cdot CO \times m_{CO_2}) + (n \cdot N_2 \times m_{N_2})}{(n \cdot CO_2 + n \cdot H_2O + n \cdot O_2 + n \cdot CO + n \cdot N_2)}$$

Equation 3-16 Product Molecular Weight

Where n is the number of moles per species and the molecular masses, m of each species can be found in *appendix 11.1*. *Figures 3-16 & 3-17* show how these masses change with varying FER.

From *equation 3-12* the gas constant for the reactant and product therefore the unburnt mixture and burnt mixture can be given as:

$$R_{un} = \frac{\bar{R}}{m_{reactant}}$$

$$R_b = \frac{\bar{R}}{m_{product}}$$

Equation 3-17 Unburnt and Burnt Gas Constants

Fuel Ratio	RPM	Mol Wt (Kg/mol)	Mol Wt RGF	C	H	H2O	R.Un
0.90	1000	30.12446312	30.11644929	7.207207	16.21622	0	276.0618
0.90	1250	30.12446312	30.12446312	7.207207	16.21622	0	275.9883
0.91	1500	30.13586606	30.13586606	7.272727	16.36364	0	275.8839
0.97	1750	30.22178679	28.59602508	7.76699	17.47573	0	290.7397
1.01	2000	30.27624856	28.89881063	8.080808	18.18182	0	287.6935
1.01	2250	30.27624856	30.27624856	8.080808	18.18182	0	274.6047
1.01	2500	30.27624856	30.27624856	8.080808	18.18182	0	274.6047
1.00	3000	30.2622314	30.2622314	8	18	0	274.7319
1.06	3500	30.35072932	30.35072932	8.510638	19.14894	0	273.9308
1.03	4000	30.30513514	30.30513514	8.247423	18.5567	0	274.3429
1.05	4500	30.33521686	30.33521686	8.421053	18.94737	0	274.0709
1.09	5000	30.38274776	30.38274776	8.695652	19.56522	0	273.6421
1.09	5500	30.38274776	30.38274776	8.695652	19.56522	0	273.6421
1.11	6000	30.41616315	30.41616315	8.888889	20	0	273.3415
1.11	6500	30.41616315	30.41616315	8.888889	20	0	273.3415

Figure 3-16 Reactant Molecular weight and Gas Constant

RPM	Free O2	Free CO	Mol Wt (Kg/mol)	a+b (CO2)/(C)	c (H2O)	2a+b	a (CO2)	b (CO)	Mol wt	R.b
1000	1.25	0	28.63047309	7.207207207	8.108108	16.89189				290.3899
1250	1.25		28.63047309	7.207207207	8.108108	16.89189				290.3899
1500	1.125	0	28.62739339	7.272727273	8.181818	16.81818				290.4211
1750	0.375		28.61445702	7.766990291	8.737864	16.26214				290.5524
2000	0	0.252525253	28.54869621	8.080808081	9.090909	15.90909	7.828283	0.252525	28.54576657	291.2217
2250		0.252525253	28.54869621	8.080808081	9.090909	15.90909	7.828283	0.252525	28.54576657	291.2217
2500	0	0.252525253	28.54869621	8.080808081	9.090909	15.90909	7.828283	0.252525	28.54576657	291.2217
3000	0	0	28.60726563	8	9	16	8	0	28.60432813	290.6255
3500	0	1.595744681	28.24235077	8.510638298	9.574468	15.42553	6.914894	1.595745	28.23946224	294.3806
4000	0	0.773195876	28.42891852	8.24742268	9.278351	15.72165	7.474227	0.773196	28.42600495	292.4487
4500	0	1.315789474	28.30548824	8.421052632	9.473684	15.52632	7.105263	1.315789	28.30259124	293.724
5000	0	2.173913043	28.11312019	8.695652174	9.782609	15.21739	6.521739	2.173913	28.110249	295.7338
5500	0	2.173913043	28.11312019	8.695652174	9.782609	15.21739	6.521739	2.173913	28.110249	295.7338
6000	0	2.777777778	27.97979258	8.888888889	10	15	6.111111	2.777778	27.97693929	297.143
6500	0	2.777777778	27.97979258	8.888888889	10	15	6.111111	2.777778	27.97693929	297.143

Figure 3-17 Product Molecular Weight and Gas Constant

Using the MFB and the two combustion states gas constant, the average gas constant throughout combustion can now be determined:

$$R_{Av} = (MFB \times R_b) + [(1 - MFB) \times R_{un}]$$

Equation 3-18 Average Gas Constant throughout Combustion

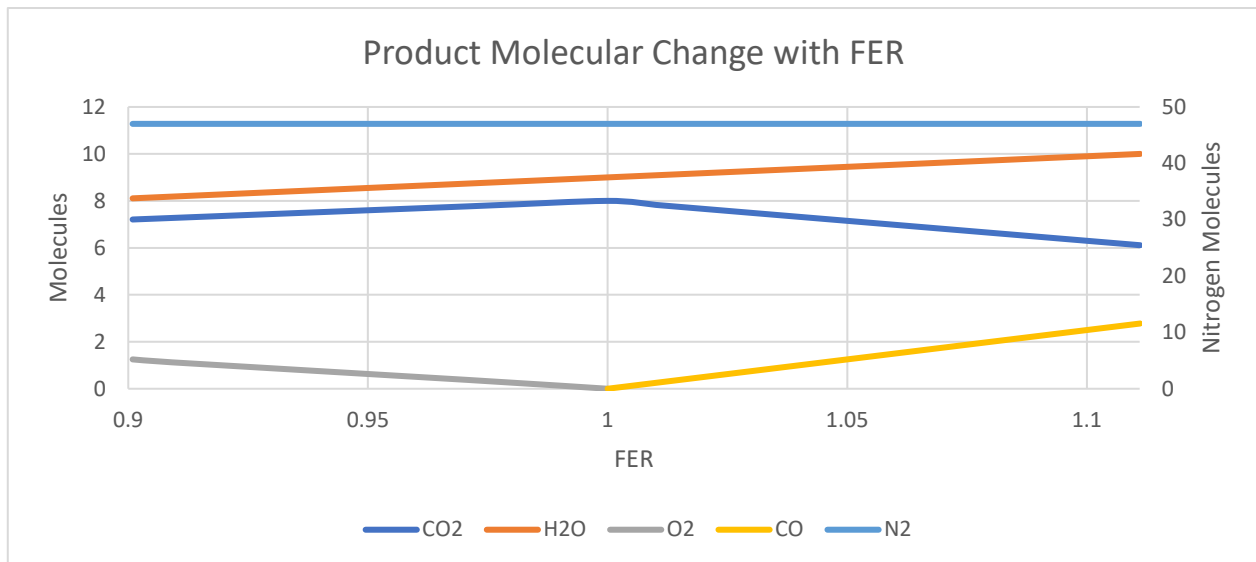


Figure 3-18 Product Composition Change with FER

The nitrogen content stays the same throughout the changes in FER however, oxygen is seen to reduce until stoichiometric this is because as the mixture increases in leanness there is less free O₂ as more of it is being used to oxidise the fuel. As the mixture becomes richer past stoichiometric, CO starts to rise as there is not enough oxygen present during combustion to fully oxidise the fuel as the outer layers of fuel droplets will burn and oxidise however the inner layers do not burn and stay as fuel molecules. This resultant rise in CO partnered with the fact that the hydrogen atoms are also bonding to available oxygen molecules is therefore responsible for the decline in CO₂.

3.7 Average Temperature

With the gas constant and mass of the mixture entering the cylinder calculated the average temperature of the combustion cylinder can now be determined using:

$$T_{Av} = \frac{pV}{m_{total} \times R}$$

Equation 3-19 Average Temperature

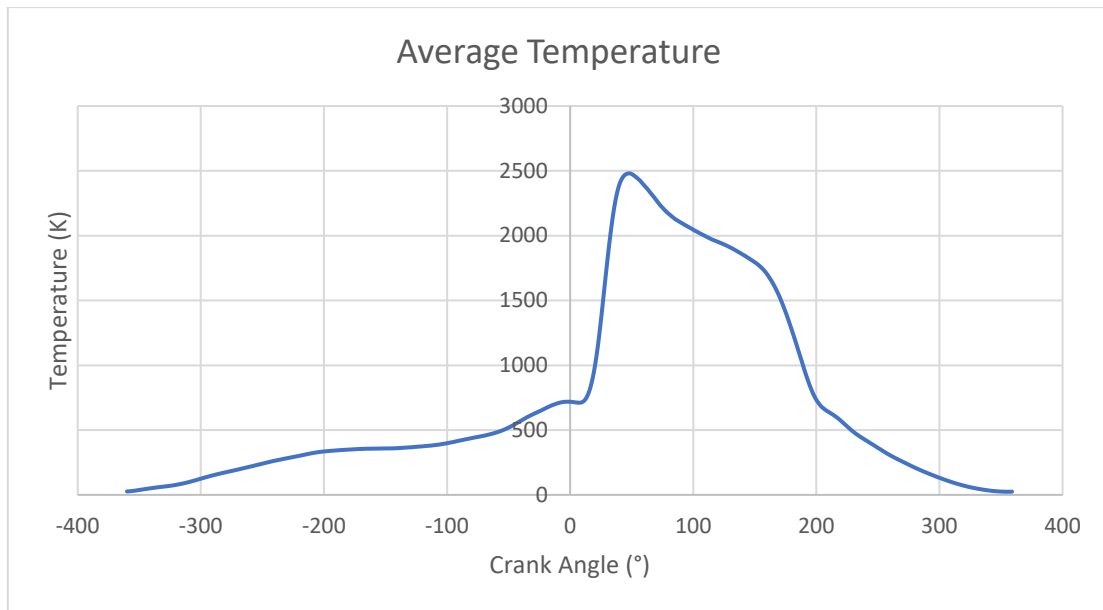


Figure 3-19 Average Temperature at 3000 RPM on the Ford Fox

Up to SOC R_{un} is used then during combustion R_{avg} will be then then R_b after EOC. *Figure 3-19* can be seen to largely follow a pressure/crank angle trace as seen in *figure 3-5* in that after combustion is finished roughly after 60° ATDC pressure begins to drop from the expansion process and then around 20° ABDC the exhaust valve opens resulting in the final rapid heat loss of the system.

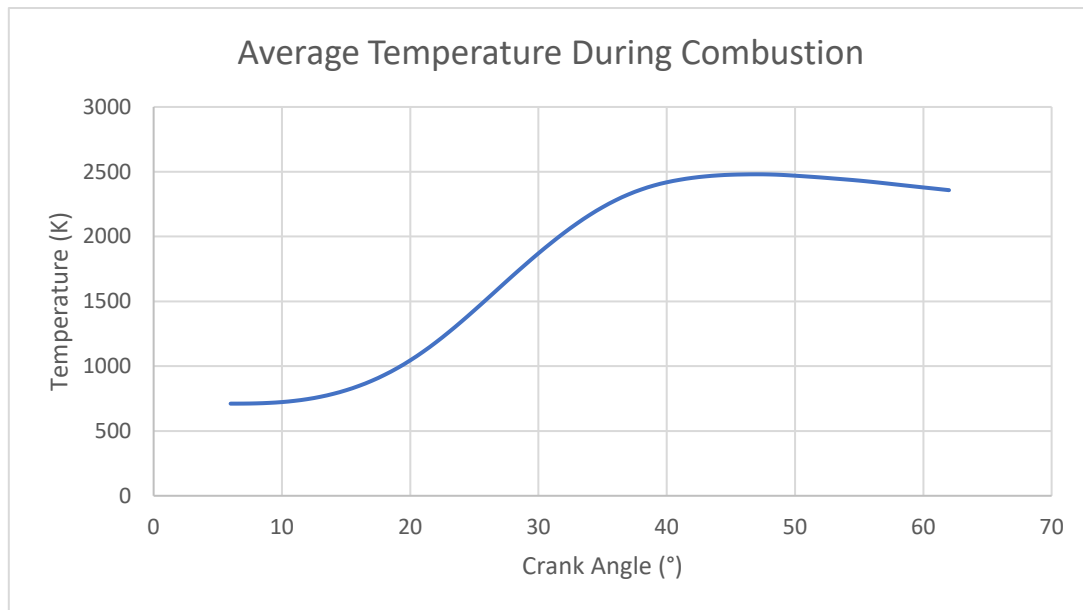


Figure 3-20 Average Temperature during Combustion at 3000 RPM on the Ford Fox

Figure 3-20 follows closely to a MFB curve in that there is a period where the temperature steadily increases as the flame develops, followed by a rapid increase in temperature as the flame front spreads increasing the pressure. Thus, the temperature in the cylinder and then tailing off at the end as most of the mixture has burnt and expansion is occurring, decreasing the pressure and temperature of the system.

4. Two-Zone Model

Previously, the one-zone model assumed the entire cylinder volume as one body to obtain the average temperature, a two-zone model attempts to split this body into two zones; the unburnt and burnt zone with the flame front as the dividing factor. Whilst these two zones will have different volumes and temperatures they will still share the same pressure.

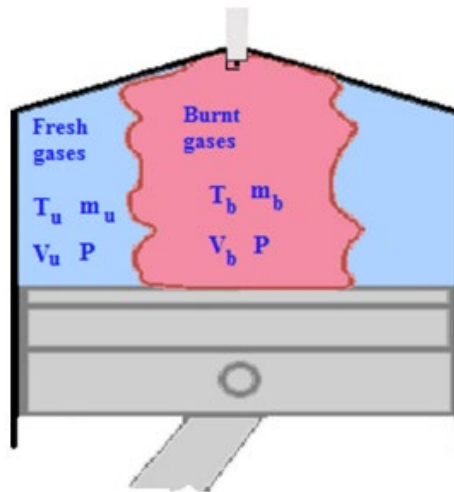


Figure 4-1 Two-Zone Combustion Model (Karthikeyan, et al., 2015)

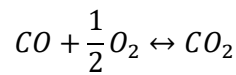
A two-zone model is important for NO_x prediction as it forms in both the flame front and the post flame gases which is the burnt zone. This is because as the flame front progresses the cylinder pressure increases so the burnt gases produced early during the combustion process are compressed to a higher temperature and because NO_x formation depends on the amount of free O₂ and the temperature, post flame gases NO_x production dominates flame produced NO_x. (Heywood, 1988, p. 574) In regard to the flame front it can itself be represented as its own zone. However, because of simple assumptions about the reaction kinetics, lack of solved balance equations and that it is assumed to be extremely thin ~0.1mm, with no mass, this zone is not usually considered to be an independent zone (Merker, et al., 2006, p. 187) and as such it just serves as a boundary for the model.

One of the main assumptions of this model is that the mixture is homogenous; the air and fuel is perfectly mixed meaning that there are no lean or rich patches present in the cylinder. Whilst this could be possible in a port injection engine due to both these engines being GDI there is rarely enough time for the mixture to fully atomize leading to lean and rich spots that can cause issues for NO_x prediction. This is because these different patches change the combustion characteristics due to their differing chemical composition which also can influence flame speed and temperature.

4.1 Specific Heat of Reactants

To calculate the specific heat, two assumptions must be made in that the unburnt mixture is frozen in composition as the chemical reactions are so slow that they have a negligible effect on composition, whilst the second assumption is that the burnt mixture is in chemical equilibrium due to the reactions being so rapid that the mixture state changes. (Heywood, 1988, p. 85)

Chemical equilibrium is the process in which species in a mixture react together, producing and removing species at equal rates. An example would be CO₂, at a sufficient enough temperature for dissociation to occur which will be covered later. The molecules would dissociate into CO and O₂ molecules respectively, however, due to chemical equilibrium occurring whilst CO₂ is dissociating, CO & O₂ are both recombining creating CO₂ satisfying the equation:



Equation 4-1 Carbon Dioxide Chemical Equilibrium (Heywood, 1988, p. 86)

With this in mind, for each species in its standard state at a given temperature its specific heat can be given as:

$$\begin{aligned} \frac{\tilde{C}_{p,i}}{\tilde{R}} &= a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4 \\ \therefore \tilde{C}_{p,i} &= \tilde{R}(a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4) \end{aligned}$$

Equation 4-2 Specific Heat for a Given Species (Heywood, 1988, p. 130)

The coefficients a_i are provided by Heywood and were obtained from JANAF originally taken from the NASA equilibrium program found in *appendix 11.4*. (Heywood, 1988, p. 130) For each species there are two sets of coefficients, a set for temperature ranges between 300-1000K which will be used in the unburnt zone and a set for temperatures between 1000-5000K for the burnt zone. The temperature T in the equation relates to the average temperature before SOC in the cylinder as the specific heat ratio is needed to determine the temperatures of the unburnt zone and then it will use the previous unburnt temperature thereafter until EOC. Similarly, the specific heat for a given fuel in the vapour phase can be determined with:

$$\tilde{C}_{p,fuel} = 4184 \times (A_{f1} + A_{f2}t + A_{f3}t^2 + A_{f3}t^2 + A_{f4}t^3 + \frac{A_{f5}}{t^2})$$

Equation 4-3 Specific Heat for a Given Fuel (Heywood, 1988, p. 130)

The coefficients A_f provided by Heywood were originally found by fitting *equation 4-3* to data from Rossini *et al* (Rossini, et al., 1953). The value 4184 is used to convert the specific heat value from cal/gmol.K to J/Kmol.K and $t = T_{Av}/1000$.

Once the specific heat for each species is determined, the average value can be determined using:

$$\tilde{C}_{p,Avg} = \frac{(\tilde{C}_{p,fuel} \times \phi) + 12.5(\tilde{C}_{p,O_2} + (3.76 \times \tilde{C}_{p,N_2}))}{\phi + (12.5 \times (1 + 3.76))}$$

Equation 4-4 Average Specific Heat of the Mixture

To find the specific heat ratio of the mixture:

$$\tilde{C}_v = \tilde{C}_{p.Avg} - \tilde{R}$$

$$\gamma = \frac{\tilde{C}_{p.Avg}}{\tilde{C}_v}$$

Equation 4-5 Ratio of Specific Heats

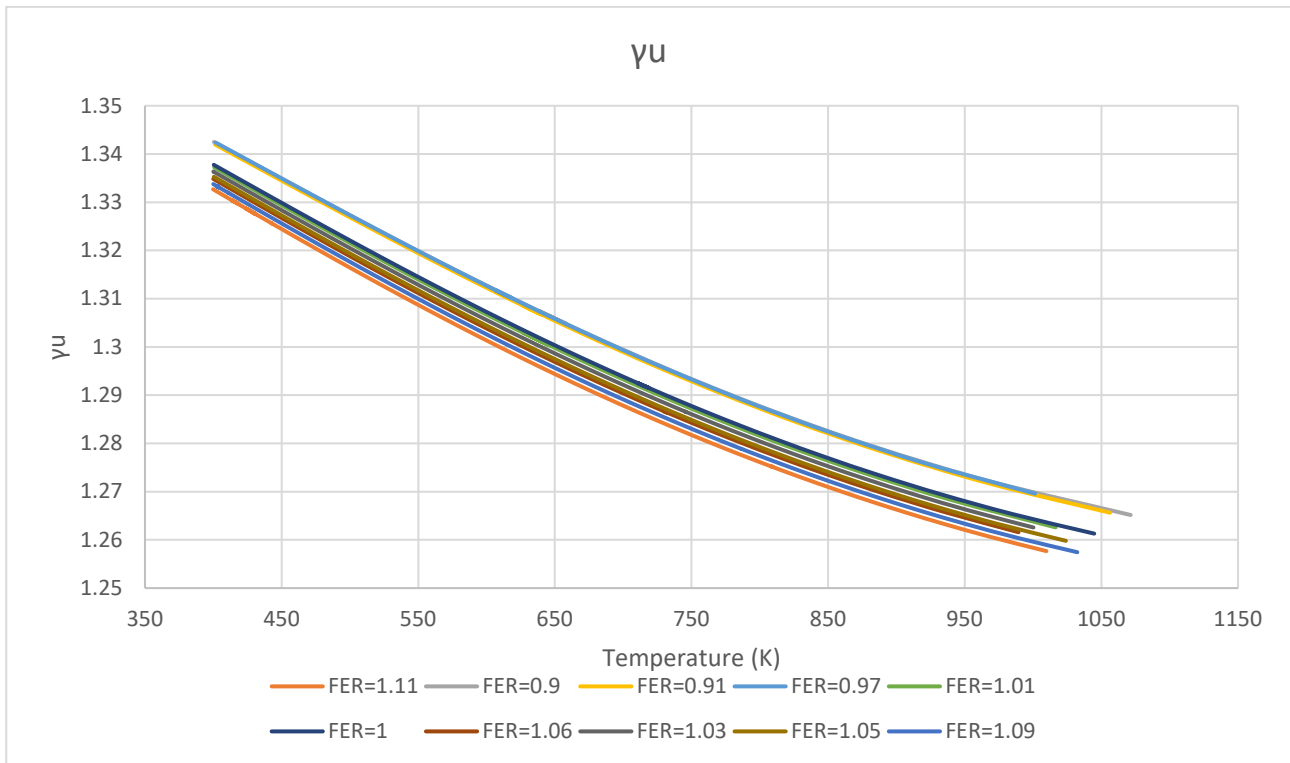


Figure 4-2 Calculated Ratio of Specific Heats for each FER on the Ford Fox

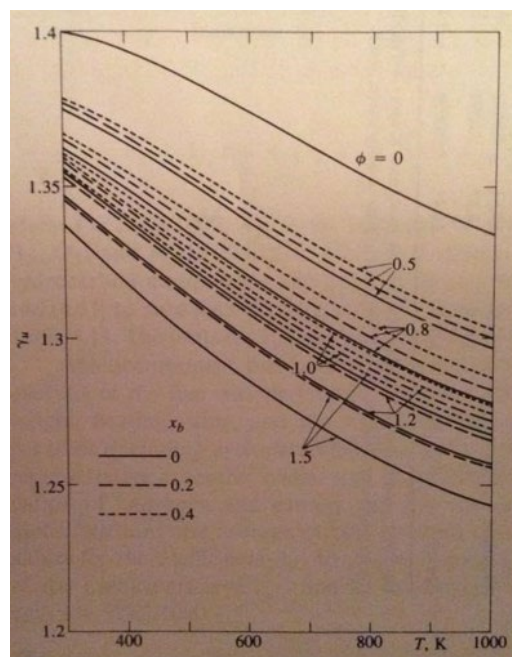


Figure 4-3 Ratio of Specific Heat as Given by Heywood (Heywood, 1988, p. 134)

4.3 Unburnt and Burnt Zone Temperatures

Previously the temperature calculated was an average of the two zones combined and was related to the change in pressure and volume in the cylinder. Firstly, when the unburnt zone is calculated in this model it is assumed that no heat transfer is occurring between the two zones where in reality heat energy would be transferring between the burnt zone into the unburnt zone, with this in mind the unburnt temperature can be given as:

$$T_{un2} = T_{un1} \left(\frac{p_2}{p_1} \right)^{\frac{\gamma-1}{\gamma}}$$

Equation 4-6 Unburnt Temperature

As previously mentioned γ is a function of T_{un} however, T_{un} is also a function of γ . Therefore, to calculate the first γ before SOC the average temperature is used enabling the first unburnt temperature to be calculated at SOC which allows a new γ gamma to be calculated to be then used for the next T_{un} . Unfortunately, this means the model is one step behind γ and as such would benefit from small crank angle intervals. Now that the unburnt temperature has been determined we can now obtain the unburnt volume from the ideal gas law:

$$pV_{un} = (1 - MFB) \times m_{total} \times R_{un} \times T_{un}$$

$$\therefore V_{un} = \frac{(1 - MFB) \times m_{total} \times R_{un} \times T_{un}}{p}$$

Equation 4-7 Volume of the Unburnt Zone

Because of the assumption that the unburnt zone and the burnt zone equal the total volume the volume of the burnt zone can therefore be defined as:

$$V_{total} = V_{un} + V_b$$

$$V_b = V_{total} - V_{un}$$

Equation 4-8 Volume of the Burnt Zone

Therefore:

$$pV_b = MFB \times m_{total} \times R_b \times T_b$$

$$T_b = \frac{pV_b}{MFB \times m_{total} \times R_b}$$

Equation 4-9 Burnt Temperature

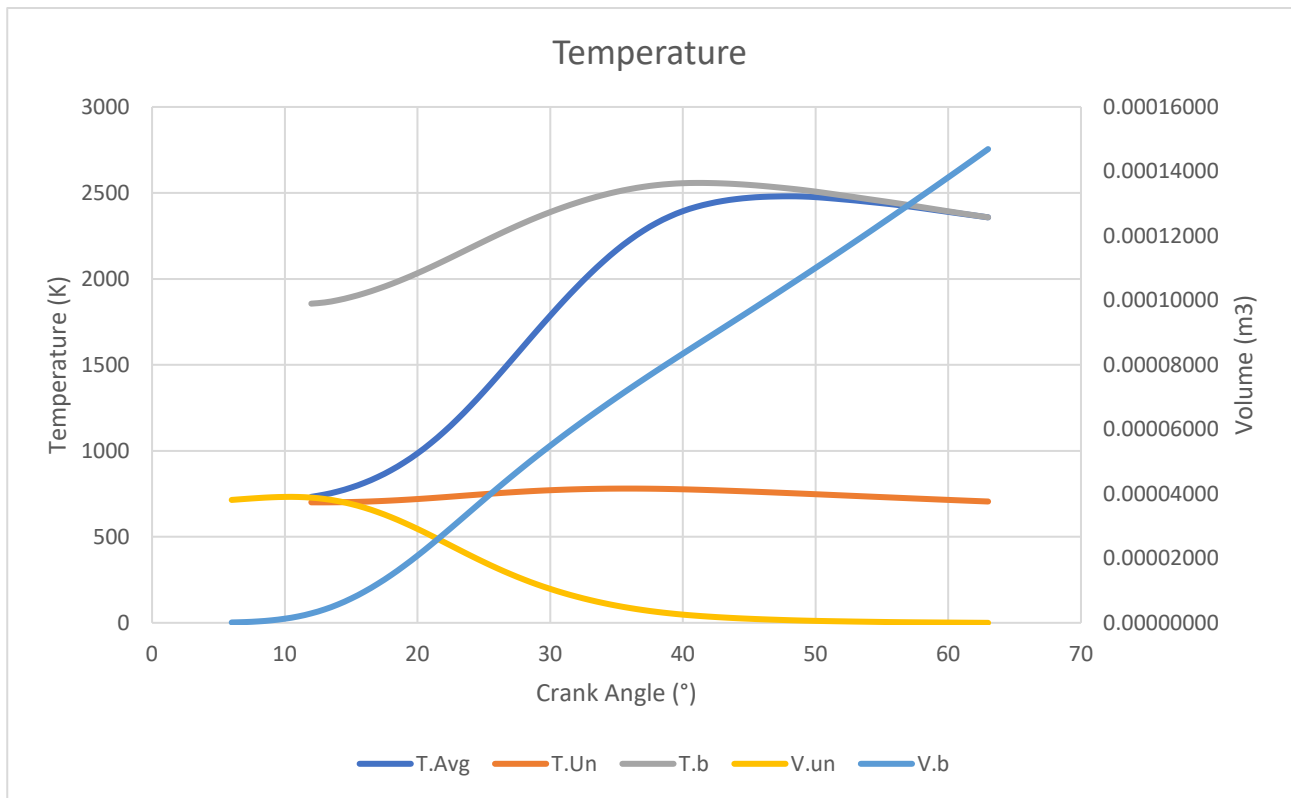


Figure 4-4 Temperatures and Volumes of the Ford Fox during combustion at 3000 RPM

Another limitation of this model in relation to the homogeneous assumption is that the temperature in the unburnt and burnt zone is assumed to be uniform. This can provide complications in predictions as NO_x formation is dependent on temperature adding to the limitations of the model.

Studying *figure 4-5* peak temperature of the burnt zone is 2558 K at 41° ATDC and 780 K at 36° ATDC in the unburnt zone. This delay could be due to heat transfer between the two zones with the unburnt zone experiencing peak temperature at a peak pressure of 81.294 bar. The unburnt temperature stays under 1000 K to prevent auto ignition from occurring and as the volume of the unburnt zone decreases and pressure begins to drop so too does the unburnt temperature as the combustion process is starting to slow down as it comes to an end. As combustion does start coming to an end, the average and burnt zone temperatures come together, showing that the burnt zone is predominant in the cylinder at that point. The unburnt volume at the start of combustion is the volume of the cylinder and as combustion occurs and this volume shrinks, the burnt volume rapidly increases as the flame front progresses and the piston travels back down increasing the volume of the cylinder.

A problem was encountered when calculating the burnt temperature as seen in *figure 4-6*, it is believed this is caused by a calculation error of the MFB in that an incorrect SOC was chosen, as MFB at SOC is small and is the denominator for the burnt temperature, this results in a higher burnt temperature and thus is removed from any further calculations which is apparent in *figure 4-5*, fortunately NO_x formation <2000 K is low which will be seen later on so the removal of this outlier in temperature does not have negative consequences in later calculations.

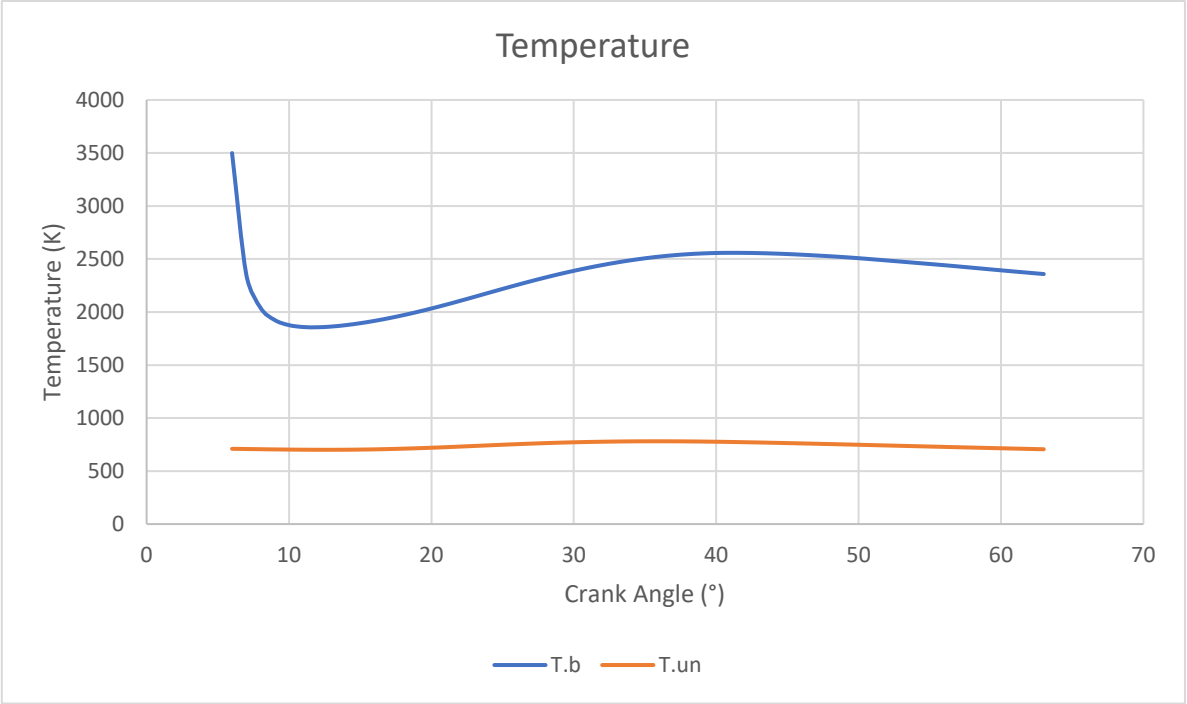
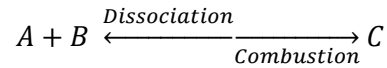


Figure 4-5 Unburnt and Burnt Temperatures on the Ford Fox

5. Dissociation

For temperatures of 1700 K dissociation of products must be accounted for. (Backman, 2011) At this point thermal agitation occurs meaning that combustion products begin to dissociate back to their reactant materials giving a reversibility to the reaction. This can be visualised as:



Equation 5-1 Dynamic equilibrium (Goodger, 2000, p. 284)

When a high temperature is sustained a state of equilibrium occurs which means that the reactant and product materials proportion remains constant. These proportions can be determined using partial pressure equilibrium constants at given temperatures. (Goodger, 2000, p. 284)

5.1 Reaction Rate Constants

Through experiment the rate of combustion/dissociation can be determined and have been found to be proportional to the instantaneous concentration of each species in that:

$$\text{Forward Reaction Rate} = K_f \times [A]^a \times [B]^b$$

$$\text{Reverse Reaction Rate} = K_r \times [C]^c$$

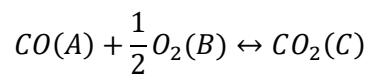
Equation 5-2 Forward and Reverse Reaction Rates

Where:

[X]- Instantaneous molar concentration of species.

a,b,c- Experimentally determined powers.

Using *equation 4-1* as an example:



However, because it is at a state of equilibrium it can be seen that:

$$\frac{[C]^c}{[A]^a[B]^b} = \frac{K_f}{K_r} = K'$$

Equation 5-3 Concentration Equilibrium (Goodger, 2000, p. 284)

Using Avogadro's law which states that under the same conditions of temperature and pressure, equal volumes of different gases contain an equal number of molecules (Encyclopaedia Britannica, 2016) it is therefore seen that the partial pressure equilibrium constant for the reversible reaction is:

$$\frac{p \cdot C^c}{p \cdot A^a \times p \cdot B^b} = K,$$

Equation 5-4 Partial Pressure Equilibrium (Goodger, 2000, p. 284)

With the partial pressure of the number of molecules in the system being:

$$p_x = p \left(\frac{n_x}{n_t} \right)$$

Equation 5-5 Partial Pressure (Goodger, 2000, p. 284)

Combining all this together for carbon dioxide gives us:

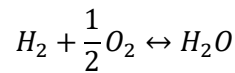
$$\frac{p \cdot CO_2}{p \cdot CO \times (p \cdot O_2)^{0.5}} = \frac{n \cdot CO_2}{n \cdot CO \times (p \cdot \frac{n \cdot O_2}{n_t})^{0.5}}$$

Therefore:

$$K_{CO_2} = \frac{n_1}{n_3 \left(p \cdot \frac{n_5}{n_t} \right)^{0.5}}$$

Equation 5-6 Carbon Dioxide Constant (Goodger, 2000, p. 285)

Water follows the same system in that:



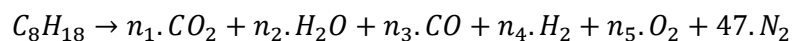
Equation 5-7 Water Chemical Equilibrium

$$K_{H_2O} = \frac{n_2}{n_4 \left(p \cdot \frac{n_5}{n_t} \right)^{0.5}}$$

Equation 5-8 Water Constant (Goodger, 2000, p. 285)

Whilst the dissociation process creates other free radicals, using the formula below gives an initial realistic idea of what is being created by the combustion process. Due to these unknowns, known values for the partial pressure equilibrium constants derived from JANAF tables at certain temperatures will be used which can be found in *appendix 11.5*.

However, because n values are currently unknown as they are calculated in the dissociation process as:



Equation 5-9 Combustion Chemical Equilibrium

To start solving for the unknown n values we must first assume a starting value such as 0.001 for the equation:

$$\text{Assumed Value} = \frac{n_5}{n_t}$$

Equation 5-10 Assumed Value

Then add the pressure and evaluate giving:

$$\left(p \times \frac{n_5}{n_t}\right)^{0.5}$$

Equation 5-11 Assumed Value with Pressure

If the total amount of carbon can be seen as n_1+n_3 then to get the carbon balance:

$$\frac{n_1}{n_3} = K_{CO_2} \times \left(p \times \frac{n_5}{n_t}\right)^{0.5}$$

Equation 5-12 Carbon Balance

Therefore, the amount of CO in the mixture is:

$$n_3 = \frac{C_{total}}{\frac{n_1}{n_3} + 1}$$

Equation 5-13 Carbon Monoxide in Equation

Which means the total CO_2 can be found as:

$$n_1 = C_{total} - n_3$$

Equation 5-14 Carbon Dioxide in Equation

As the amount of hydrogen in the mixture is n_2+n_4 then the hydrogen balance follows in a similar fashion that:

$$\frac{n_2}{n_4} = K_{H_2O} \times \left(p \times \frac{n_5}{n_t}\right)^{0.5}$$

Equation 5-15 Hydrogen Balance

Meaning the total amount of H_2 and H_2O can be found as:

$$n_4 = \frac{H_{total}}{\frac{n_2}{n_4} + 1}$$

Equation 5-16 Hydrogen in Equation

$$n_2 = H_{total} - n_4$$

Equation 5-17 Water in Equation

To find the total free oxygen in the products:

$$n_5 = \frac{O_{total} - 2n_1 - n_2 - n_3}{2}$$

Equation 5-18 Oxygen in Equation

Therefore, the total number of atoms found in the balance equation for the products is:

$$n_t = n_1 + n_2 + n_3 + n_4 + n_5 + 47$$

Equation 5-19 Total Product Atoms

With n_5 and n_t calculated, n_5/n_t can be re-evaluated and an error column put into place to determine the error between the assumed value and the calculated value. This error column will employ the Excel function 'goal seek' in which it sets the error cell to match the value '0' by changing the assumed n_5/n_t value which would then change the calculations as this value changes. It was set to try a maximum of 500 iterations with a maximum change of 1×10^{-8} , these values were chosen as it provided a good balance of accuracy to computational time.

This process was carried out for each temperature that there was a CO_2 and H_2O constant for and pressures from 10 bar up to 110 bar in 5 bar increments for each FER.

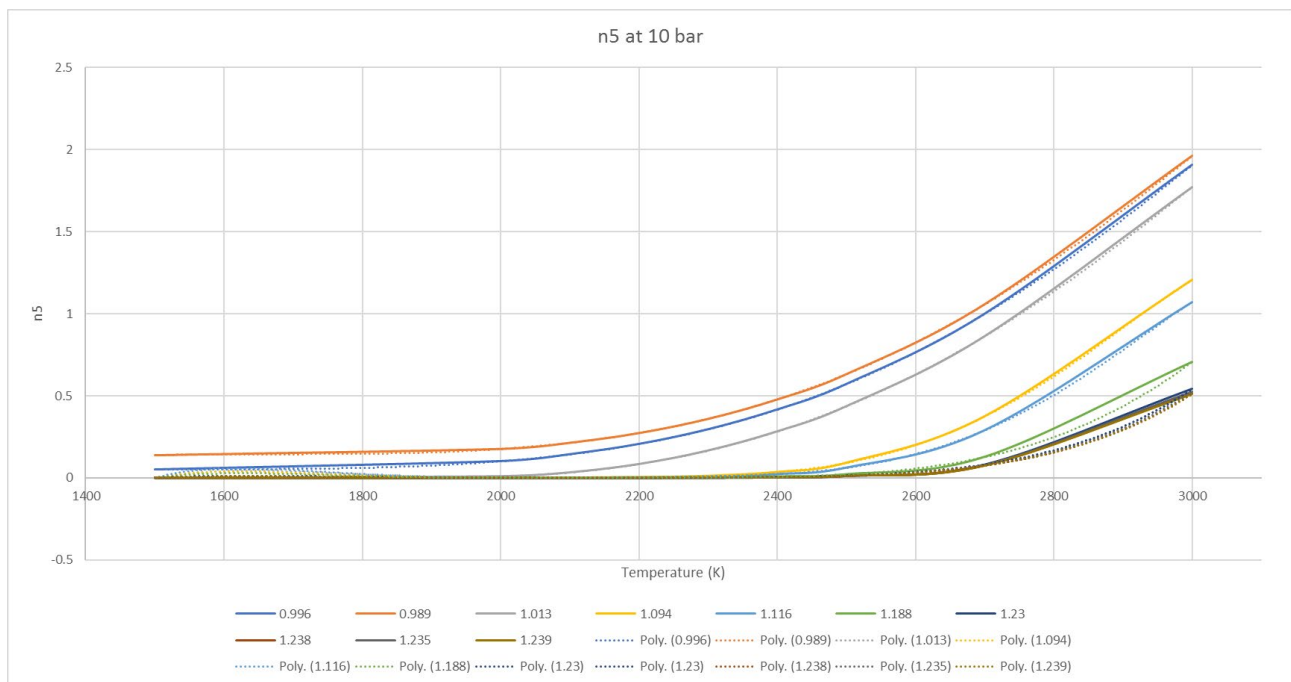


Figure 5-1 Oxygen Content for each Ford Sigma FER at 10 Bar

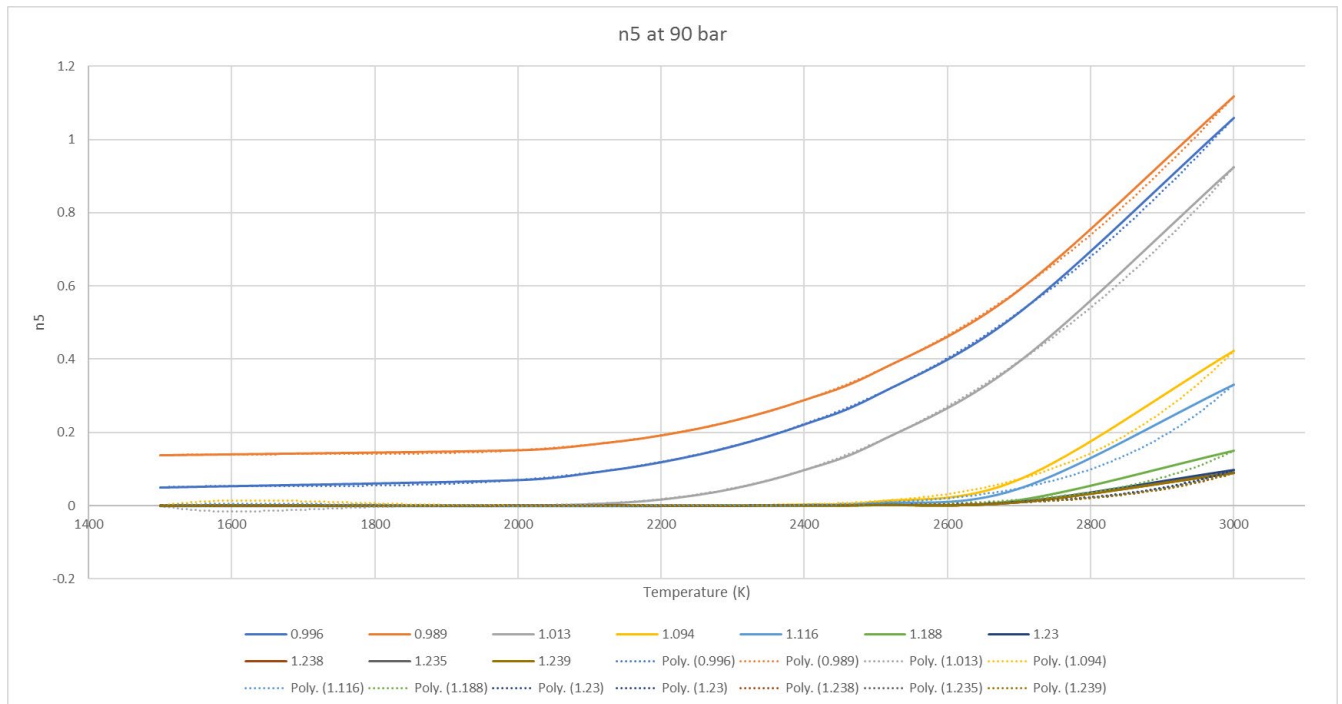


Figure 5-2 Oxygen Content for each Ford Sigma FER at 90 Bar

Figures 5-1 & 5-2 show that the amount of free oxygen available depends on three things: pressure, temperature and FER. As the temperature increases, oxygen levels increase due to increased dissociation with it starting to rapidly occur at 2200 K at lean FER. As the pressure increases oxygen levels decrease, this is because the calculations are a product of pressure because the assumed n_5/n_t is multiplied by the cylinder pressure.

10 bar												
Guess n_5/n_t	$(n_5/n_t) \cdot P$	$(n_5/n_t) \cdot P^2$	n_1/n_3	n_3	n_1	n_2/n_4	n_4	n_2	n_5	n_t	n_5/n_t	error
0.028450676	0.2845068	0.533392	1.629458468	3.042452	4.957548	11.75009	0.705877540	8.29412246	1.874165	65.874165	0.028450677	0.00
90 bar												
Guess n_5/n_t	$(n_5/n_t) \cdot P$	$(n_5/n_t) \cdot P^2$	n_1/n_3	n_3	n_1	n_2/n_4	n_4	n_2	n_5	n_t	n_5/n_t	error
0.015790486	1.4211438	1.192117	3.641799265	1.72347	6.27653	26.26115	0.33014011	8.66985989	1.026804863	65.026805	0.015790486	0.00

Figure 5-3 Difference Between 10 Bar and 90 Bar at $\lambda=1$

Figure 5-3 gives an idea of what this pressure is doing to the products, at 90 bar pressure n_1 and n_2 are higher, and this is because from equations 4-1 & 5-7. During equilibrium the reactant and product materials proportions remain constant. An increase in pressure means an increase in density as:

$$\rho = \frac{p}{RT}$$

Equation 5-20 Density

If the density within the cylinder increases it means that the reactant molecules will now be closer together which increases the likelihood of them joining together to form the product material in this case CO_2 and H_2O . (McDonald, 2018) Because these both require oxygen to form it stands that there will be less free oxygen in the cylinder. According to Le Châtelier's principle this is one of the changes imposed from outside the system that displaces the equilibrium, the other two being that excess

oxygen, so lean conditions would cause the reaction to move in the forward direction as this would reduce the concentration of oxygen and the other which *figures 5-1 & 5-2* show is that if the temperature is raised the reaction moves in the direction that absorbs heat which in this case would be the forward direction. (Stone, 1999, p. 67)

For each FER at 5 bar intervals polynomials were constructed to the 6th order with 30 decimal points for the most accuracy, examples of these polynomials can be found in *appendix 11.6*. These polynomials would then be used for linear interpolation to determine n_5 at each temperature and pressure. An example would be to determine n_5 at 53.7 bar 2568.3 K:

$$n_5 = n_{5.50 \text{ bar}} + \left(\frac{53.7 - 50}{55 - 50} \right) \times (n_{5.55 \text{ bar}} - n_{5.50 \text{ bar}})$$

Equation 5-21 Linear Interpolation

However, due to the number of polynomial equations created increasing computational time, and by the fact that the polynomials do not perfectly line up with the n_5 results as seen in *figures 5-1 & 5-2* it was decided to approach the problem in another manner.

It was decided to use polynomials based on the constant values of CO_2 and H_2O to determine the value for each temperature at each degree of crank angle as shown in *figure 5-4*.

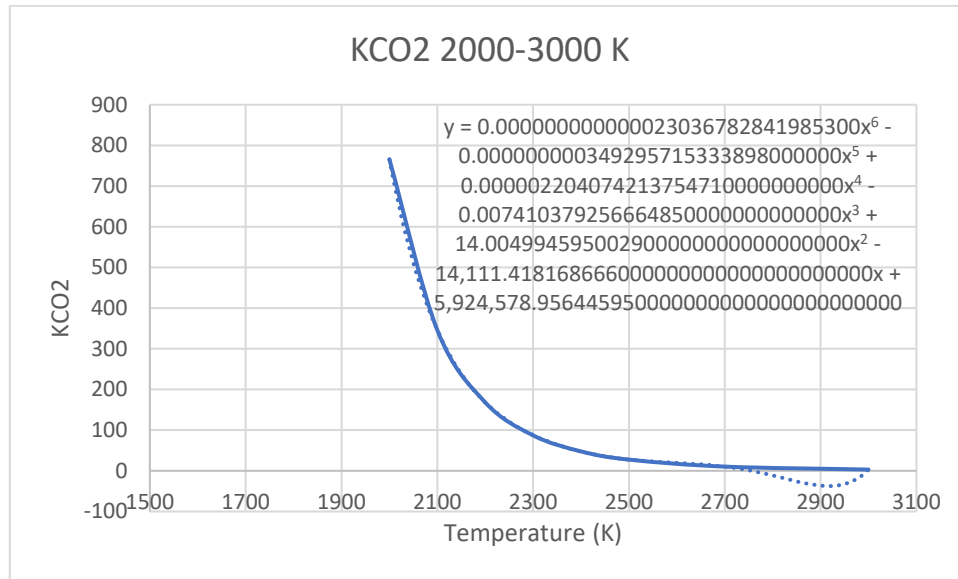


Figure 5-4 Polynomial for Carbon Dioxide Equilibrium Constant

However, the polynomial cannot fit perfectly to the data due to the JANAF tables missing out 2800-2900 K and a polynomial could not be constructed for 1500-2000 K also due to a lack of data. Fortunately, the Gibbs free energy for each 100 K is provided allowing each constant value for every 100 K to be determined allowing for more accurate polynomials. From the Gibbs function (Stone, 1999, p. 67):

$$K_x = \exp\left(\frac{-G_{\text{overall}}^0}{RT}\right)$$

Equation 5-22 Equilibrium Constant from Gibbs Function

If the example at 3000 K in *equation 2-14* is used then K_{CO_2} :

$$K_{CO_2} = \exp\left(\frac{-(-27645000)}{8314 \times 3000}\right)$$

$$K_{CO_2} = 3.029$$

Equation 5-23 Carbon Dioxide Equilibrium Constant using the Gibbs Function

Which is similar to the 3.0549 provided by the JANAF tables so it was seen that this was an acceptable method of calculation which then provided the graphs and polynomials seen in *figure 5-5*:

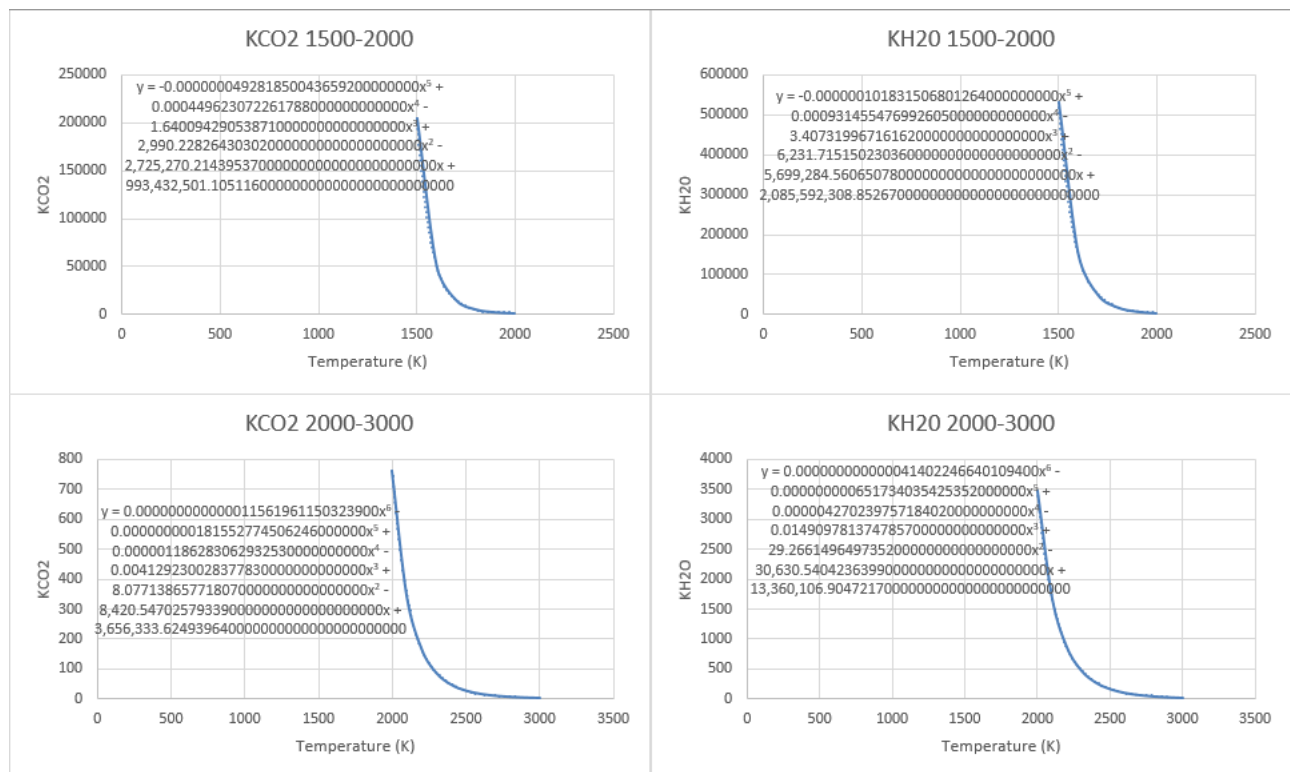


Figure 5-5 Equilibrium Constant Graphs

By using if statements to select the polynomial dependent on the temperature range the equivalent constant value can be determined. However, there was still a slight error detected using this method, the trend is that as the temperature decreases the equilibrium constant decreases as seen in *figure 5-6*:

1858.443	KCO2	KH2O	Guess n5/nt	[n5/nt]*P	[n5/nt]*P	n1/n3	n3	n1	n2/n4	n4	n2	n5	nt	n5/nt	error
1856.187	2286.183	10214.6	0.000290755	0.013758	0.117294	268.155	0.029722646	7.970277	1198.109	0.007505572	8.992494428	0.018614	64.019	0.000291	0.00
1863.009	2122.044	9593.509	0.000305104	0.014428	0.120117	254.8925	0.031263122	7.968737	1152.339	0.007803430	8.992196570	0.019533	64.020	0.000305	0.00
1876.329	1903.958	8630.479	0.000327365	0.015544	0.124677	237.3791	0.033559996	7.966440	1076.019	0.008356400	8.991643600	0.020958	64.021	0.000327	0.00
1894.427	1816.28	7824.342	0.000339139	0.016245	0.127457	231.4978	0.034408922	7.965591	997.2684	0.009015611	8.990984389	0.021712	64.022	0.000339	0.00
1916.227	1973.223	7491.148	0.000325447	0.015801	0.125703	248.0405	0.032123289	7.967877	941.6614	0.009547436	8.990452564	0.020835	64.021	0.000325	0.00
1941.45	2308.594	7545.283	0.000298524	0.014764	0.121509	280.5153	0.028417635	7.971582	916.8211	0.009805832	8.990194168	0.019112	64.019	0.000299	0.00
1969.428	2335.382	7058.128	0.000298051	0.015086	0.122824	286.841	0.02779312	7.972207	866.9076	0.010369768	8.989630232	0.019081	64.019	0.000298	0.00
2000.227	758.3474	3458.72	0.000584886	0.030433	0.17445	132.2937	0.060017828	7.939982	603.3737	0.014891448	8.985108552	0.037455	64.037	0.000585	0.00
2033.136	583.9213	2724.691	0.000686364	0.036849	0.19196	112.0895	0.070740441	7.929260	523.0314	0.017174542	8.982825458	0.043957	64.044	0.000686	0.00
2068.174	442.2468	2117.574	0.00081236	0.045194	0.212589	94.01681	0.084195629	7.915804	450.1729	0.019948005	8.980051995	0.052072	64.052	0.000813	0.00

Figure 5-6 Equilibrium Constant Error

It can be observed that the constant begins to increase again and then dropping after 2000 K, it was thought that this was due to a calculation input error in the cells so the function was checked against the known temperatures of 1800 K and 1900 K which have CO₂ constants of 4884.256 and 1832.993 respectively.

1858.443	KCO2	KH2O	Guess n5/nt	(n5/nt)*P	(n5/nt)*P	n1/n3	n3	n1	n2/n4	n4	n2	n5	nt	n5/nt	error
1856.187	2286.183	10214.6	0.000290755	0.013758	0.117294	268.155	0.029722646	7.970277	1198.109	0.007505572	8.992494428	0.018614	64.019	0.000291	0.00
1863.009	2122.044	9593.509	0.000305104	0.014428	0.120117	254.8925	0.031263122	7.968737	1152.339	0.007803430	8.992196570	0.019533	64.020	0.000305	0.00
1876.329	1903.958	8630.479	0.000327365	0.015544	0.124677	237.3791	0.033559996	7.966440	1076.019	0.008356400	8.991643600	0.020958	64.021	0.000327	0.00
1800	4884.256	18586.78	0.000339139	0.016245	0.127457	622.5334	0.012830107	7.987170	2369.019	0.003797438	8.996202562	0.008314	64.008	0.00013	0.00
1900	1832.993	7681.311	0.000325447	0.015801	0.125703	230.4131	0.034570207	7.965430	965.5655	0.009311320	8.990688680	0.021941	64.022	0.000343	0.00
1941.45	2308.594	7545.283	0.000298524	0.014764	0.121509	280.5153	0.028417635	7.971582	916.8211	0.009805832	8.990194168	0.019112	64.019	0.000299	0.00
1969.428	2335.382	7058.128	0.000298051	0.015086	0.122824	286.841	0.02779312	7.972207	866.9076	0.010369768	8.989630232	0.019081	64.019	0.000298	0.00
2000.227	758.3474	3458.72	0.000584886	0.030433	0.17445	132.2937	0.060017828	7.939982	603.3737	0.014891448	8.985108552	0.037455	64.037	0.000585	0.00
2033.136	583.9213	2724.691	0.000686364	0.036849	0.19196	112.0895	0.070740441	7.929260	523.0314	0.017174542	8.982825458	0.043957	64.044	0.000686	0.00

Figure 5-7 Equilibrium Constant Error Input Check

When these temperatures are inputted they, both give the correct CO₂ value therefore the equation and polynomial input are correct however it shows that there is a slight discrepancy in the polynomial trend line between 1900 K and 2000 K in which it increases above the actual calculated values. Fortunately, as shown in figures 5-1 & 5-2 for the most part oxygen levels at these temperatures is minimal for rich values however this has the potential to throw off the lean values.

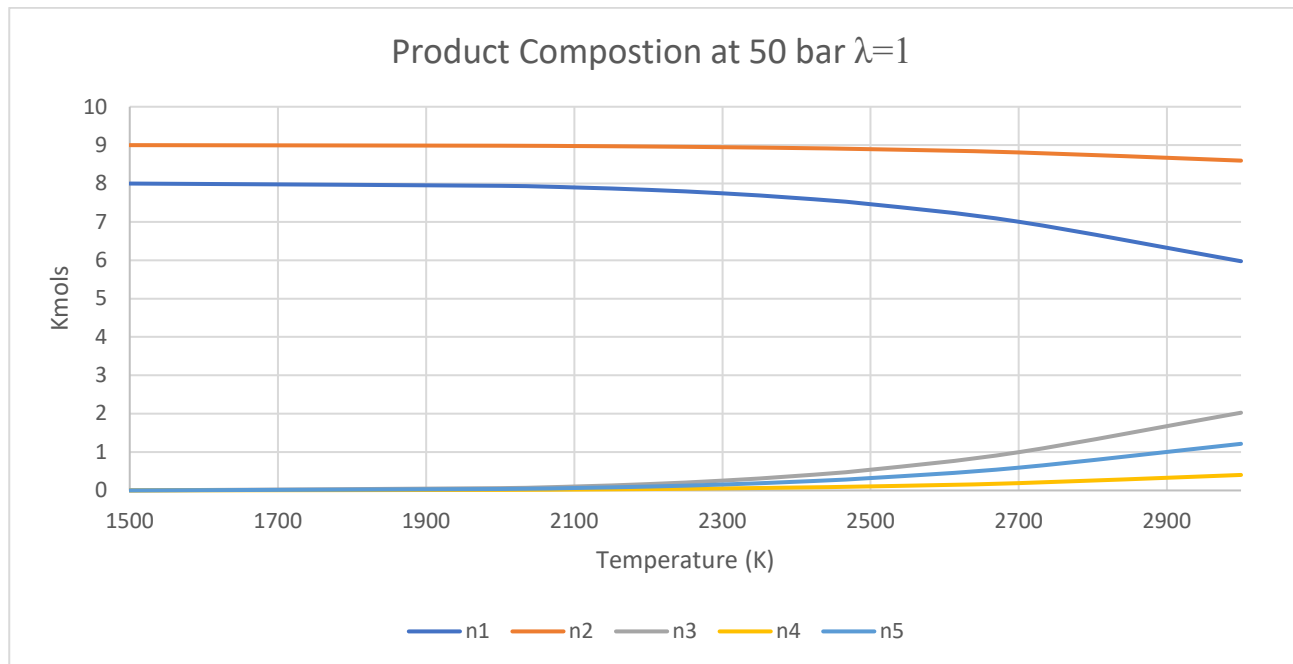


Figure 5-8 Product Composition at 50 Bar Stoichiometric

Figure 5-9 gives a good overview of the dissociation process at a set pressure and λ , as CO₂ begins to decrease CO and oxygen begin to increase and at high temperatures when H₂O begins to break down H₂ begins to increase.

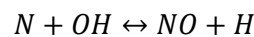
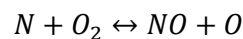
6. NO_x Formation

6.1 Background

There are three ways NO_x can form during combustion:

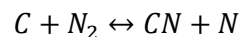
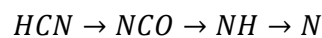
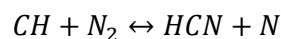
- 1) Thermal NO_x. This is the process where nitrogen in the air reacts with free oxygen during combustion to produce NO_x. This process is due to dissociation and is dependent on very high temperatures, in practice is a nonlinear process in which hot spots can have a large effect on the amount of NO_x produced which therefore means that the maximum temperature in the cylinder is more important than the average which is further backed up by *figures 5-1 & 5-2* in which oxygen levels increase exponentially with temperature. This process is mostly governed by three equations called the Zeldovich mechanism which will be used to predict the NO_x produced later.

These three equations are:



Equation 6-1 Zeldovich Mechanism

- 2) Fuel NO_x. This is process where the nitrogen in the fuel reacts with the oxygen in the air to form NO_x. Gas fuels have minimal nitrogen and thus produce negligible NO_x compared to thermal formation and as such will not be investigated further.
- 3) Prompt NO_x. Radical hydrocarbons produced during combustion in the flame front react with the nitrogen in the air to form substances that then oxidize to NO_x when they react with oxygen and accounts for 5-10% of the total NO_x produced. (Merker, et al., 2006, p. 140) This process usually only occurs at low temperature and in rich operating conditions.



Equation 6-2 Prompt NO_x Formation Mechanism

(Schwerdt, 2006)

This model assumes homogeneity throughout the mixture but in reality, there will be the presence of rich and lean patches throughout the cylinder. Zhao, et al suggests that in a stratified charge that due to the inclusion of rich and stoichiometric patches that the local temperature will remain high increasing NO_x production. (Zhao, et al., 1997) Reddy and Mallikarjuna who studied the effect of increasing injector pressure and timing, also seem to suggest that as the pressure was increasing NO_x increased due to better atomisation producing finer droplets aiding combustion causing higher temperatures. By injecting earlier as well it gave the fuel more time to mix with the air becoming more

homogenous increasing NO_x. (Reddy & Mallikarjuna, 2017) It is this authors own view aided by figures 2-2, 5-1 & 5-2 that the inclusion of lean patches will aid in NO_x production due to the increased oxygen concentration.

6.2 Reverse Reactions

If one of Zeldovich's mechanisms are taken:



It is known that as the temperature increases NO formation increases and according to La Châtelier the position of equilibrium will move in a way to counteract the change. (Clarke, 2013) When the temperature increases it will always favour the endothermic reaction which is when energy is absorbed from the surroundings giving the oxygen enough energy to bond with the nitrogen to form NO. This energy absorption will therefore decrease the surrounding temperature and is known as the charge cooling effect. (Cao, et al., 2006) If the temperature starts to gradually decrease the reaction will begin to favour the exothermic side of the equation and begins attempting to reach equilibrium, from this it sees that NO levels will begin to decrease given enough time.

The equilibrium NO is found immediately after SOC and rises rapidly with temperature, because of this dependency a kinetic reaction model is usually referred to. And according to Zeldovich less NO is produced than the equilibrium model however due to the slow process at lower temperatures kinetic NO does not regress over the reverse reaction, i.e. the reaction is said to have frozen.

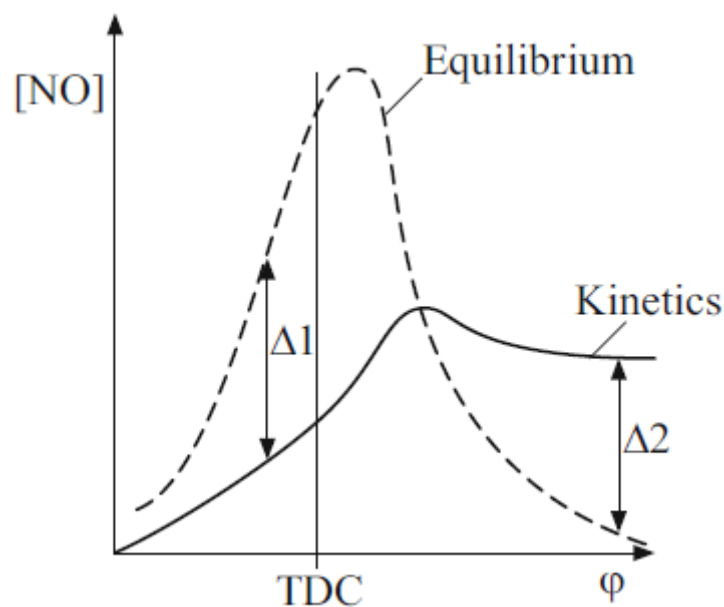


Figure 6-1 NO Concentrations under Condition of Equilibrium/Kinetically Controlled NO Formation (Merker, et al., 2006, p. 136)

6.3 Extended Zeldovich Model

The EZM can be given as:

$$\frac{d[NO]}{dt} = (4.7 \times 10^{13}) \times [N_2] \times [O_2]^{0.5} \times \exp\left(-\frac{67837}{T}\right)$$

Equation 6-3 Extended Zeldovich Model (McDonald, 2017)

This equation makes clear of NO's production being heavily dependent on the concentration of nitrogen and oxygen but also on the temperature. The exponential component of the equation is the rate constant which has been measured in experimental studies. (Heywood, 1988, p. 573) It is unknown what kind of engines were used in the experiments or how long ago and with rapid advancement of engine technology this empirical figure may be completely out, however, for the purposes of this report it will be used to give a rough estimation of the NO formation rate.

Currently the amount of oxygen and nitrogen calculated through dissociation are in Kmols, converting them to Kmols/m³ which gives the concentration of each denoted as [O₂] and [N₂] respectively the number of Kmols in the cylinder must be determined through:

$$\alpha = \frac{m_{fuel}}{\Phi \times ((C_{total} \times C_{mass}) + (H_{total} + H_{mass}))}$$

Equation 6-4 Kmols in the Cylinder

Then to find the concentration of [O₂] and [N₂] in the burnt zone:

$$[O_2] = \frac{\alpha \times MFB \times n_5}{V_b}$$

$$[N_2] = \frac{\alpha \times MFB \times 47}{V_b}$$

Equation 6-5 Oxygen and Nitrogen Concentration

These values are then placed into the EZM and then converted from Kmols/s to Kmols/m³/θ:

$$\frac{d[NO]}{d\theta} = \frac{d[NO]}{dt} \times \frac{1}{(6 \times RPM)}$$

$$NO_\theta = \frac{d[NO]}{d\theta} \times V_b$$

Equation 6-6 Sum of NO per Degree of Crank Angle

Then to finally convert the NO to ppm:

$$NO_{ppm} = \frac{(NO_\theta \sum SOC \rightarrow T_{max})^{10^6}}{\alpha \times n_t}$$

Equation 6-7 NO ppm to Maximum Temperature

For later comparison:

$$NO_{ppm} = \frac{(NO_{\theta} \sum SOC \rightarrow EOC)^{10^6}}{\alpha \times n_t}$$

Equation 6-8 NO ppm to EOC

6.4 Arrhenius Equation

Arrhenius put forth a theory that states that only molecules that possess energy greater than a certain amount, E_A , will react. These molecules acquire the energy from the thermal conditions present in the engine. (Glassman & Yetter, 2008, p. 45) Arrhenius equation can be seen as:

$$k = Ae^{\left(\frac{-E_a}{RT}\right)}$$

Equation 6-9 Arrhenius Equation

To determine how this equation changes the reaction rate two examples will be compared, an assumed activation energy of 50 KJ/mol with the gas constant being 8.314 J/mol.K and temperatures of 1800 K and 2500 K with A staying as a constant so it can be ignored so that it can be seen how temperature affects the reaction rate:

$$e^{\left(\frac{-50000}{8.31 \times 1800}\right)} = 0.035$$

$$e^{\left(\frac{-50000}{8.31 \times 2500}\right)} = 0.09$$

Equation 6-10 Arrhenius Equation Example

As seen, the number of molecules able to react has more than doubled at a higher temperature which leads to the conclusion that a higher temperature means that a reaction will occur at a faster rate due to two things, the probability of collision is increased and the molecules will have more energy surpassing E_A allowing reaction to occur.

7. NOx Prediction

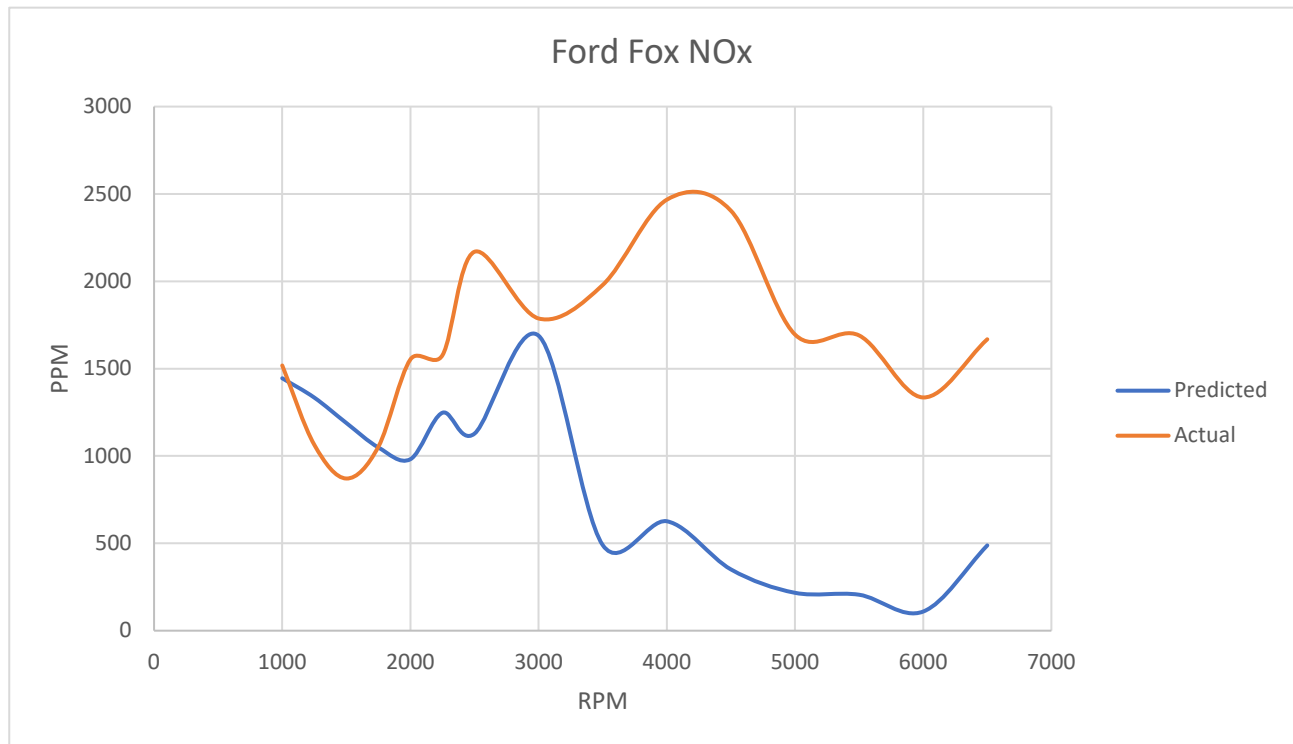


Figure 7-1 Ford Fox NOx to Maximum Temperature Prediction

From *figure 7-1* it can be seen that the NOx is over-predicting or very similar to what is being measured by the engine between 1000-1750 RPM, at these points the engine is running lean and then it begins to run rich after that until and after 3000 RPM where there was a lack of data so it was assumed stoichiometric which brings the prediction close to the actual value. During rich operation it can be seen to be under predicting with it getting lower as the A/F ratio decreases with an increase at 4000 RPM as it is slightly less rich. 6000 & 6500 RPM the engine is running at its most rich with a FER of 1.11 and although there is a dip at 6000 RPM, 6500 RPM seems to rapidly increase. Predicted peak temperature at 6000 RPM is 2535 K whilst predicted for 6500 RPM is 2634 K which can help explain the rapid rise. Another explanation could be that there is simply not enough time for reverse reactions to occur due to how fast everything is moving in the engine. 1500 RPM appears to be over predicting by 36%, 4000 RPM under predicting by 74% and 6500 RPM under predicting by 26%, according to Miller, et al the EZM was shown to under predict NO levels by 30-60% depending on operating conditions. (Miller, et al., 1998) With 6000 RPM under predicting by 91% it can be said that the predicted temperature was too low, most likely from an MFB miscalculation which will be investigated in the sensitivity analysis. It could also be due to the mixture time being too small causing lean and rich patches which would increase measured NOx levels but would not be taken into the account in this model due to the assumption that the mixture consists of just two zones that are homogeneous in nature with the predicted temperatures being assumed to be the same throughout their respective zone. It is important to note however, that although the

majority of the time it is under predicting, the trend of the predicated data matches that of the measured data meaning that the model is accurately predicting how NO is being formed in the engine just without taking into account the quality of the mixture.

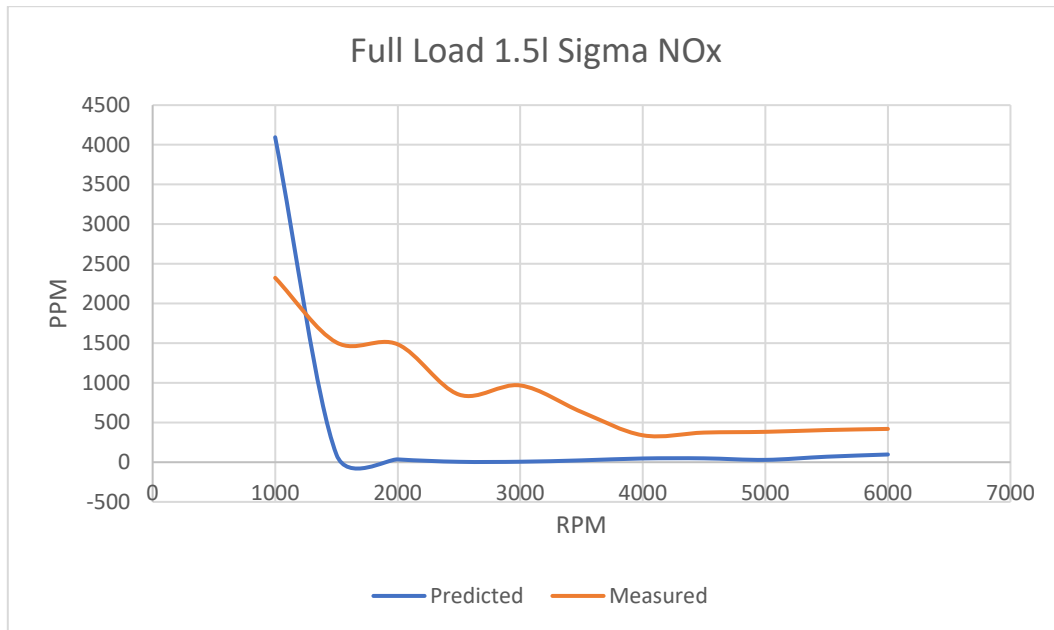


Figure 7-2 Ford Sigma to Maximum Temperature Prediction

Figure 7-2 shows the predicted NO for the Ford Sigma, at 1000 RPM there is dramatic over prediction when it is running lean, this is because at this speed everything is moving slowly giving more time for reverse reaction to occur as the NO_x is reverting back to O₂ and N₂. Whereas in the model NO_x levels keep adding up to the maximum temperature. Coupled with the fact that the turbo is not operational at this speed meaning that timing is advanced with SOC at 1000 RPM at -4 CA° compared to SOC at 1500 RPM at 3 CA° causing an increase in temperature due to the ideal gas equation.

$$pV = mRT$$

$$T = \frac{pV}{mR}$$

Equation 7-1 Temperature from Ideal Gas Law

Due to ignition starting as the piston is moving up, pressure is still increasing and because the turbo is not operational at this point the mass is a lot less compared to later RPM's with 1000 RPM's total intake mass being 0.0003994 Kg and 1500 RPM being 0.0008686 Kg. Also, the temperature of the intake charge is also unaccounted for.. As the intake air is being compressed by the turbo charger it will rise in temperature which will have a knock-on effect of increasing the in-cylinder mixture, this air temperature increase can be seen in *figure 7-3*:

AFTCOMPT deg C

	0	1000	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000
FL			110.350	95.111	86.892	80.482	90.212	101.713	100.431	106.415	104.672	104.457
1.5			101.381	91.439	86.106	80.360				106.413		
1.4			92.211	81.554	77.426	77.405	88.782	97.333	94.751	95.719	97.846	105.803
1.3			79.834	73.613	67.910	77.021	80.309	86.970	84.592	85.164	86.780	92.517
1.2			64.116	66.540	73.414	69.860	72.449	77.980	73.516	72.214	73.794	76.923
1.1			66.901	66.221	62.567	59.960	64.042	65.211	62.705	64.629	69.041	73.206
1		37.407	58.999	65.455	57.277	49.785	52.050	56.852	57.994	61.870	64.968	69.386
0.9		34.653	54.876	53.979	46.956	41.037	47.193	52.040	52.975	56.948	59.318	64.098
0.8		29.707	46.750	45.959	36.751	33.620	44.129	47.560	48.701	52.709	55.081	58.595
0.7		27.228	29.678	29.173	29.422	31.086	41.488	45.270	46.042	47.601	49.458	53.157
0.6		27.021	27.030	27.331	26.906	28.410	37.757	41.679	41.832	42.517	44.419	46.682
0.5		26.595	25.937	25.936	25.494	26.539	35.645	37.542	38.038	37.212	39.552	40.372
0.4		26.095	25.228	24.777	24.173	25.038	33.175	34.095	34.229	32.068	34.004	
0.3		27.025	25.011	23.631	23.234	23.584	31.149	31.343	30.420	27.535	29.245	
0.2		26.803	26.450	25.789	25.043	27.566	36.715	39.267	39.805	39.961	43.471	

Figure 7-3 Ford Sigma Air Temperature after Turbo charger

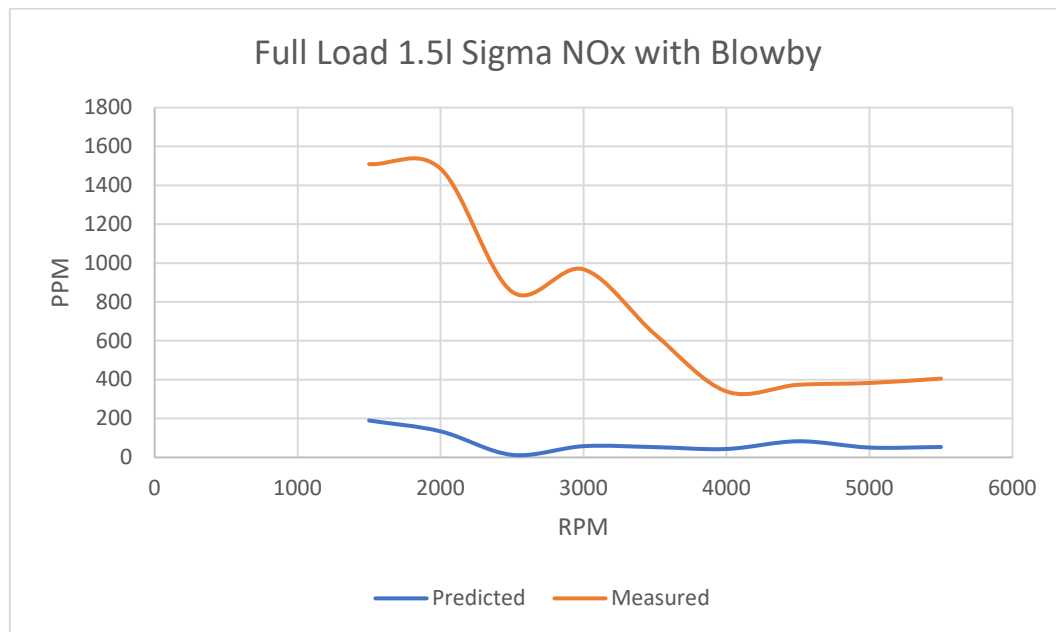


Figure 7-4 Ford Sigma Predicted Results with Blowby Included

Figure 7-4 removes 1000 RPM to better see the rest of the results but these results also include the blowby occurring which is the amount of mixture escaping past the piston rings into the crankcase, reducing the mass of the in-cylinder mixture, increasing the temperature. It can be seen that this has brought NOx levels up slightly but it is still drastically under predicting, however, like the Fox it still follows the same trend as the measured data. For most of the engines operating conditions it is running extremely rich, which is most likely done in effort to cool combustion due to the increased charge temperature from the turbo charger with 6000 RPM seeing an FER of 1.239. Due to this high FER value it would see that this model would drastically under predict the amount of free oxygen being produced when in reality as previously mentioned there would be lean patches with high concentrations of oxygen and more stoichiometric patches increasing temperature therefore increasing the actual NOx produced.

What was interesting to note however in figure 7-1 is when the mixture was stoichiometric the predicted and measured NOx were reasonably close to further investigate this, part load data was analysed for the Ford Sigma which operated close to stoichiometric being slightly rich.

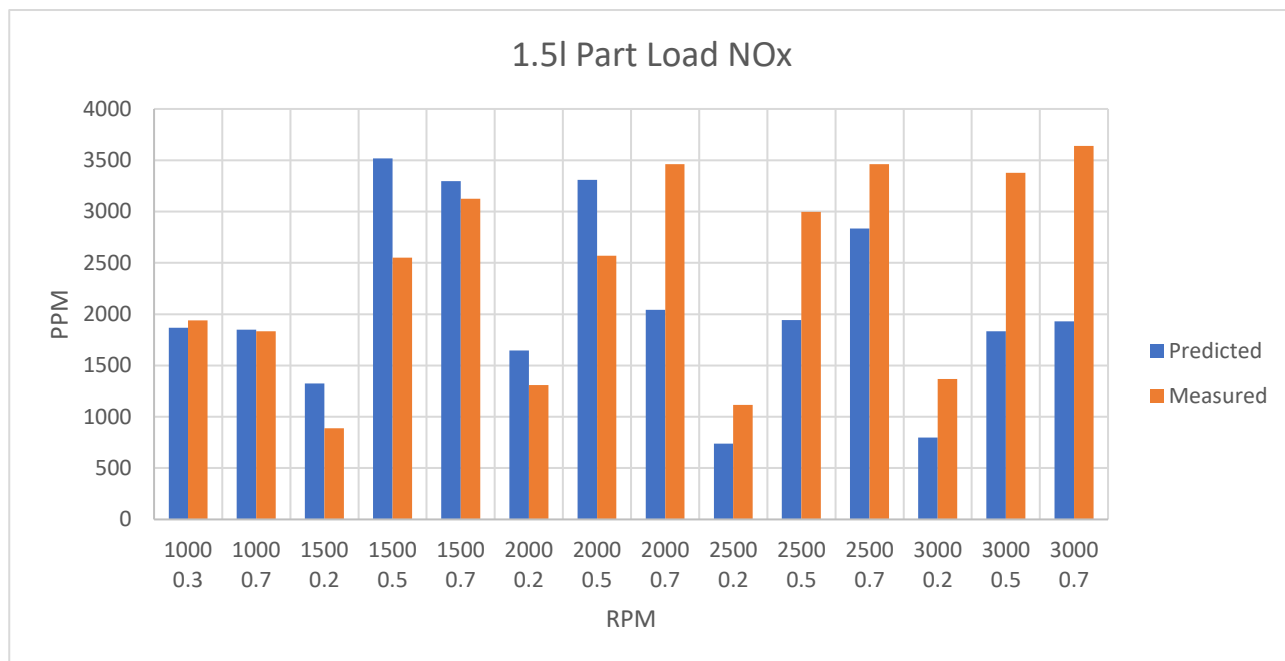


Figure 7-5 Ford Sigma Part Load Predictions

It is believed that the model works better at stoichiometric due there being less chance of under predicting the amount of free oxygen created during combustion.

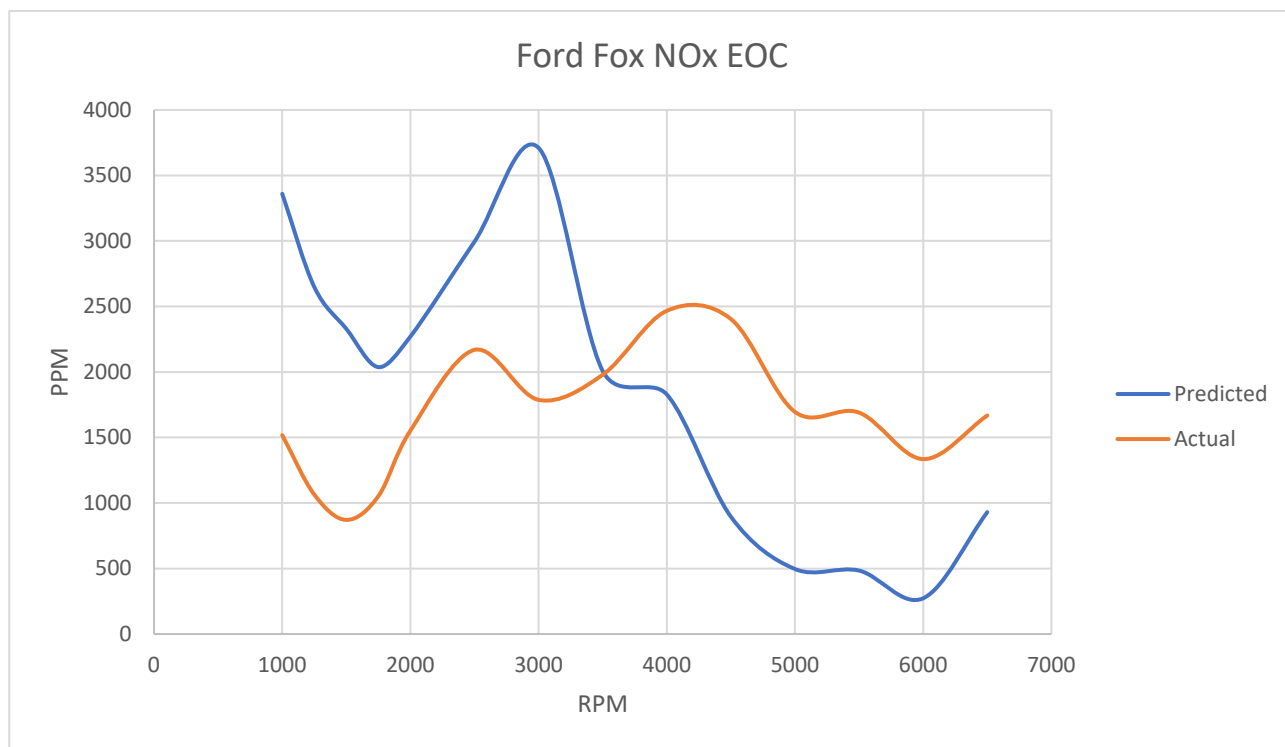


Figure 7-6 Ford Fox NOx Prediction to EOC

If NOx production didn't 'freeze' or experience from reverse reactions and carried on being produced throughout the entire combustion process then as *figure 7-6* shows the model would over predict NOx levels until it starts to become sufficiently rich.

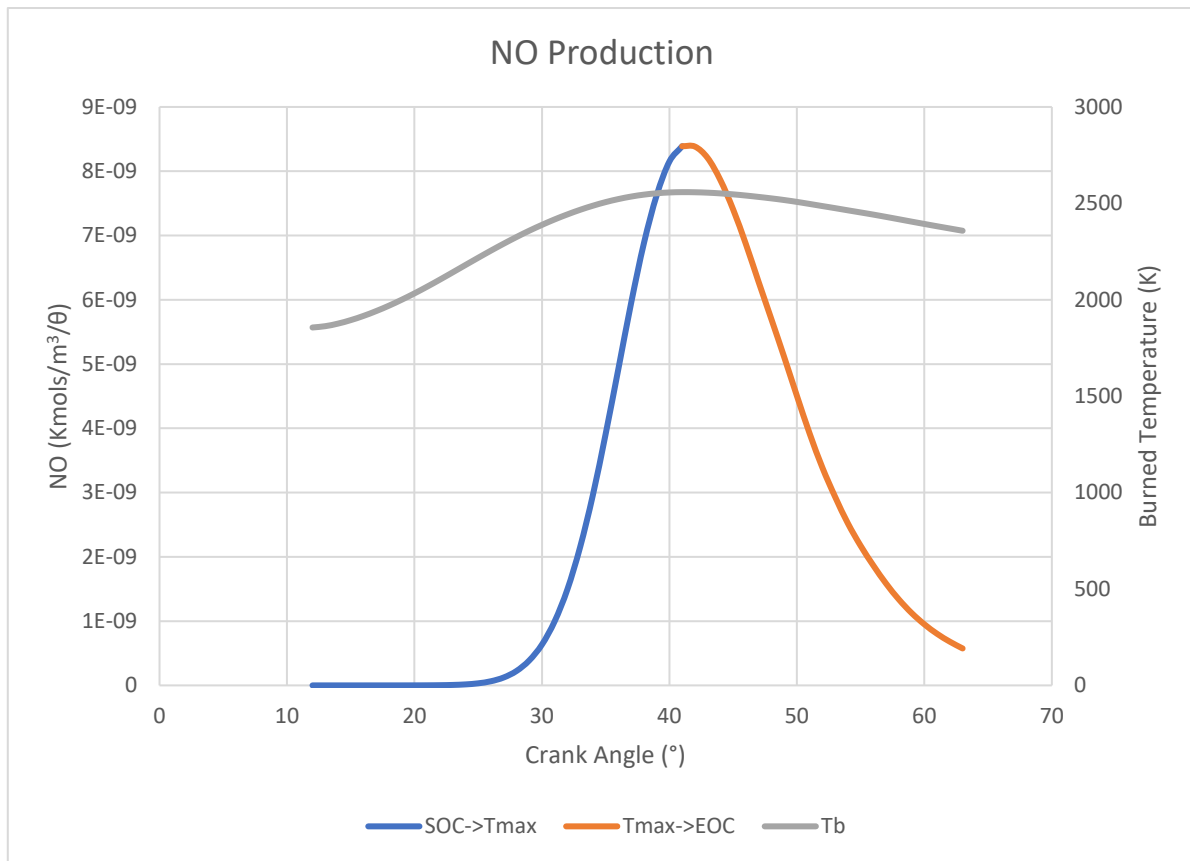


Figure 7-7 Ford Fox NO Production at 3000 RPM

Figure 7-7 shows the burnt temperature against the NO production, NO is still being produced after peak temperature has been reached but soon quickly starts to rapidly decrease and at this point reverse reactions would start to occur as peak temperature can be found at 91% MFB. According to Schwerdt using the equilibrium equations means that NO_x formation will drop when the temperature drops simply because the equilibrium approach does not consider the freezing phenomenon. (Schwerdt, 2006)

7.1 Sensitivity Analysis

As previously determined by the ideal gas law the first thing that was to be investigated was the effect of the pressure on NO_x levels.

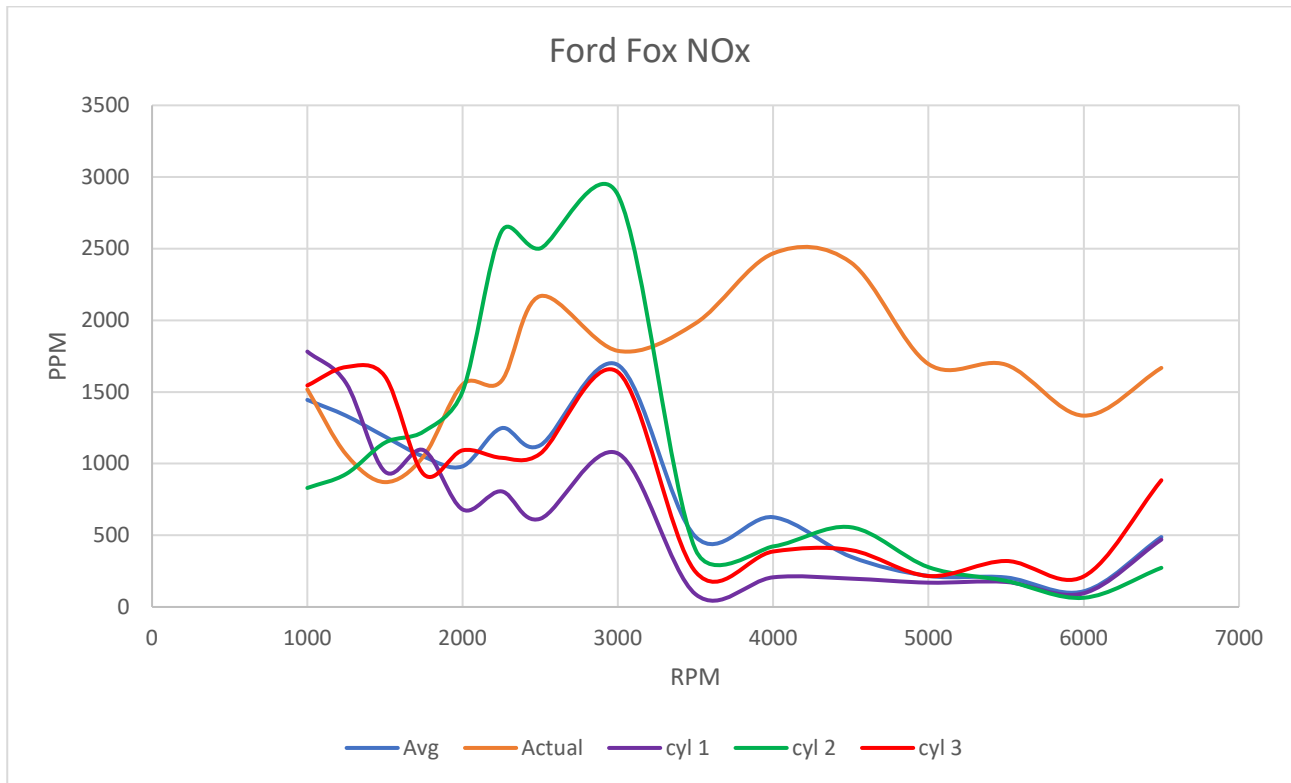


Figure 7-8 Ford Fox NO_x Prediction for each Cylinder

As previously discussed, pressure plays an important role in not only the temperature but also in increasing forward reaction probability to create NO_x from the free radicals. It is important to note that the pressure data and measured NO_x is an average taken over 300 cycles which can be the cause for such large differences as seen in cylinder 2, this could be caused by a variety of unknown reasons but as cylinder 2 is in the middle of the engine block it could be experiencing heat transfer from the outer cylinders increasing the mixture temperature, this would occur more at low-mid RPM where there is more time for heat transfer to occur.

Another factor that can affect the data is the polytropic index which affects the MFB which will then have an effect on the burn temperatures and as such the NO_x production. Three RPM's on the Ford Fox will be compared, 1000, 3000 and 6500 RPM and will compare the calculated polytropic index to 1.25 and 1.35.

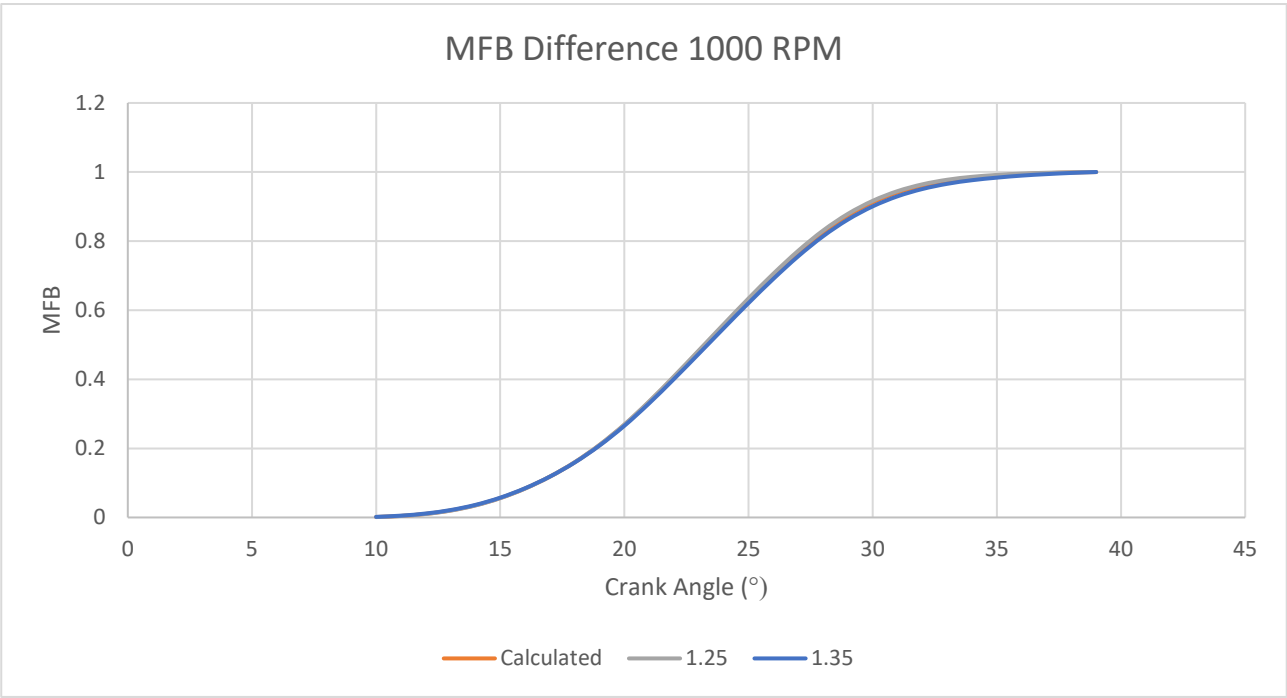


Figure 7-9 Different MFB for 1000 RPM

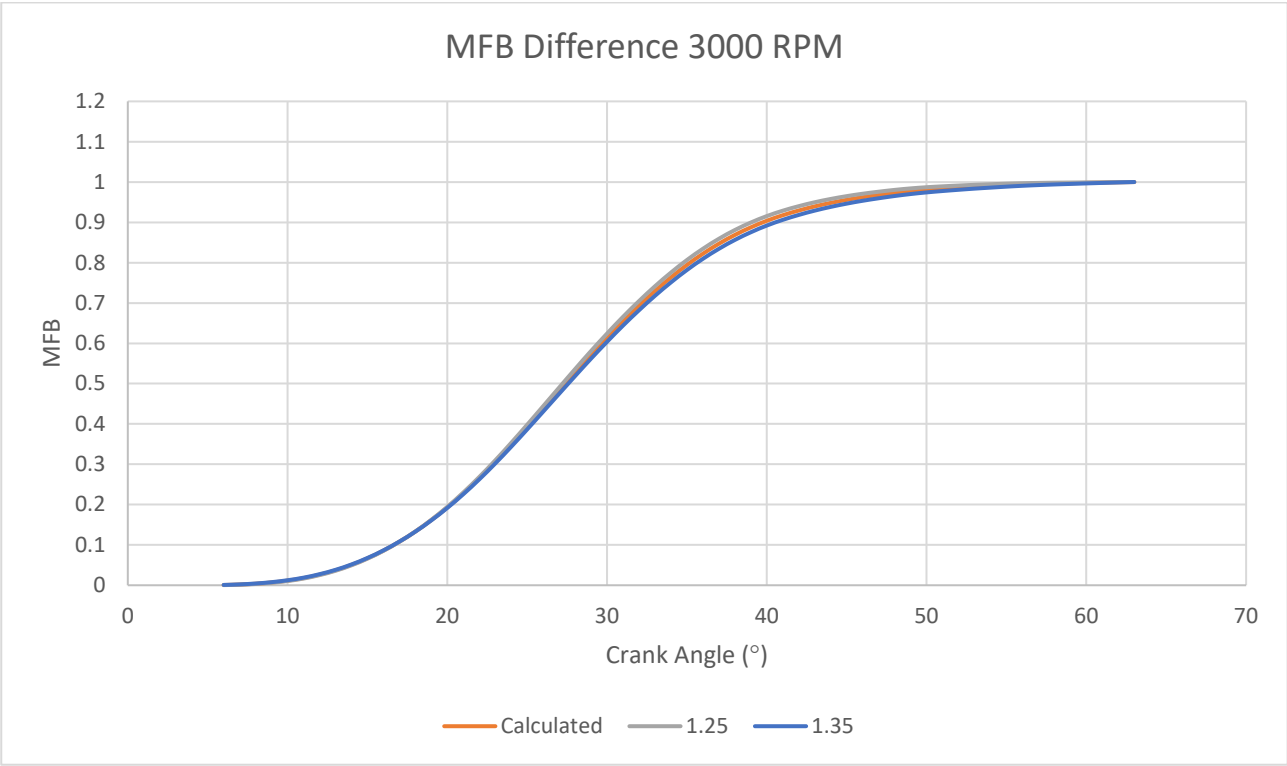


Figure 7-10 Different MFB for 3000 RPM

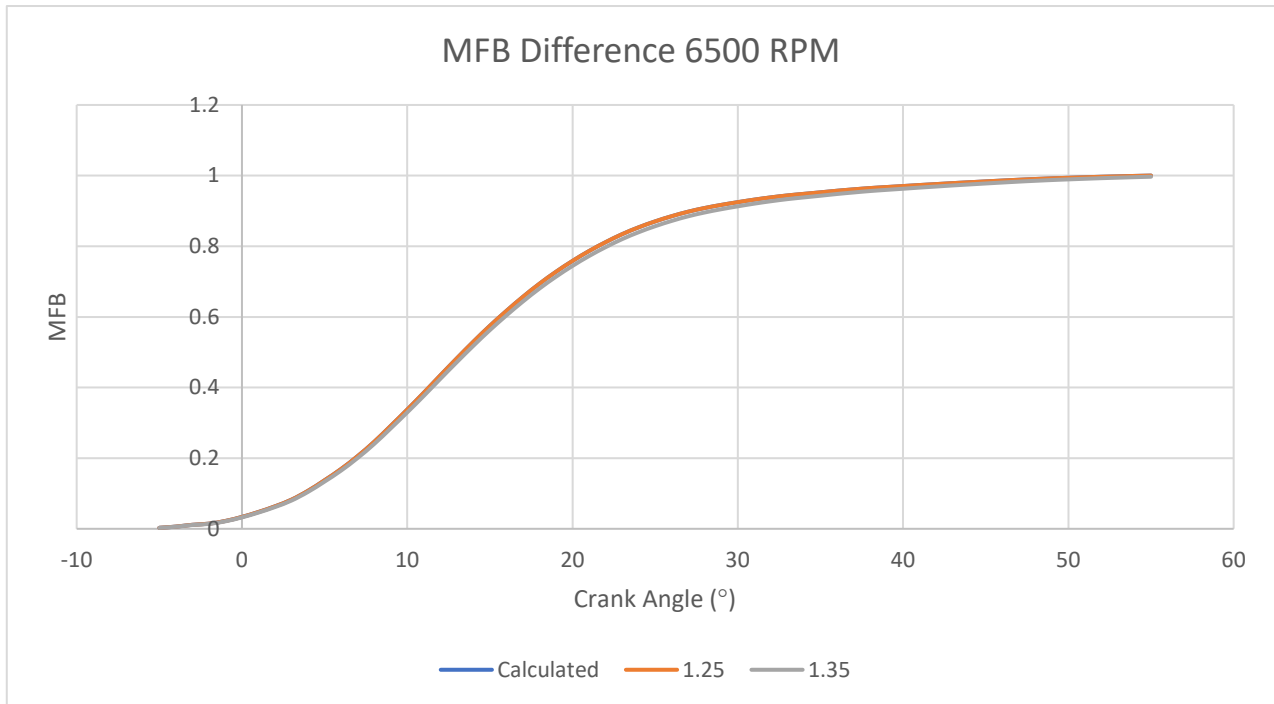


Figure 7-11 Different MFB for 6500 RPM

A different polytropic index only has a slight effect on the MFB however what can be noted is that an index of 1.35 after 50% MFB can be seen to start burning more slowly than the other polytropic index's indicating that the higher the index the slower the burn rate is.

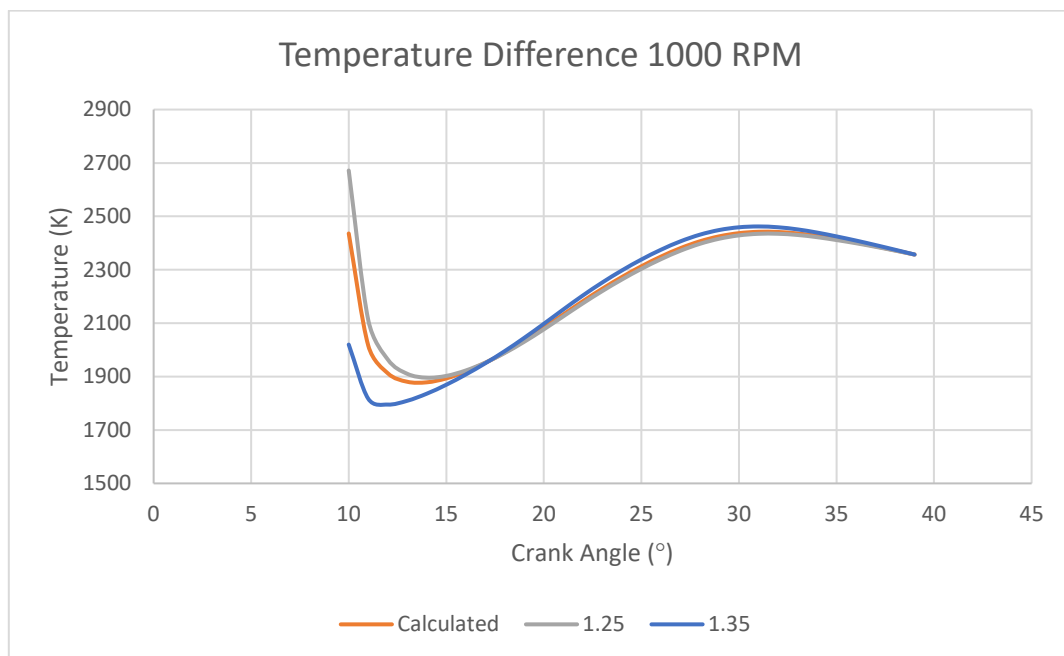


Figure 7-12 Temperature Difference at 1000 RPM

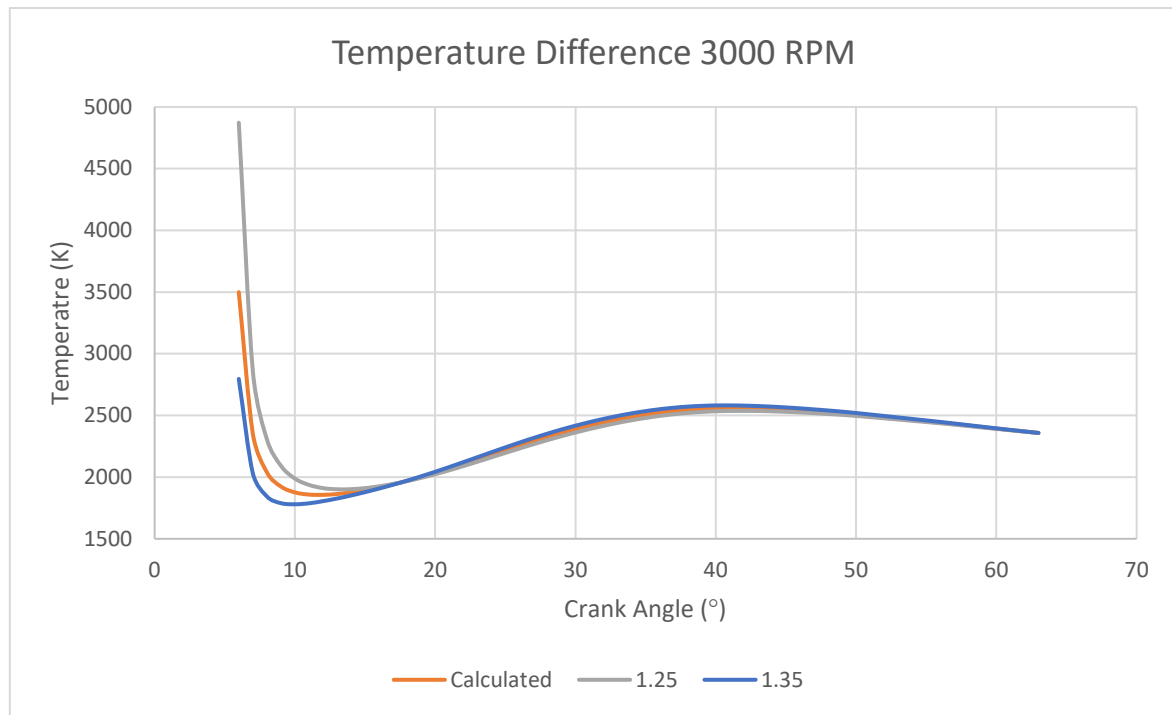


Figure 7-13 Temperature Difference at 3000 RPM

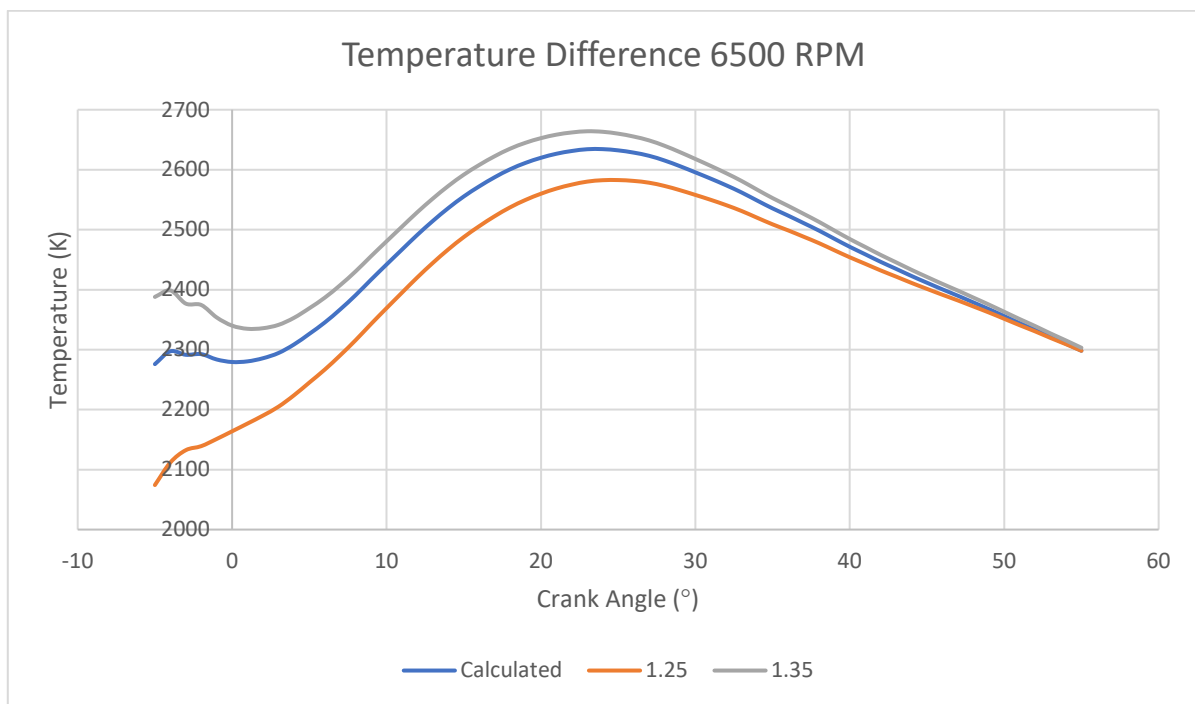


Figure 7-14 Temperature Difference at 6500 RPM

A larger index gives greater maximum temperatures indicating that there is less heat transfer out of the engine occurring, what is also interesting is that a greater polytropic index also helps remove the initial spike seen in *figures 7-12 & 7-13*, this is due to the MFB causing the calculations to predict a larger burnt volume in these early stages and the increase in temperature is due to a smaller burnt volume but increased pressure at the same CA degree compared to the other two indexes.

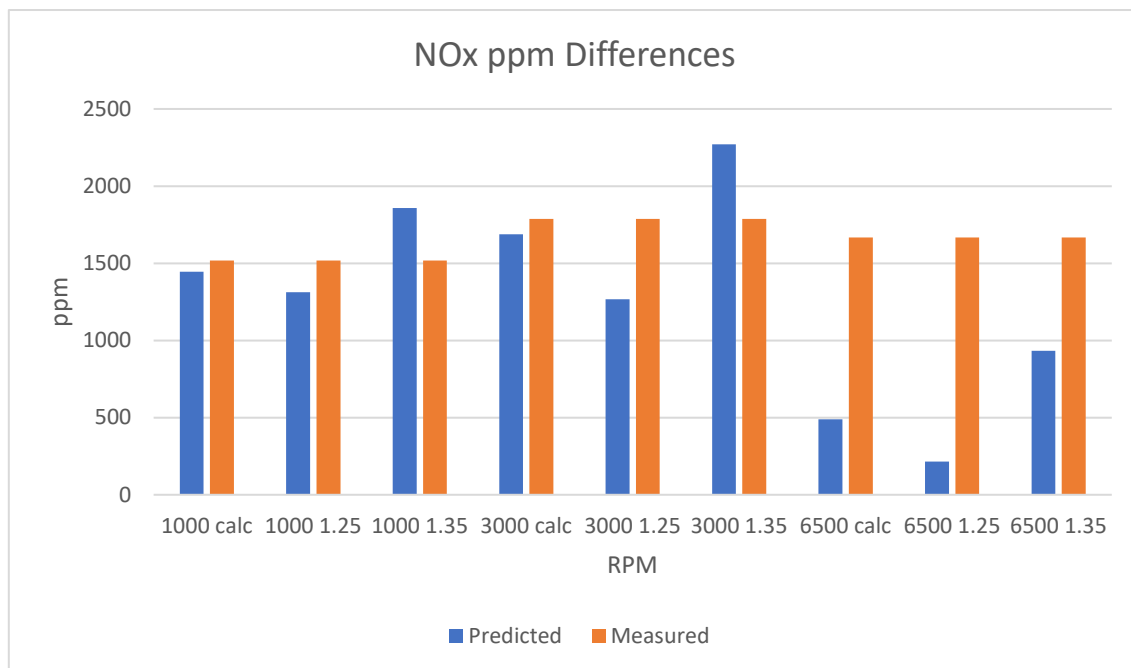


Figure 7-15 NOx Difference due to Polytropic Index

As a result of the increased burnt temperature from the larger polytropic index it can be seen that NOx levels are a lot higher and sometimes over predicts compared to the measured data, suggesting that more heat transfer is occurring in the real engine which as previously discussed with the NOx predictions in the separate cylinders can play an important role in the reduction of NOx.

Finally, the FER was changed so that the Ford Fox ran constantly at stoichiometric to determine how much effect an increase or decrease in oxygen concentration would have on the NOx.

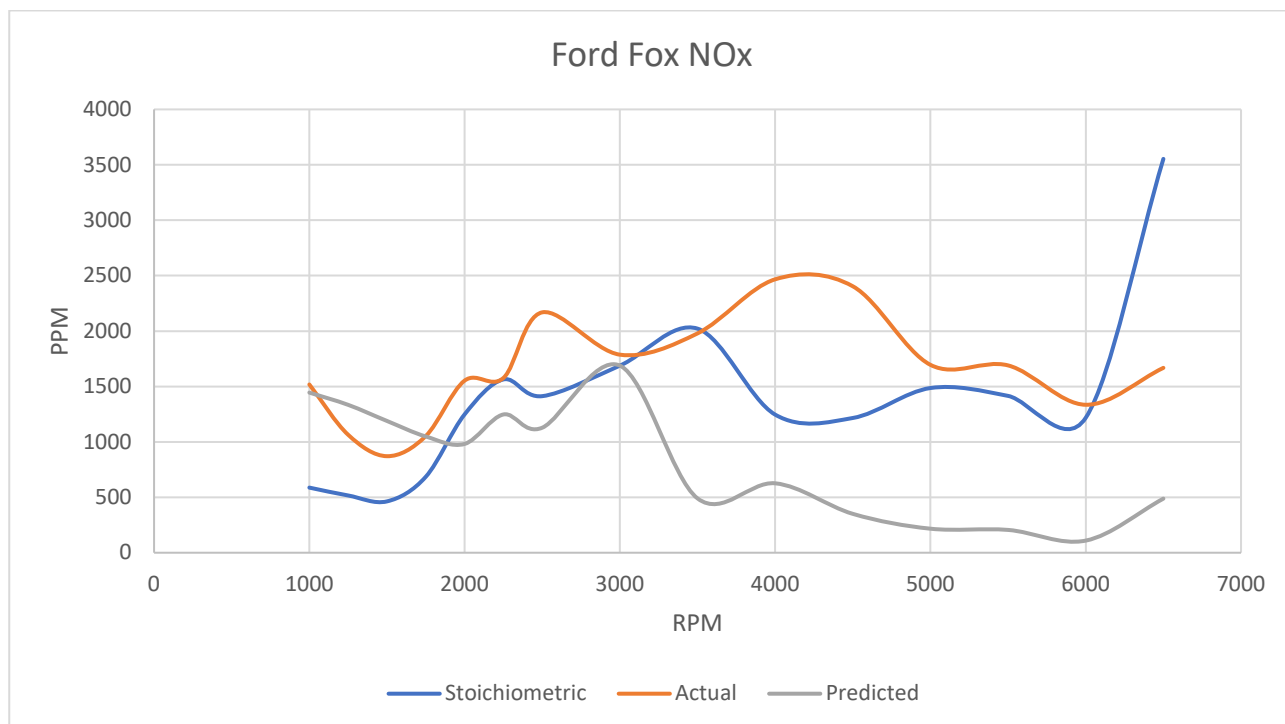


Figure 7-16 Ford Fox Running at Stoichiometric

Figure 7-16 shows drastic changes in NO_x formation, where the engine was previously running lean at low RPM, running stoichiometric has decreased NO_x levels due to the oxygen concentration being reduced and whilst running stoichiometric where the engine was originally rich has predicted closer to the measured value it still seems to be under predicting indicating that the in-cylinder mixture is far from homogeneous and is suffering from lean patches thus increased oxygen concentration. At 6500 RPM it is believed that it is drastically over predicting the oxygen concentration due to the speed at which everything is moving meaning that there would not be enough time for equilibrium to occur in the engine leading to the over prediction.

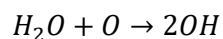
8. Water Injection

8.2 Water Injection Literature Review

Because of increasingly stringent emission standards being imposed on the automotive industry, manufacturers must come up with new means of reducing emissions whilst still producing vehicles that are attractive to customers. Because of this the automotive industry has seen a shift to downsized boosted engines with Gerty and Heywood suggesting that this method can increase engine efficiency by 16% (Gerty & Heywood, 2006) however a boosted engine will experience higher in-cylinder pressures and temperatures increasing the NOx problem.

A widely used method of reducing NOx is to employ the use of EGR to reduce the in-cylinder temperature which has the benefits of reducing the oxygen concentration (Dec, et al., 2009) but also by increasing the heat capacity of the mixture as there is a greater number of kmols experiencing burning which in turn lowers peak temperatures. (Dimitriou, et al., 2015) However, this reduction in oxygen concentration leads to performance loss due to incomplete oxidation of the fuel which is why it can be seen in *appendix 11.6* that EGR is shut off at FL. EGR also simultaneously increases HC emissions due to reduced oxidation and lower combustion temperatures. However, whilst Liu, et al suggests that the inclusion of EGR slows down the combustion process and increases its duration which could cause combustion efficiency to drop, (Liu, et al., 2013) Olsson, et al suggest EGR can increase efficiency if the EGR intake temperature is high enough and Khalef, et al suggest low pressure EGR also increases efficiency. (Olsson, et al., 2003) (Khalef, et al., 2016) However, manufacturers are looking at ways to reduce emissions whilst also increasing performance, one of these methods is to employ the use of water injection.

A common approach to reducing NOx levels from gas turbines is by adding water to the combustion process as the water vapour reduces the oxygen concentration by the following equation:



Equation 8-1 Reaction between Water and Oxygen

These hydroxide radicals do not efficiently 'attack' N₂ preventing NOx being formed however most of the NOx reduction will come from the temperature reduction. (Glassman & Yetter, 2008, p. 436) It is because of the benefits experienced by these engines that the automotive industry is now looking towards water injection as a viable solution.

Currently the BMW M4 GTS runs a BOSCH water injection system in which they are claiming 13% increased fuel economy reducing CO₂ by 4% and increasing power by 5%. (Sheehan, 2016)

Inlet Manifold Water Injection for Control of Nitrogen Oxides-Theory and Experiment- J. E. Nicholls, I. A. El-Messiri and H. K. Newhall

There are three main mechanisms helping to reduce NO_x, the charge cooling effect due to the high latent heat of evaporation meaning that energy must be expended to evaporate the water, the increase in the overall heat capacity and the reduction in the adiabatic flame temperature due to the water dilution. This paper shows the effect of varying levels of water injection at different FER to determine the effectiveness of reducing NO_x on a carbureted single cylinder engine where the water is injected continuously into the induction pipe.

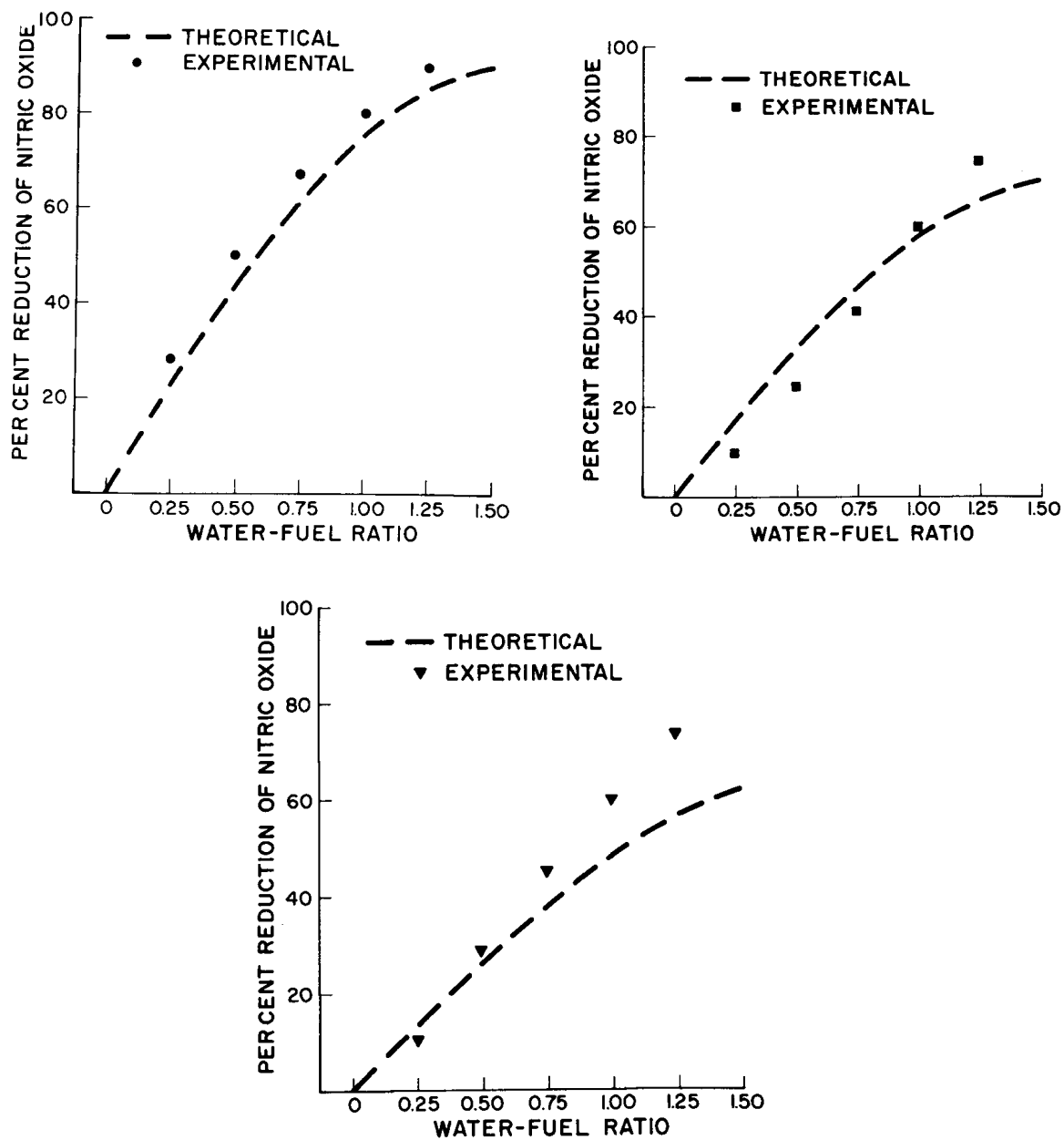


Figure 8-1 NO_x % Reduction with Varying Amounts of Water Injection at FER 1) 1.08 2) 1.0 3) 0.93

Analysing *figure 8-1* it is evident that the effect of water injection is a lot more prevalent during rich operation with a reduction of over 90% at a FER of 1.08 with a W/F of 1.25. Interestingly, water injection appeared to have a positive effect on the BMEP of the engine increasing it up to a W/F before dropping back down to base levels, it was also believed that theoretically because the water was cooling the charge in the induction stage that an increase in V.E was to be expected prior to the inlet valve closing. However, upon studying the experimental results shown that there was no variation in the air flow rates and as such V.E remained unchanged.

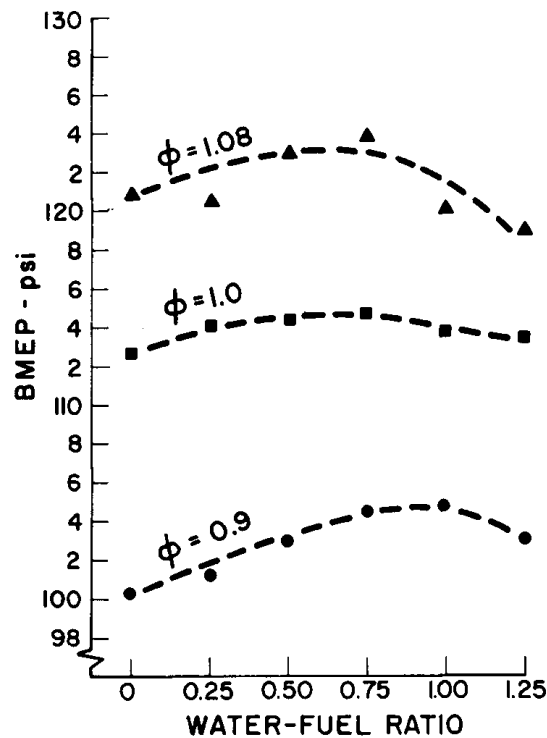


Figure 8-2 Effects of Water Injection on BMEP

The paper begins to conclude that temperature reduction is primarily due to the dilution of the molar and energy densities by the water vapour and that whilst evaporation does have a cooling effect it is minor compared to dilution. Because of this reduction of temperature, the dissociation of products has decreased leading to the expansion process efficiency improving and reducing overall fuel consumption and fortunately as the total moles in the expansion process has increased the combustion pressure and work output of the engine cycle remain unchanged even with the reduced temperature. It was seen that effectiveness of water injection in lean mixtures was reduced, this is most likely since the nitric oxide equilibrium equation is less sensitive to temperature variation compared to rich mixtures. However, in the paper they theoretically under predicted the effectiveness at lean mixture due to the assumption that flame velocity would not be altered when there is a greater reduction in temperature due to flame speed retardation.

(Nicholls, et al., 1969)

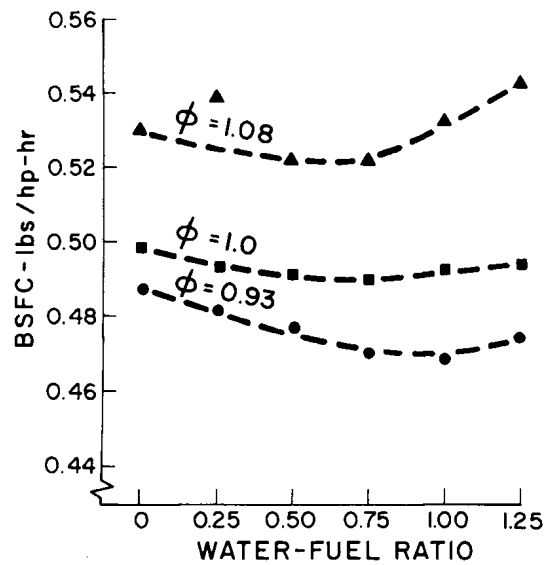


Figure 8-3 Water Injection Effect on BSFC

Whilst this paper gives a good understanding of the effect of water injection, the fact that it was port injection means that what was effective here might not necessarily work on a GDI engine, however because the water is being inducted into the cylinder along with the A/F mixture it follows the same behaviour that will be exhibited in the simple water injection model later in the report.

Emissions from a Direct-Cylinder Water-Injected Spark-Ignition Engine- S. S. Lestz, W. E. Meyer and C. M. Colony

This paper utilised a direct injection water injection system to study the effects of not only the amount of water to inject but also the importance of the injection timing, it also mentions the possibility of worsening other emissions at the expense of reducing NOx.

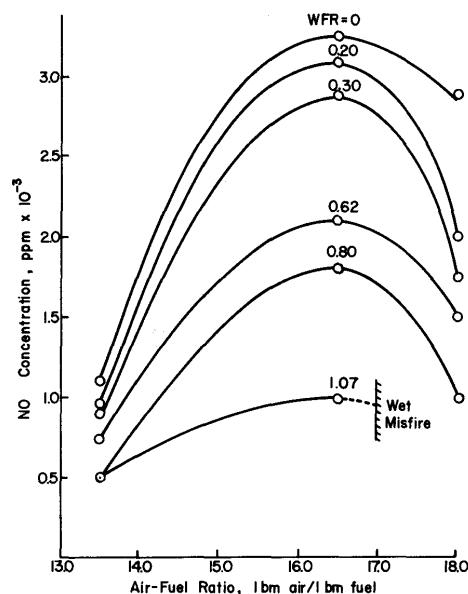


Figure 8-4 NO Emissions versus A/F with varying W/F with an Injection Timing of 45° BTDC at MBT Spark Advance

Figure 8-4 shows that with the timing set to MBT the NO production as a function of the A/F ratio follows the same trend as the W/F ratio, it also proves at W/F=0 that NO production heavily depends on the A/F ratio which further backs up figure 2-2. As it was determined that NO production was highest at an A/F ratio of 16.5:1 further experiments were carried out at this operating condition with variation in the injection timing of the water.

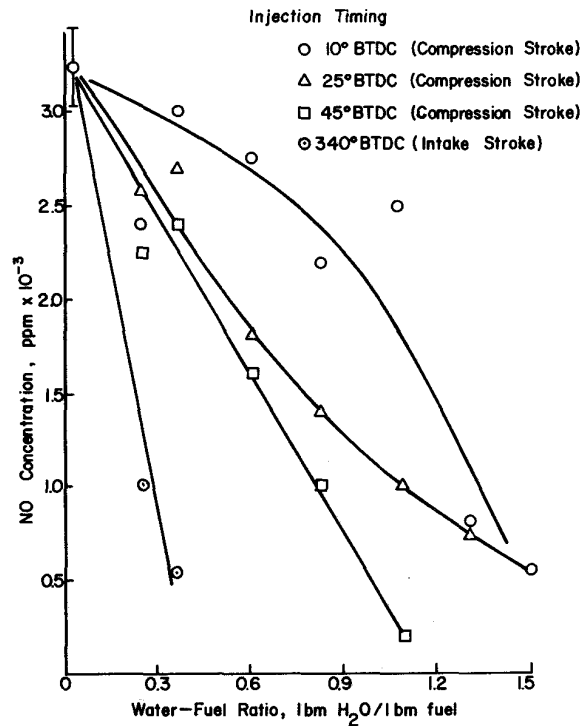


Figure 8-5 NO Emissions versus A/F ratio of 16.5:1 with a 30° Spark Advance

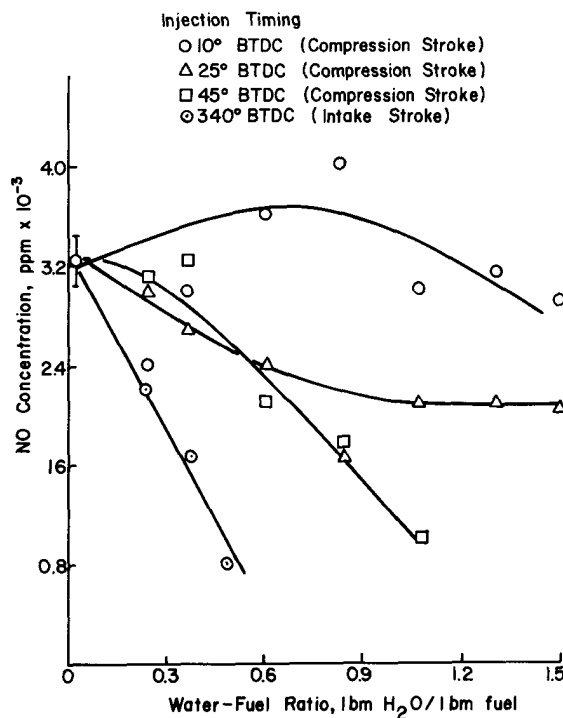


Figure 8-6 NO Emissions versus A/F ratio of 16.5:1 with MBT Timing

Figure 8-5 shows that a 90% reduction is possible with water injection and it found that the rate of reduction is greater when injected in the intake stroke and it was also found that injection at this point used considerably less water to achieve substantial reduction. Whilst not theorised in the paper, it is this author's theory that due to the increased mixture time it is more likely that the water can effectively dilute more of the cylinder. Thus, reducing the concentration of oxygen over a much greater area compared to a late injection timing which would suffer from the same issues GDI finds with lean and rich patches, in that the water will only be effective in certain patches while other patches will see minimal benefit from the water not mixing into it.

For this constant spark timing however, it was found that that the power output degenerated with water injection meaning that to recover the lost energy timing must be advanced to MBT for each operating condition.

Condition	Injection Angle, deg bt/dc	Water Fuel Ratio							
		0.0	0.24	0.36	0.60	0.83	1.07	1.30	1.54
30 deg bt/dc	10	22.0	21.8	21.8	21.6	21.5	21.0	19.6	15.5
Spark	45	22.0	22.8	22.7	21.0	21.0	16.6	miss	
Advance	340	22.0	20.1	19.2	16.3	miss			
MBT	10	22.0	21.8	21.8	22.1	21.6	21.3	20.6	19.7
Spark	45	22.0	22.9	22.9	22.6	22.7	21.3	miss	
Advance	340	22.0	21.5	21.3	19.2	miss			

Figure 8-7 Brake Torque in ft-lbf with Water Injection

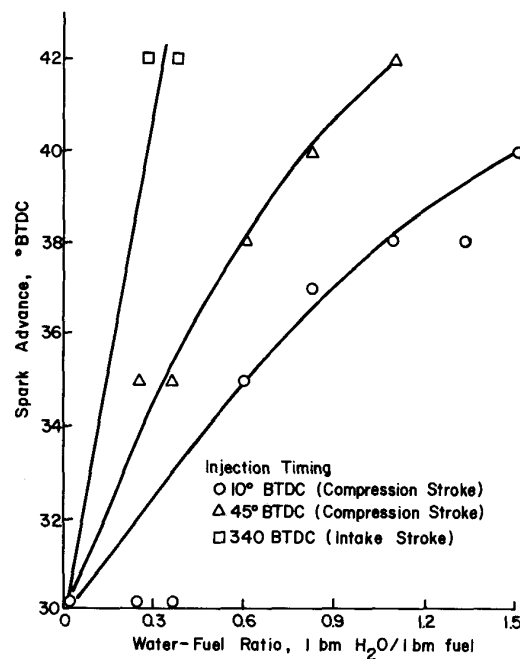


Figure 8-8 Spark Advanced Required to Achieve MBT Timing

Figure 8-7 shows the measured torque for all operating conditions for an A/F ratio of 16.5:1, it can be seen that injecting earlier deteriorates the performance rapidly and requires heavy advancement of the timing with minimal water. However, it was found that an NO reduction of 50% with an increase in performance could be achieved with injection timings between 10-40° before the passage of the spark. Interestingly to note by looking at figure 8-6 is that NO production seems to increase with the inclusion of water injection although this is not discussed further although it could be attributed by the increase in torque.

While the lower temperatures contribute to the reduction of NOx it can be seen that it coincides with an increase of unburnt HC levels due to incomplete combustion.

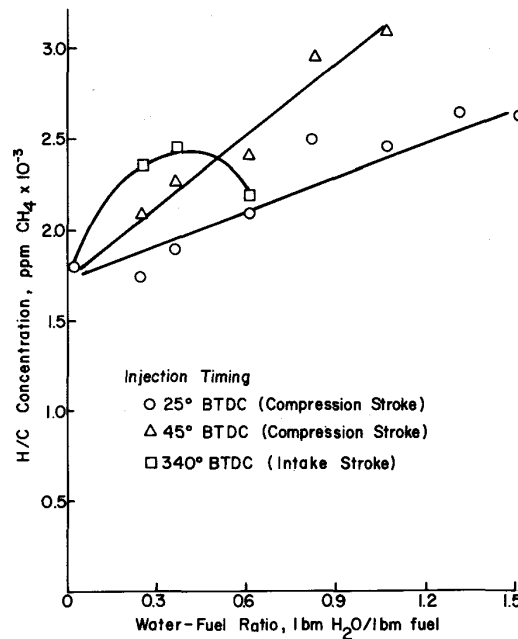


Figure 8-9 HC Emissions at an A/F Ratio of 16.5:1 MBT Timing

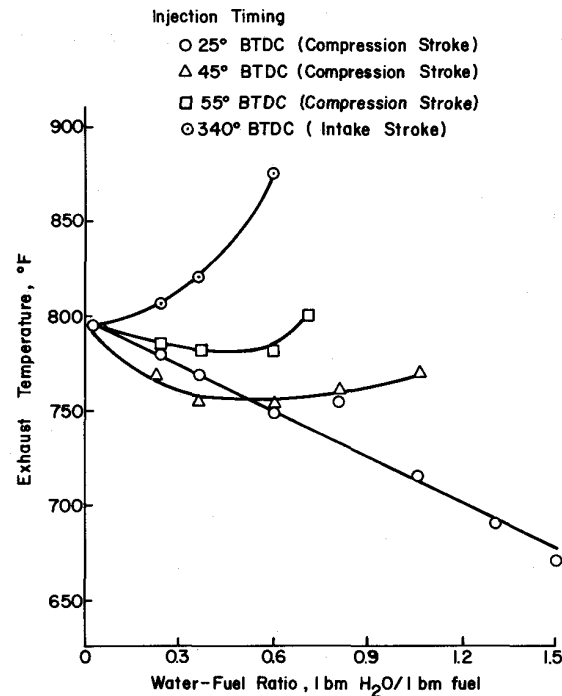


Figure 8-10 Exhaust Temperatures at an A/F Ratio of 16.5:1 MBT Timing

For MBT timing later injections cause a pronounced increase in HC emissions with earlier injections causing a peak and then reducing. This can be caused due to combustion still occurring during the expansion and exhaust stroke burning off the excess HC whilst not discussed in this paper, from the previous paper this phenomenon can be theorised due to the fact that the flame speed is retarded due to the inclusion of an assumed homogenous mixture of the water suggesting that perhaps a study of the MFB with different injection timings can give a greater understanding of how water injection effects the combustion process.

It was later stated that CO₂ and CO levels were unaffected by the presence of water and that the expense of a water injection system means that at the time of writing the authors cannot deem this system of emission control viable. However, with advances in technology which has brought the cost of control systems down significantly in recent years this final remark by no longer hold true.

(Lestz, et al., 1972)

Water Injection: A Technology to Improve Performance and Emissions of Downsized Turbocharged Spark Ignited Engines- Cinzia Tornatore, Daniela Siano, Luca Marchitto, Arturo Iacobacci and Gerado Valentino

This paper seeks to use water injection to advance the spark but also make the engine run stoichiometric from various rich mixtures, looking at the knock reduction and improvement in fuel efficiency. The water to gasoline mass was kept at a constant mass ratio of 0.2 which was determined by a previous experiment injected at a temperature of 298 K at the same time as the fuel. Spark timing was then advanced by one-degree CA until the knock limit was reached.

Speed [rpm]	SA [CAD ATDC]	W/G [%]	SOI _G =SOI _W [CAD ATDC]	λ [± 0.01]
2500	-8	0	-140	0.89
2500	-9 to -11	0.2	-140	1.00
3000	-8.5	0	-165	0.92
3000	-9.5 to -14.5	0.2	-165	1.00
3500	-12	0	-179	0.89
3500	-13 to -17	0.2	-179	1.00
4000	-13	0	-199	0.92
4000	-14 to -19	0.2	-199	1.00
4500	-14	0	-233	0.89
4500	-15 to -21	0.2	-233	1.00

Figure 8-11 Test Operating Parameters

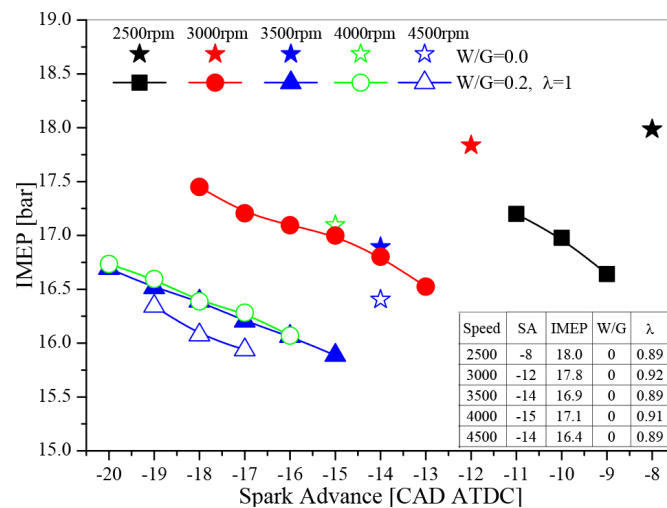


Figure 8-12 IMEP against Spark Advance

Figure 8-12 shows the effect of water injection on the IMEP showing that as the timing is advanced IMEP increases however, it still sees an overall reduction over no water, rich conditions.

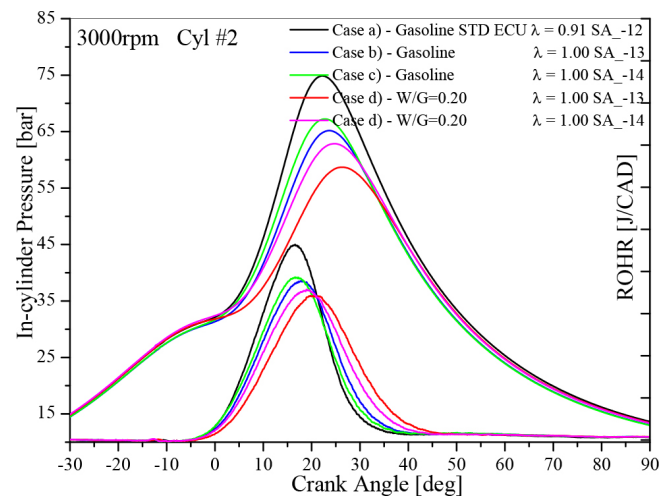


Figure 8-13 In-Cylinder Pressure

Figure 8-13 gives an idea on how the inclusion of water injection can affect the in-cylinder pressure, it is theorised that the heat energy absorbed by the water reduces the peak pressure and decreasing the rate of heat release causing the increase of the burn duration.

It was found that due to the mixture being run at stoichiometric made possible by the inclusion of water injection that CO emissions were drastically reduced however, because of this reduction, CO₂ saw a drastic increase however, both were not affected by the spark timing but by simply running at stoichiometric. Hydrocarbon levels however, were also seen to decrease thanks to the leaner mixture and was only slightly affected by the advanced timing.

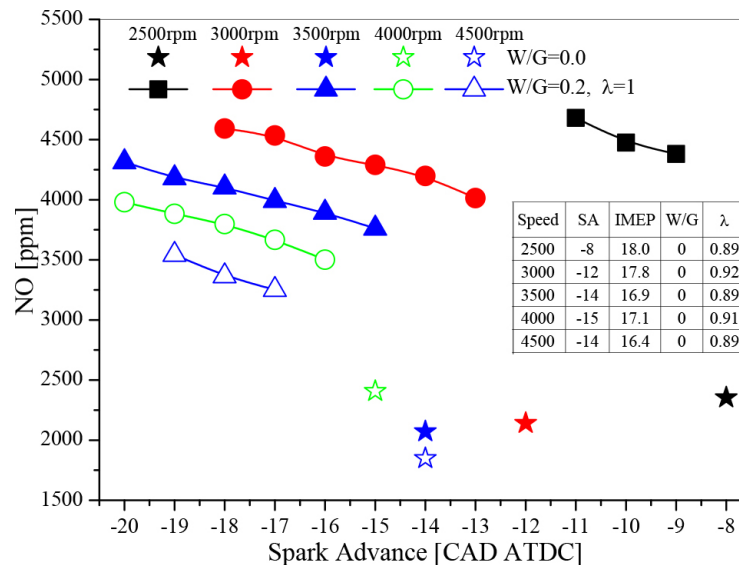


Figure 8-14 NO Emissions against Spark Advance

Interestingly, in this experiment the inclusion of water injection increases NO production. As the timing is advanced increased pressure and thus temperature that will be experienced in the cylinder and even though the cylinder would have undergone cooling from the vaporisation of water NO can be seen to increase. NO production is dependent on temperature and available oxygen, the oxygen concentration will be the limiting factor for NO production which in the case of the rich operating is drastically lower. This means that because water injection has permitted a leaner operation of the engine because the cooling effect of the fuel is no longer necessary the amount of free oxygen will have increased allowing NO reactions to take place.

Naturally if operation was made leaner without the addition of water injection NO production would be higher still however, this paper shows an interesting concept of using water injection to lean out the engine which saw a fuel consumption reduction of 6-12% and the leaner operation saw heavy reduction in HC emissions in which previous papers saw an increase in with the addition of water injection.

(Tornatore, et al., 2017)

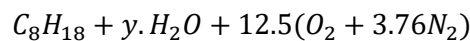
Interestingly all three papers have each approached water injection in different ways, the first simply changing the amount of water injected at different FER's, the second changes the amount of water

injected but mainly focuses on when injection should occur and the third paper keeps the amount of water the same but uses it to advance the timing but more importantly, uses it to change the FER.

Each paper has seen some improvement in emissions and performance but the final paper which found an increase in NO_x suggests to this author that although the Zeldovich mechanism relies heavily on the temperature it relies further on the oxygen concentration which further backs up *figure 7-16* in the sensitivity analysis.

8.3 Methodology

There are multiple stages to this simple water injection model, the first stage is to consider the added mass and then to consider the water's latent heat of vaporisation which is 40 MJ/Kmol as its enthalpy of formation as a liquid is -282 MJ/Kmol and as a gas it is -242 MJ/Kmol compared to isooctane which is -259 MJ/Kmol and -224 MJ/Kmol respectively. Four amounts of injected water will be considered, 10%, 15%, 20% and 25% to the amount of fuel injected, for example for 10%:

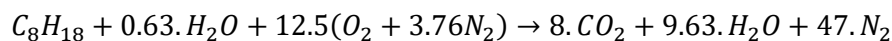


$$\frac{m_{water}}{m_{fuel}} = 10\%$$

$$\frac{y \times 18}{114} = 0.1$$

$$y = \frac{0.1 \times 114}{18}$$

$$y = 0.63$$



Equation 8-2 10% Water Addition Chemical Equilibrium

Now using *equation 3-15* the new molecular weight of the mixture can be determined:

$$m_{product} = \frac{m_{fuel} + m_{air} + m_{water}}{\phi + y + [x(1 + 3.76)]}$$

Equation 8-3 Molecular Weight with Water

Reactant		C8 H18									Water added to fuel (y.H2O)			
Fuel Ratio	RPM	Mol Wt (K)	Mol Wt RGF	C	H	H2O	R.Un	RPM			10%	15%	20%	25%
0.90	1000	30.0111	30.00327156	7.20721	16.2162	0.5706	277.103	1000			0.570598324	0.8559	1.1412	1.4265
0.90	1250	30.0111	30.0111374	7.20721	16.2162	0.5706	277.03	1250			0.570598324	0.8559	1.1412	1.4265
0.91	1500	30.0215	30.02145133	7.27273	16.3636	0.57566	276.935	1500			0.575664679	0.8635	1.15133	1.43916
0.97	1750	30.099	28.49757075	7.76699	17.4757	0.6143	291.744	1750			0.614295643	0.92144	1.22859	1.53574
1.01	2000	30.148	28.56955431	8.08081	18.1818	0.63963	291.009	2000			0.639627422	0.95944	1.27925	1.59907
1.01	2250	30.148	30.14799565	8.08081	18.1818	0.63963	275.773	2250			0.639627422	0.95944	1.27925	1.59907
1.01	2500	30.148	30.14799565	8.08081	18.1818	0.63963	275.773	2500			0.639627422	0.95944	1.27925	1.59907
1.00	3000	30.1354	30.13535939	8	18	0.63329	275.889	3000			0.633294477	0.94994	1.26659	1.58324
1.06	3500	30.215	30.21499377	8.51064	19.1489	0.67383	275.161	3500			0.673825323	1.01074	1.34765	1.68456
1.03	4000	30.1762	30.17623354	8.24742	18.5567	0.64159	275.515	4000			0.641590634	0.96239	1.28318	1.60398
1.05	4500	30.201	30.20101371	8.42105	18.9474	0.66686	275.289	4500			0.666859084	1.00029	1.33372	1.66715
1.09	5000	30.2438	30.24380367	8.69565	19.5652	0.68839	274.899	5000			0.688391096	1.03259	1.37678	1.72098
1.09	5500	30.2438	30.24380367	8.69565	19.5652	0.68839	274.899	5500			0.688391096	1.03259	1.37678	1.72098
1.11	6000	30.2739	30.273859	8.88889	20	0.70359	274.626	6000			0.703590164	1.05539	1.40718	1.75898
1.11	6500	30.2739	30.273859	8.88889	20	0.70359	274.626	6500			0.703590164	1.05539	1.40718	1.75898

Figure 8-15 Molecular Weight with 10% Water Injection

Comparing figures 3-16 & 8-1 it can be seen that the molecular weight of the mixture has decreased thus increasing the gas constant. This can also be seen in the products molecular weight and R_b and as the temperatures calculated require the gas constant this increase will decrease the calculated temperatures.

In addition to the molecular weight, the total mass will increase in that:

$$m_{total} = (C_{total} \times C_{mass}) + (H_{total} + H_{mass}) + (H_2O_{total} \times H_2O_{mass})$$

Equation 8-4 Total Mass with Water

With an increase in mass, α will decrease causing a decrease in the total NO_x produced.

Next it will be determined how the evaporation of the water affects the temperature, to change 0.63 kmols of H₂O from a liquid to a gas it can be calculated as:

$$0.63 \times 40 = 25.2 \text{ MJ}$$

Equation 8-5 Energy Required to Change Water State

Therefore, the total net heat release is:

$$5100 - (0.63 \times 40) = 5074.8 \text{ MJ}$$

Equation 8-6 Heat Release of the water

Meaning that the total energy reduction caused by the water evaporating:

$$\frac{25.2}{100} \times 100 = 0.5\%$$

Equation 8-7 Total Heat Reduction

The next stage involves increasing the specific heat capacity using equation 4-2 except with constant values for H₂O. With the C_p values calculated for every degree CA the new $C_{p,avg}$ could be calculated:

$$\tilde{C}_{p,Avg} = \frac{(\tilde{C}_{p,fuel} \times \phi) + (\tilde{C}_{p,H_2O} \times y) + 12.5(\tilde{C}_{p,O_2} + (3.76 \times \tilde{C}_{p,N_2}))}{\phi + y + (12.5 \times 3.76)}$$

Figure 8-16 Average Specific Heat with Water Injection Included

With this the ratio of specific heat decreases due to the increase of specific heats as seen in figure 8-6:

Temp K	H2O	Cp N2	J/Kmol.K O2	J/Kmol.K C8H18	J/Kmol.K Cp.Av	J/Kmol.K Cv.Av	Gamma
2000	51036.7	36016.2	37841.9	563782	44265.9	35951.9	1.23125

Temp K	H2O	Cp N2	J/Kmol.K O2	J/Kmol.K C8H18	J/Kmol.K Cp.Av	J/Kmol.K Cv.Av	Gamma
2000	51036.7	36016.2	37841.9	563782	44422.1	36108.1	1.23025

Figure 8-17 Ratio of Specific Heat at 1) 0% Water Injection 2) 25% Water Injection

However, it was observed that this decrease had a negligible effect on the burnt temperature.

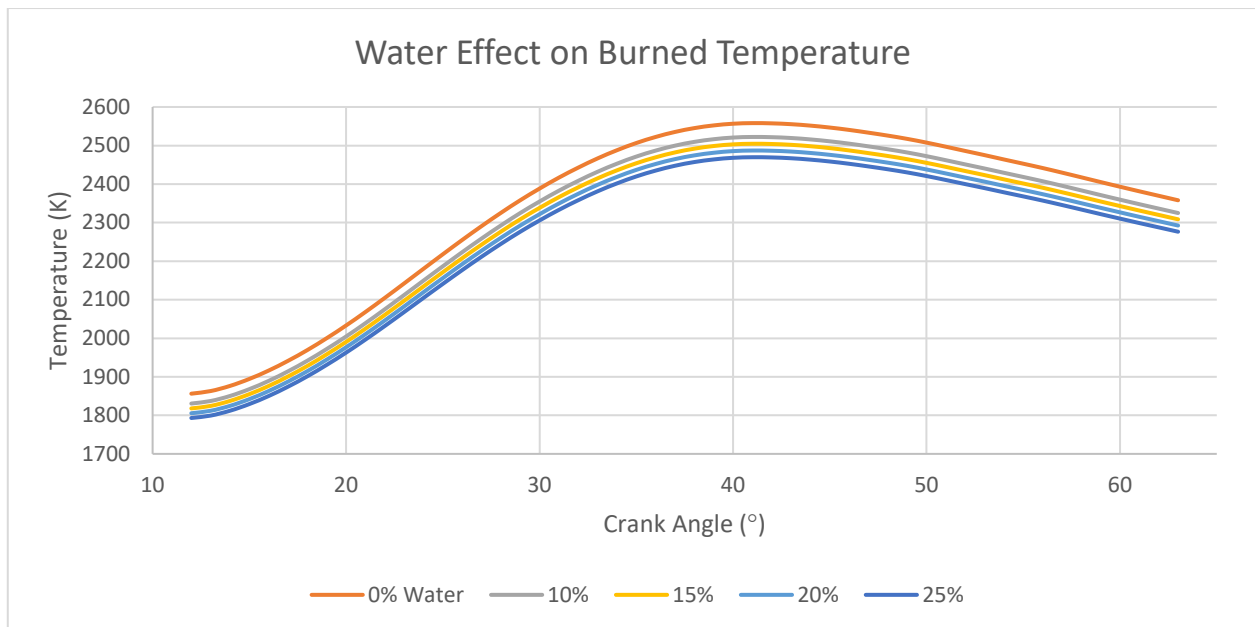


Figure 8-18 Water Effect on Temperature

The peak temperature at 3000 RPM with 0% water injection is 2558 K and with an inclusion of 25% water this temperature is reduced to 2470 K.

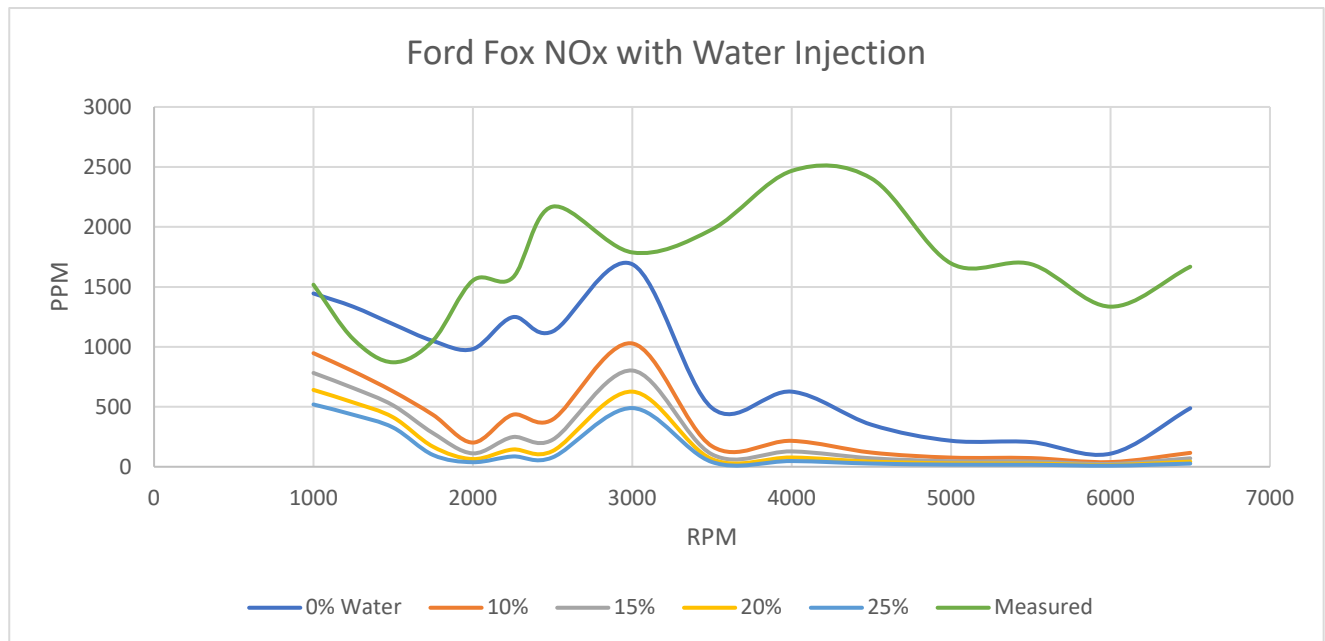


Figure 8-19 Water Effect on NOx

Even with only a peak temperature reduction of 88 K it is evident that it has a dramatic effect on the NOx levels reducing the produced NOx by 71% at 3000 RPM FER=1 and a 98% reduction at 5000 RPM FER=1.09. This seems to follow the trend suggested by Nicholls, et al in which *figure 8-1* shows a reduction in NOx at FER=1 between 60-80% and whilst it also shows a reduction for FER=1.08 of over 90% it seems that the calculated predicted result of 98% may be too high however this may be due to the under prediction caused by the rich mixture

9. Conclusion

This report can be split into three sections, combustion analysis, NO_x analysis and water injection. Temperatures in both the unburnt zone and burnt zone have been calculated from a simple single zone model based on first principles. If this sections work was repeated, particular attention would be placed on determining the SOC, EOC and MFB as it was found that these can have a large effect on the final temperatures even with an apparent minimal change in MFB.

With regards to the NO_x prediction it was seen to drastically under-predict at rich mixtures and even when changed to stoichiometric there was still some degree of under-prediction. This suggests to the author that both engines analysed suffer from poor mixing meaning that large amounts of rich and lean patches exist in-cylinder. Unfortunately, the method used in this report cannot predict these patches and as such if this investigation was carried out again a CFD simulation would be employed to determine how the fuel is mixing with the air therefore determining the A/F ratio in each patch. This would allow the user to measure how much NO_x each patch would produce during each cycle.

The final part of this report was to study how water injection affects NO_x production, whilst this model employed a simple method it was shown that it was possible to drastically decrease NO_x formation through a reduction in temperature and increase in mass. It was found through research that the concept of water injection has been around for some time but has been picking up interest lately and has been shown to improve emissions whilst also increasing the power output on the engine. Because a lot of water injections benefits come from changing the spark timing and water injection timing it seems fit that whilst a simple numerical model can be done, it would be best to carry it out experimentally.

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11. Appendix

11.1 Molecular Mass

Species	Mass
Carbon	12.011
Hydrogen	1.008
Oxygen	15.999
Nitrogen	14.007
CO ₂	44.009
H ₂ O	18.015
O ₂	31.998
CO	28.01

Figure 11-1 Molecular Masses

11.2 Polytropic Index

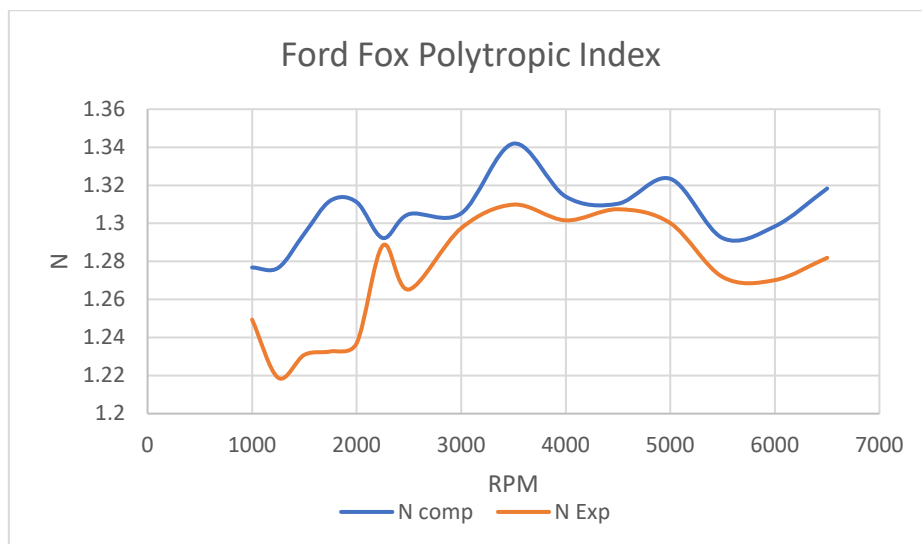


Figure 11-2 Ford Fox Polytropic Index

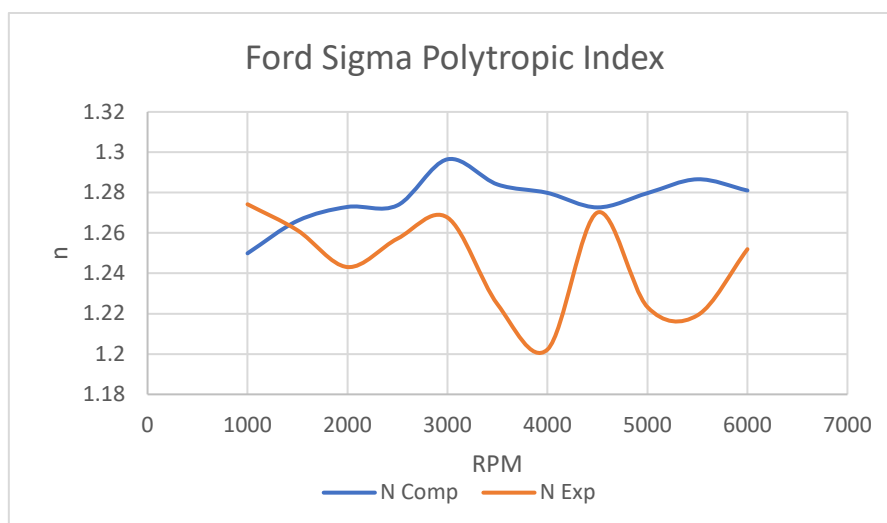


Figure 11-3 Ford Sigma Polytropic Index

11.3 Matlab Curve Fitting

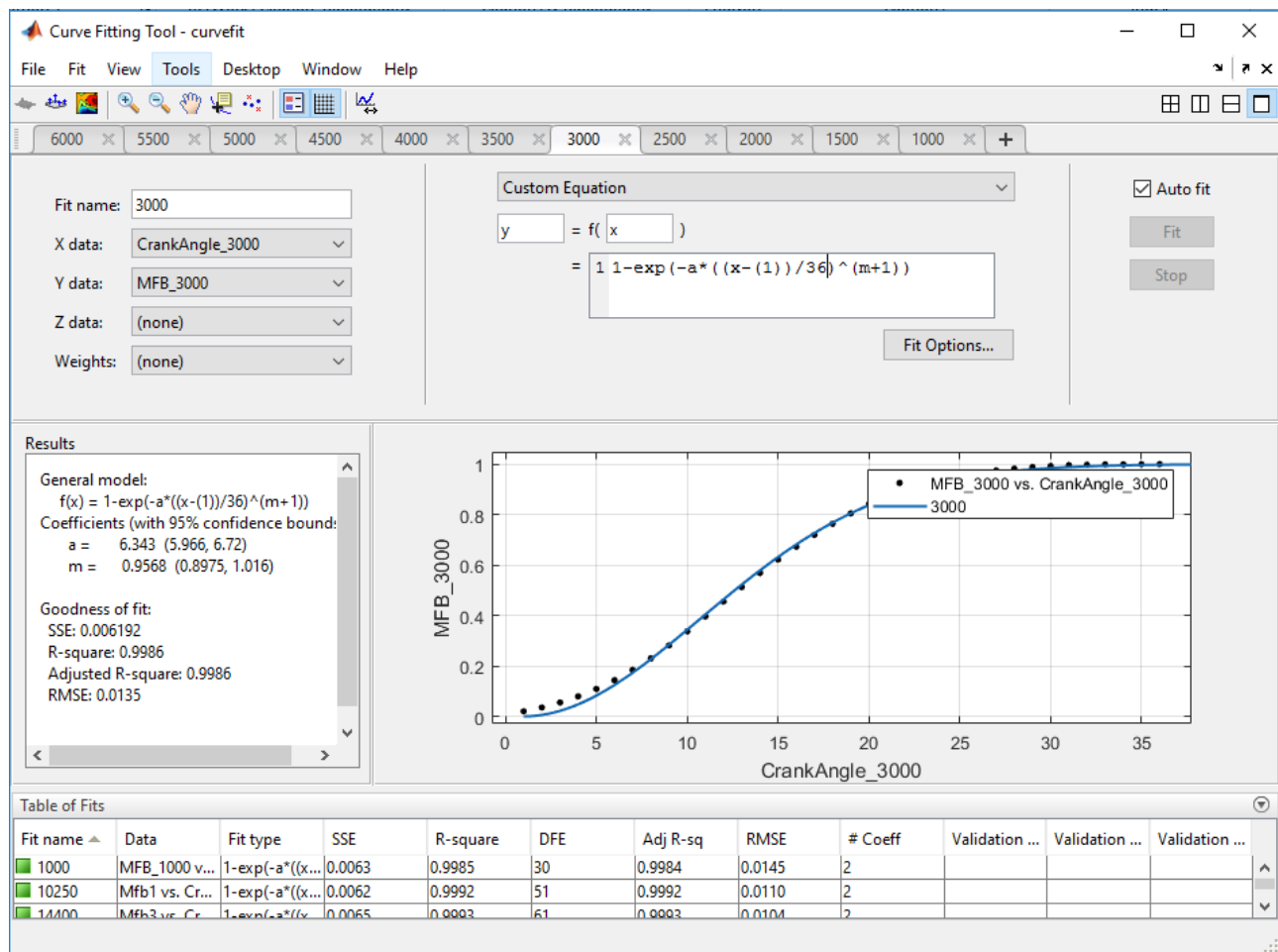


Figure 11-4 Matlab Curve Fit

Workspace	
Name	Value
Crank1	53x1 double
Crank2	53x1 double
Crank3	63x1 double
CrankAngle1000	38x1 double
CrankAngle1500	38x1 double
CrankAngle2000	41x1 double
CrankAngle2500	44x1 double
CrankAngle3000	37x1 double
CrankAngle3500	39x1 double
CrankAngle4000	45x1 double
CrankAngle4500	44x1 double
CrankAngle5000	42x1 double
CrankAngle5500	49x1 double
CrankAngle6000	48x1 double
Mfb1	53x1 double
MFB1000	38x1 double
MFB1500	38x1 double
Mfb2	53x1 double
MFB2000	41x1 double
MFB2500	44x1 double
Mfb3	63x1 double
MFB3000	37x1 double
MFB3500	39x1 double
MFB4000	45x1 double
MFB4500	44x1 double
MFB5000	42x1 double
MFB5500	49x1 double
MFB6000	48x1 double

Figure 11-5 Data Import of Crank Angle and MFB to Supply Curve Fit Tool

11.4 JANAF Tables

CO2	T range (K)	ai1	ai2	ai3	ai4	ai5
	1000-5000	4.4608	0.003098	-1.2E-06	2.27E-10	-1.6E-14
	300-1000	2.4008	0.008735	-6.6E-06	2E-09	6.33E-16
H2O	1000-5000	2.7168	0.002945	-8E-07	1.02E-10	-4.8E-15
	300-1000	4.0701	-0.00111	4.15E-06	-3E-09	8.07E-13
CO	1000-5000	2.9841	0.001489	-5.8E-07	1.04E-10	-6.9E-15
	300-1000	3.7101	-0.00162	3.69E-06	-2E-09	2.4E-13
O2	1000-5000	3.622	0.000736	-2E-07	3.62E-11	-2.9E-15
	300-1000	3.6256	-0.00188	7.06E-06	-6.8E-09	2.16E-12
N2	1000-5000	2.8963	0.001516	-5.7E-07	9.98E-11	-6.5E-15
	300-1000	3.6748	-0.00121	2.32E-06	-6.3E-10	-2.3E-13
	Af1	Af2	Af3	Af4	Af5	
C8H18	-0.55313	181.62	-97.787	20.402	-0.03095	

Figure 11-6 Coefficients for Polynomials for Specific Heat Equations

N₂ If statement:

=IF(AA3<1000,8314*(Coefficients!\$C\$15+(Coefficients!\$D\$15*AA3)+(Coefficients!\$E\$15*(AA3^2))+
(Coefficients!\$F\$15*(AA3^3))+(Coefficients!\$G\$15*(AA3^4))),8314*(Coefficients!\$C\$14+(Coefficient
s!\$D\$14*AA3)+(Coefficients!\$E\$14*(AA3^2))+(Coefficients!\$F\$14*(AA3^3))+(Coefficients!\$G\$14*(A
A3^4))))

O₂ If statement:

=IF(AA3<1000,8314*(Coefficients!\$C\$12+(Coefficients!\$D\$12*AA3)+(Coefficients!\$E\$12*(AA3^2))+
(Coefficients!\$F\$12*(AA3^3))+(Coefficients!\$G\$12*(AA3^4))),8314*(Coefficients!\$C\$11+(Coefficient
s!\$D\$11*AA3)+(Coefficients!\$E\$11*(AA3^2))+(Coefficients!\$F\$11*(AA3^3))+(Coefficients!\$G\$11*(A
A3^4))))

H₂O If statement:

=IF(AA3<1000,8314*(Coefficients!\$C\$6+(Coefficients!\$D\$6*AA3)+(Coefficients!\$E\$6*(AA3^2))+
(Coefficients!\$F\$6*(AA3^3))+(Coefficients!\$G\$6*(AA3^4))),8314*(Coefficients!\$C\$5+(Coefficients!\$D\$5*
AA3)+(Coefficients!\$E\$5*(AA3^2))+(Coefficients!\$F\$5*(AA3^3))+(Coefficients!\$G\$5*(AA3^4))))

Isooctane equation:

=4184*(Coefficients!\$B\$18+(Coefficients!\$C\$18*(AA3/1000))+(Coefficients!\$D\$18*((AA3/1000)^2))
+(Coefficients!\$E\$18*((AA3/1000)^3))+(Coefficients!\$F\$18/((AA3/1000)^2)))

11.5 Equilibrium Constants

Temperature K	K _{CO2}	Temperature K	K _{H2O}	Temperature K	K _{WGS}
298.15	1.16E+45	298.15	1.12E+40	298.15	9.5945E-06
300	5.75E+44	300	6.11E+39	300	0.000010617
500	1.06E+25	500	7.69E+22	500	0.0072607
1000	1.66E+10	1000	1.15E+10	1000	0.6935
1500	207010	1500	530880	1500	2.5645
2000	765.6	2000	3467	2000	4.5285
2100	345.94	2100	1686.6	2100	4.8754
2200	168.27	2200	874.98	2200	5.1999
2300	87.097	2300	480.84	2300	5.5207
2400	47.753	2400	277.43	2400	5.8097
2500	27.543	2500	167.49	2500	6.081
2700	10.351	2700	68.077	2700	6.5769
3000	3.0549	3000	22.029	3000	7.211

Figure 11-7 Partial Pressure Equilibrium Constants

Using Gibbs Function:

Temp K	ΔG CO KJ/mol	ΔG CO ₂ MJ/Kmol	ΔG Overall MJ/Kmol	ΔG Overall J/Kmol	KCO ₂
300	-137.328	-394.394	257.066	257066000	5.76E+44
400	-146.338	-394.675	248.337	248337000	2.7E+32
500	-155.414	-394.939	239.525	239525000	1.06E+25
600	-164.486	-395.182	230.696	230696000	1.22E+20
700	-173.518	-395.398	221.88	221880000	3.61E+16
800	-182.497	-395.586	213.089	213089000	8.2E+13
900	-191.416	-395.748	204.332	204332000	7.24E+11
1000	-200.275	-395.886	195.611	195611000	1.65E+10
1100	-209.075	-396.001	186.926	186926000	7.53E+08
1200	-217.819	-396.098	178.279	178279000	57618653
1300	-226.509	-396.177	169.668	169668000	6570373
1400	-235.149	-396.24	161.091	161091000	1024698
1500	-243.74	-396.288	152.548	152548000	205298.2
1600	-252.284	-396.323	144.039	144039000	50415.1
1700	-260.784	-396.344	135.56	135560000	14635.32
1800	-269.242	-396.353	127.111	127111000	4884.256
1900	-277.658	-396.349	118.691	118691000	1832.993
2000	-286.034	-396.333	110.299	110299000	760.0083
2100	-294.372	-396.304	101.932	101932000	343.1715
2200	-302.672	-396.262	93.59	93590000	166.7974
2300	-310.936	-396.209	85.273	85273000	86.4332
2400	-319.164	-396.142	76.978	76978000	47.36342
2500	-327.356	-396.062	68.706	68706000	27.26372
2600	-335.514	-395.969	60.455	60455000	16.39078
2700	-343.638	-395.862	52.224	52224000	10.24166
2800	-351.729	-395.742	44.013	44013000	6.623724
2900	-359.789	-395.609	35.82	35820000	4.417852
3000	-367.816	-395.461	27.645	27645000	3.029421

Figure 11-8 Equilibrium Constants for CO₂ from Gibbs Function

Temp	ΔG_{H_2O}	ΔG_{H_2O}	K_{H_2O}
K	MJ/Kmol	J/Kmol	
300	-228.5	-2.3E+08	6.12098E+39
400	-223.901	-2.2E+08	1.73591E+29
500	-219.051	-2.2E+08	7.67232E+22
600	-214.007	-2.1E+08	4.28191E+18
700	-208.612	-2.1E+08	3.69301E+15
800	-203.496	-2E+08	1.93823E+13
900	-198.083	-2E+08	3.13945E+11
1000	-192.59	-1.9E+08	11487688537
1100	-187.033	-1.9E+08	761687121.6
1200	-181.425	-1.8E+08	78978678.16
1300	-175.774	-1.8E+08	11559550.31
1400	-170.089	-1.7E+08	2219870.033
1500	-164.376	-1.6E+08	530014.2273
1600	-158.639	-1.6E+08	151084.1695
1700	-152.883	-1.5E+08	49853.11379
1800	-147.111	-1.5E+08	18586.78416
1900	-141.325	-1.4E+08	7681.310573
2000	-135.528	-1.4E+08	3465.42087
2100	-129.721	-1.3E+08	1685.581455
2200	-123.905	-1.2E+08	874.9533943
2300	-118.082	-1.2E+08	480.643722
2400	-112.252	-1.1E+08	277.4529895
2500	-106.416	-1.1E+08	167.3096091
2600	-100.575	-1E+08	104.8695693
2700	-94.729	-9.5E+07	68.03131431
2800	-88.878	-8.9E+07	45.50920918
2900	-83.023	-8.3E+07	31.29390107
3000	-77.163	-7.7E+07	22.05848594

Figure 11-9 Equilibrium Constants for H_2O from Gibbs Function

Polynomial for K_{CO_2} 1500-2000 K:

$$y = -0.000000049281850043659200000000x^5 + 0.000449623072261788000000000000x^4 - 1.640094290538710000000000000000x^3 + 2,990.2282643030200000000000000000x^2 - 2,725,270.2143953700000000000000000000x + 993,432,501.1051160000000000000000000000$$

Polynomial for K_{CO_2} 2000-3000 K:

$$y = 0.000000000000011561961150323900x^6 - 0.000000000181552774506246000000x^5 + 0.000001186283062932530000000000x^4 - 0.004129230028377830000000000000x^3 + 8.077138657718070000000000000000x^2 - 8,420.547025793900000000000000000x + 3,656,333.6249396400000000000000000000$$

0.0149097813747857*AM375^3 + 29.2661496497352*AM375^2 - 30630.5404236399*AM375 + 13360106.9047217))))))

11.6 Pressure Polynomials

	Coefficients						
PER	x6	x5	x4	x3	x2	x	c
0.996	-1.331E-19	1.70561E-15	-9.01472E-12	2.55941E-08	-4.12926E-05	0.035769	-12.87402
0.989	-1.974E-20	1.41466E-16	-1.45606E-13	-8.24479E-10	2.242E-06	-0.001836	0.51719
1.013	9.777E-19	-1.36457E-14	7.83935E-11	-2.36623E-07	0.000395443	-0.346928	124.8676
1.094	-5.1E-19	7.34215E-14	-4.29703E-11	1.31455E-07	0.000222317	0.197399	71.95528
1.116	-1.164E-20	1.01128E-15	-7.70549E-12	2.77802E-08	5.25929E-05	0.050707	19.8768
1.188	2.366E-19	-2.941E-15	1.5205E-11	-4.18189E-08	6.44882E-05	-0.052828	17.94563
1.230	1.864E-19	-2.3473E-15	1.22872E-11	-3.41984E-08	5.33381E-05	-0.044166	15.15494
1.238	1.759E-19	-2.21792E-15	1.16238E-11	-3.23887E-08	5.05692E-05	-0.041914	14.39579
1.235	1.798E-19	-2.2663E-15	1.18725E-11	-3.30684E-08	5.16114E-05	-0.042764	14.68269
1.239	1.746E-19	-2.20191E-15	1.15415E-11	-3.21634E-08	5.02236E-05	-0.041633	14.30052
	+	+	+	+	+	+	+
Current polynomials							
0.996	-1.33131182092894E-19x6+1.70560667150519E-15x5+9.01471560270762E-12x4+2.55941329171256E-08x3+4.129260047405037x2+0.0357691920063855x-12.8740212513686						
0.989	-1.97407537196508E-20x6+1.41466013153212E-16x5+1.4560637049173E-13x4-8.24479168168314E-10x3+2.24200058682836E-06x2-0.00183585164629393x+0.51718999170481						
1.013	9.7766090036465E-19x6+1.3645745039685E-14x5+7.8393516981262E-11x4-2.36623209129529E-07x3+0.000395443116854288x2+0.34692824979165x+124.86768985434						
1.094	-5.100258006564E-19x6+7.342148064356E-14x5+2.270341049558E-11x4+1.31455209422505E-07x3+0.0002231672505586x2+0.197399300525359x-71.9552836544667						
1.116	-4.16399664189044E-20x6+1.01127632325195E-15x5+7.706494868884E-12x4+2.77801571094969E-08x3+5.25929136957754E-05x2+0.0507067609290734x-19.876509609047						
1.188	2.36570995257328E-19x6+2.941001249984E-15x5+1.52050455274713E-11x4+4.1818907996429E-08x3+6.44881654361159E-05x2+0.0528281273415682x+17.945672038745						
1.230	1.86394766023552E-19x6+2.3473964650373E-15x5+1.2287222005546E-11x4+3.4198444725649E-08x3+5.3338113817649E-05x2+0.044165846011809x+15.15494026165						
1.238	1.758959333677E-19x6+2.2179187780919E-15x5+1.16238419265124E-11x4+3.23886659548953E-08x3+5.0569200654988E-05x2+0.0419144981078371x+14.395786183786						
1.235	1.79816447195679E-19x6+2.2630472105392E-15x5+1.18724783241904E-11x4+3.30684225354827E-08x3+5.000506161401815467x2+0.04276354617103415x+14.682694169875						
1.239	1.7460532782589E-19x6+2.20191158751389E-15x5+1.15415319051719E-11x4+3.21634447704582E-08x3+5.02236197854321E-05x2+0.041632760905359x+14.3005198900919						
10 bar							
0.996	-1.5931242106031E-19x6+1.78300094497947E-15x5+8.1166698932049E-12x4+1.98571696416819E-08x3+2.80596298052125E-05x2+0.0218043768076571x-7.19971479230418						
0.989	-1.8404130090992E-19x6+2.19955033664222E-15x5+1.09060295686666E-11x4+2.96956394733808E-08x3+0.0004719505882845x2+0.0412233589922325x+11.15734171338472						
1.013	-6.40475187114041E-19x6+8.72131177005922E-15x5+5.13190345628049E-11x4+1.59140246385724E-07x3+0.000278107258526711x2+0.258269174305353x-99.0354822145055						
1.094	-3.41148566492621E-19x6+5.1793505989939E-14x5+2.4622944868031E-11x4+7.07828620223237E-07x3+0.0011328753330186x2+0.957567992978181x+333.9801557695						
1.116	-3.64099756234191E-19x6+4.9349158786589E-14x5+2.7206512808969E-11x4+7.9525707546281E-07x3+0.00193368453993x2+1.11143860726057x+393.68725552542						
1.188	-1.09460182991786E-19x6+1.5473732246381E-14x5+8.933250422666E-11x4+2.7038426347041E-07x3+0.000453394463742003x2+0.398803178304969x+144.909192473458						
1.230	-2.1473508453152E-19x6+3.59457018119579E-15x5+2.32231373891012E-11x4+7.61865194653443E-08x3+0.00135712996545919x2+0.12541062846709x+47.1743712768884						
1.238	-1.09363098544869E-19x6+2.164401087534E-15x5+1.5198152501631E-11x4+5.24435120687722E-08x3+9.66298402796014E-05x2+0.0914686314171816x+35.0268315278517						
1.235	-1.4722252951693E-19x6+2.674691300664E-15x5+1.80641917196705E-11x4+6.0928049843534E-08x3+0.00110608503205519x2+0.103615536820054x-39.3762783971497						
1.239	-9.78731506847854E-20x6+2.00096596741334E-15x5+1.4279518629602E-11x4+4.97217021246013E-08x3+9.21440085803727E-05x2+0.0875687941947311x+33.6298526855113						
20 bar							
0.996015936	-1.72543292507393E-19x6+2.07707232880659E-15x5+1.02933082911708E-11x4+2.75038212397537E-08x3+4.20814114648676E-05x2+0.0348855142432627x+12.1177901746786						
0.989119683	-1.52747396551179E-19x6+1.8563189351373E-15x5+9.3752485328258E-12x4+2.59500021182031E-08x3+4.17872486932178E-05x2+0.036866089870691x+13.6083101371752						
1.013171226	-1.873211571685E-19x6+2.664258774449E-15x5+1.6097181076031E-11x4+5.3204383571808E-08x3+0.00100277065243314x2+0.100606842465392x+41.4605874778286						
1.09401904	-2.88466126734055E-19x6+3.8919619295043E-14x5+2.1608567548841E-11x4+6.32650454198297E-07x3+0.0010308256109288x2+0.886503942614557x+314.347604380223						
1.116784429	-4.14700810588809E-19x6+6.2974425763187E-14x5+1.65153186876374E-11x4+4.89081862576983E-07x3+0.00080523103872589x2+0.69939379618896x+250.040444540014						
1.187648456	-1.32750050531442E-19x6+2.1492371513754E-15x5+1.48002527079095E-11x4+5.0520340169224E-08x3+0.00009238472863323x2+0.0870140569798597x+33.2000935728379						
1.2300123	-2.29289078055395E-19x6+3.58631871632404E-15x5+1.20441108454973E-11x4+2.95860060216038E-08x3+4.04077379244495E-05x2+0.0290097672794958x+8.53855744371678						
1.237623762	-2.57268939040424E-19x6+2.98658521883874E-15x5+1.43769025279642E-11x4+3.67123242670096E-08x3+5.24197715904692E-05x2+0.039661736474687x+12.4180714442091						
1.234567901	-2.47751447003464E-19x6+2.8496430067469E-15x5+1.3575339076697E-11x4+3.42589278957056E-08x3+4.82675753932432E-05x2+0.0359718075642782x+11.0718315713247						
1.239157373	-2.00198872489989E-19x6+3.0289547696157E-15x5+1.46258376005435E-11x4+3.7476428946543E-08x3+5.37158097538118E-05x2+0.0408156637743458x+12.6396394747744						
25 bar							
0.996015936	-1.70770074022758E-19x6+2.08452734845692E-15x5+1.04860525103705E-11x4+2.84203423413889E-08x3+4.40191751183594E-05x2+0.0368489567895022x+12.8973078087037						
0.989119683	-1.35285697075577E-19x6+1.8643396661834E-15x5+8.265960599018E-12x4+2.2843828031485E-08x3+3.68147323882779E-05x2+0.0325802657561x+12.0664599767443						
1.013171226	-1.3123733635525E-19x6+2.22078317605862E-17x5+1.1261976099847E-12x4+7.77348518216954E-09x3+2.33856524361807E-05x2+0.031899956416799x-16.17802992044167						
1.09401904	-2.52300834608061E-19x6+3.82408180967791E-14x5+1.90739464511726E-11x4+5.60963138039112E-07x3+0.000917606569337922x2+0.79200225041379x-281.777004031585						
1.116704129	-4.685526153528E-19x6+6.2322144409697E-14x5+1.31303160575298E-11x4+3.90869561594313E-07x3+0.000646321006397723x2+0.56324561918477x+202.115959975079						
1.187648456	-4.94542955848208E-19x6+6.0649578794329E-15x5+2.00204231684775E-12x4+1.2290719160271E-08x3+2.90054970184359E-05x2+0.0316196085378529x+13.267484526199						
1.2300123	-2.7160555298195E-19x6+3.2209977327739E-15x5+1.58708078543874E-11x4+4.1570616871036E-08x3+5.1022877573754E-05x2+0.04757112827245x+15.388065258298						
1.237623762	-2.8208076236986E-19x6+3.425893282577E-15x5+1.71213427983329E-11x4+4.55037117264748E-08x3+6.78198774387076E-05x2+0.0537184746547187x+17.656672690567						
1.234567901	-2.801288177748E-19x6+3.593124652629E-15x5+1.6705905403682E-11x4+4.1868657667316E-08x3+0.000655303601568x2+0.05164053652978x+16.885665905365						
1.239157373	-2.86499478978319E-19x6+3.4471802872515E-15x5+1.72465880626498E-11x4+4.59036110248798E-08x3+6.85185842266204E-05x2+0.0543553652936832x+17.8936857387125						
30 bar							
0.996015936	-1.67848433068831E-19x6+2.06866379496053E-15x5+1.05122880691409E-11x4+2.87642831381223E-08x3+4.49181564296038E-05x2+0.0378496422350977x+13.164453227918						
0.989119683	-1.1953750132949E-19x6+1.44217138719172E-15x5+7.125628804688E-12x4+1.9870302618668E-08x3+3.19960171300952E-05x2+0.0283626332075892x+10.5517850689608						
1.013171226	-1.62157603419341E-19x6+2.1831274992275E-15x5+1.7270003437033E-11x4+3.3544430443915E-08x3+4.30378961236524E-05x2+0.0276261748834906x+5.78811538862222						
1.09401904	-2.2098819076274E-19x6+3.9680029437784E-14x5+1.6774698732411E-11x4+4.94982872417398E-07x3+0.000812141304342293x2+0.70293472923228x+260.7220831715						
1.116704129	-4.33735014925919E-19x6+6.1856027347849E-14x5+1.0559379107838E-11x4+3.15839497519119E-07x3+0.0005245776366358x2+0.458692476280131x+165.1072593806						
1.187648456	-4.95446282146E-19x6+6.3880935734509E-15x5+5.3464650293142E-12x4+4.8383388020572E-09x3+7.9582625091118E-06x2+0.0008793736202844x+1.56101246878292						
1.2300123	-2.84330304683507E-19x6+3.4424073492576E-15x5+1.7336889757661E-11x4+4.6439778598886E-08x3+6.9748816748488E-05x2+0.055736303741421x+18.4732860897296						
1.237623762	-2.8913707209207E-19x6+3.531348714196E-15x5+1.7028640291146E-11x4+4.3435414244011E-08x3+7.339050797600E-05x2+0.059115769287141x+10.750813496891						
1.234567901	-2.79763070873823E-19x6+3.5005798052341E-15x5+1.7745313489789E-11x4+4.7805834172658E-08x3+7.3734980204571E-05x2+0.058017946175628x+17.3378957257259						
1.239157373	-2.8963771439813E-19x6+3.5383353463515E-15x5+1.79799575255225E-11x4+4.86178701506876E-08x3+7.37381697335718E-05x2+0.0594401818576633x+18.8812465273145						
35 bar							
0.996015936	-1.645308256545144E-19x6+2.04239495901858E-15x5+1.045681137638E-11x4+2.88123779617719E-08x3+4.52648766801119E-05x2+0.0383288127661012E-11.5377409753011						
0.989119683	-1.0554808979648E-19x6+1.263602023268E-15x5+5.26982628690511E-12x4+1.7132359198519E-08x3+0.00002752685686791x2+0.0244889465047333x-9.1349652662082						
1.013171226	-2.9078530365245E-19x6+4.009486526048E-14x5+2.78260206287E-11x4+5.49239614310948E-08x3+0.00101676545976x2+0.0789476368811138x+2.7179911990245						
1.09401904	-2.0088089999925E-19x6+3.62893154621375E-14x5+1.4767980185084E-11x4+4.369473975438E-07x3+0.00071891858078056x2+0.62372545307966x+222.941683944904						
1.116704129	-1.06964803243498E-19x6+2.49841419632165E-14x5+5.675998722827E-12x4+5.17618886255982E-08x3+0.00042963840710403x2+0.3371204171322x+36.17295898078						
1.187648456	-1.234567901E-19x6+2.34567901E-15x5+1.734567901E-11x4+4.734567901E-08x3+7.34567901E-05x2+0.058017946175628x+17.3378957257259						
1.2300123	-2.83921445639987E-19x6+3.47674204185E-15x5+1.778063146525E-11x4+4.789852523523E-08x3+7.2970439768512E-05x2+0.058957849652953x+19.48241972853						
1.237623762	-2.834864752457E-19x6+3.47674204185E-15x5+1.778063146525E-11x4+4.7875726396307E-08x3+0.0007454170150625x2+0.0605845825131x+10.7494159374529						
1.234567901	-2.8403732098287E-19x6+3.49125053694759E-15x5+1.7890374989966E-11x4+4.8562495285588E-08x3+7.41005273333635E-05x2+0.060087311263921x2+0.2137789013089						
1.239157373	-2.8321151805803E-19x6+3.49028781818958E-15x5+1.7861792316708E-11x4+4.88011425669907E-08x3+7.465281671305361E-05x2+0.060084068827159x+2.462951470955						
40 bar							
0.996015936	-1.6126590453144E-19x6+2.01432764763387E-15x5+1.03981084039136E-11x4+2.86469259340877E-08x3+4.52943548714703E-05x2+0.03832880792900874x-13.64103138176						
0.989119683	-9.31210059414869E-20x6+1.01574748912337E-15x5+5.4098107713547E-12x4+1.489429913039194E-08x3+0.000234430717279x2+0.020860534534097x-7.83140137828094						
1.013171226	-8.901321261765E-19x6+1.3123733635525E-19x6+2.22078317605862E-17x5+1.1261976099847E-12x4+7.77348518216954E-09x3+2.33856524361807E-05x2+0.031899956416799x-16.17802992044167						
1.09401904	-1.685723352492E-19x6+2.31901131505013E-14x5+1.30346472						

0.990016	-1.514001515962402E-19x6+1.91226030515607E-15x5+9.9640865061512E-12x4+2.79133536712351E-08x3+4.44908486279582E-05x2+0.0381290405117616x+13.5997866823723
0.98912	-6.32376259848902E-20x6+7.15000487053343E-16x5+3.29918605364898E-12x4+8.48225875260278E-09x3+1.32710970527635E-05x2+0.019455635231308x+4.55550982817202
0.103171	6.75553898283782E-19x6+9.36443721519453E-15x5+3.3287565110939E-11x4+1.58677599201073E-07x3+0.000260524623250963x2+0.223709449653418x+78.5685856460533
0.094092	-1.15645347276508E-18x6+1.6052848495292E-14x5+3.1393389362931E-11x4+2.772220120139997E-07x3+0.00043750313944651x2+0.396815274061634x+142.833192446859
1.116701	-4.47718714959114E-19x6+6.56177592016578E-15x5+3.911283720395E-11x4+1.20238199067442E-07x3+0.000204956419068259x2+0.183140289464631x+67.102729383119
1.187648	2.574925838197E-19x6-3.11597680906698E-15x5+1.58816730451799E-11x4+1.19901401271849E-08x3+6.3061159626762E-05x2+0.050335347894455x+16.6727548278901
1.230012	2.47673961177819E-19x6+3.08867908854052E-15x5+1.602729877800652E-11x4+4.42253885023964E-08x3+6.841405626345167E-05x2+0.056213055358158x+19.00136346977
1.237624	2.38771651470219E-19x6+2.98659502057442E-15x5+1.55298259574392E-11x4+1.29542558429479E-08x3+6.65993390550405E-05x2+0.048400742290634x+18.7204812504294
1.234588	2.42221894537478E-19x6+3.02670517559656E-15x5+1.5726236010804E-11x4+4.34610817398456E-08x3+6.7331332014305E-05x2+0.0554012558810066x+18.8984610536302
1.239157	2.3759861353391E-19x6+2.97245425951627E-15x5+1.54621314645155E-11x4+4.27783778818541E-08x3+6.63434298313286E-05x2+0.0546428275911508x+18.6572096951538
60 bar	
0.990016	-1.48419175427587E-19x6+1.87989086165766E-15x5+9.82393426504616E-12x4+2.75930676029477E-08x3+4.4083067767451E-05x2+0.0378564298191034x+13.5254093358894
0.98912	-5.5192956970468E-20x6+6.0953335736275E-16x5+2.7223995926993E-12x4+6.78844429042346E-09x3+1.046024798590126x2+0.0094581432575425x+3.64330176473866
0.103171	7.39389415935295E-19x6+1.02636918605142E-14x5+8.58287690382767E-11x4+1.74485854032441E-07x3+0.000288341705012849x2+0.248961085471013x+60.082726284772
0.094092	-1.02523958339671E-18x6+1.42911793752738E-14x5+8.1589793153895E-11x4+2.4473411854339E-07x3+0.0004073390282904x2+0.366590414415485x+128.700656502711
1.116701	-3.56472598494542E-19x6+5.3212705785475E-15x5+3.19686572095642E-11x4+9.74766938186902E-08x3+0.000171299847638904x2+0.153970111314882x+17.457247671256135
1.187648	2.58486196331135E-19x6+3.59014582641347E-15x5+1.55635192451025E-11x4+4.306352767398E-08x3+6.51465559076587E-05x2+0.0523803098821637x+17.4572476790055
1.230012	2.3743409876282E-19x6+2.9684486923023E-15x5+1.546313458021E-11x4+4.26667253273392E-08x3+6.61310719462587E-05x2+0.054437282938601x+18.5771854097615
1.237624	2.2783402558822E-19x6+2.85483604478727E-15x5+1.48728905524775E-11x4+4.12079331551522E-08x3+0.0006399609698915x2+0.0527781646834438x+18.0425345113921
1.234588	2.31511561879161E-19x6+2.89861628977980E-15x5+1.50894666147907E-11x4+4.1775357243031E-08x3+6.48357486362937E-05x2+0.0534356445211052x+18.2560967578815
1.239157	2.265917205979E-19x6+2.83998577818287E-15x5+1.47991089653074E-11x4+4.101299965678012E-08x3+6.37073602869321E-05x2+0.0525509416255089x+17.9683467782901
65 bar	
0.990016	-1.4557291726857947E-19x6+1.8489081371651E-15x5+9.6832573697563E-12x4+2.72613690176484E-08x3+4.36441679508577E-05x2+0.037547192799198x+13.4353490278729
0.98912	-4.7894971284754E-20x6+5.1358029578267E-16x5+2.19642770030989E-12x4+5.2401364168777E-09x3+7.8864300771756E-06x2+0.00717277092361x2+2.80540923259324
0.103171	7.94607764346259E-19x6+1.10432585604047E-14x5+6.30824569879318E-11x4+1.88930579841662E-07x3+0.0003126205028533x2+0.29104913965495x+96.2720912651832
0.094092	-9.10632350483299E-19x6+1.27500084304754E-14x5+7.3044781970854E-11x4+2.1970418812308E-07x3+0.0003

Figure 11-10 Polynomials for Linear Interpolation for each FER on the Ford Sigma

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Figure 11-11 Ford Fox Airmass Kg/h

rri w % (Residual gas ratio by internal and external EGR)

	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		0.5	0.2	0.1	0.4	0.8	0.8	1.0	1.5	1.7	2.2	2.7	3.1	3.3	3.6	4.1
200						0.8	0.8	1.0	1.4	1.8						
190						0.8	0.9	1.1	1.5	1.8						
180					0.4	0.9	0.9	1.1	1.5	1.9	2.2					
170				0.1	0.2	1.0	1.0	1.2	1.6	2.0	2.2	2.7				
160				0.2	0.2	1.1	1.1	1.3	1.7	2.0	2.2	2.6	3.0			
150				0.2	0.2	1.2	1.2	1.3	1.8	2.2	2.3	2.6	3.1	3.3		
140			0.2	0.2	0.3	1.0	1.2	1.3	2.1	2.4	2.6	2.7	3.1	3.4	3.6	
130			0.3	0.3	0.5	1.1	1.2	1.5	2.3	2.5	2.7	2.9	3.2	3.4	3.7	
120			0.3	0.5	0.8	1.2	1.4	1.7	2.5	2.7	2.9	3.0	3.2	3.5	3.8	4.2
110		0.6	0.5	0.8	1.0	1.3	1.5	1.9	2.6	3.0	3.1	3.1	3.2	3.7	3.9	4.3
100		1.1	0.9	1.1	1.4	1.6	1.8	2.1	2.8	3.4	3.4	3.3	3.3	3.7	4.1	4.5
90		1.8	1.5	1.8	2.1	2.5	2.5	2.8	3.4	3.8	3.6	3.6	3.4	3.7	4.2	4.5
80		3.5	3.0	3.2	3.3	3.2	3.5	4.7	4.9	4.6	4.3	4.1	3.6	3.8	4.4	4.6
70		5.7	5.4	6.0	6.0	5.7	6.5	6.9	6.7	6.2	5.6	5.4	4.2	4.2	4.6	4.8
60		9.7	9.9	10.0	9.9	10.3	10.4	9.4	9.0	8.5	8.0	7.6	5.5	4.6	5.0	5.1
50		14.1	14.7	14.7	14.4	14.6	14.2	12.9	11.5	11.1	10.3	9.6	7.3	5.1	5.4	5.6
40	18.6	18.1	18.4	18.6	19.3	19.5	17.0	15.2	15.1	14.3	12.7	11.2	8.9	5.7	5.9	6.0
30	19.9	19.3	18.6	20.7	21.7	21.3	18.6	16.5	17.7	17.1	14.2	12.5	10.6	6.7	6.7	6.7
20	20.6	19.0	19.0	20.1	19.8	19.5	18.5	17.4	18.0	17.2	15.5	13.1	11.4	8.6	8.3	8.2
10	25.6	24.7	23.4	23.1	21.9	21.3	21.4	21.8	19.9	17.9	16.5	14.5	13.3	11.7	10.8	10.4
5	28.0	27.8	26.1	25.7	23.9	23.8	23.7	24.0	21.7	19.7	17.2	16.1	14.9	13.4	12.8	12.1
2	33.3	29.1	27.3	27.6	26.2	25.8	25.2	25.3	23.1	21.3	18.3	17.3				

Figure 11-12 Ford Fox Residual Gas

LAMBDA

	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		1.11	1.11	1.10	1.03	0.99	0.99	0.99	**	0.94	0.97	0.95	0.92	0.92	0.90	0.90
200						0.99	0.98	0.99	**	0.99						
190						0.99	0.99	0.99	0.93	0.96						
180					1.02	0.99	0.99	0.99	0.96	0.95	0.97					
170				1.10	1.07	0.99	0.99	0.99	0.99	0.94	0.98	0.96				
160				1.11	1.07	1.00	1.00	0.99	0.99	0.99	0.99	0.96	0.93			
150				1.11	1.08	1.00	1.00	0.99	0.99	0.99	0.99	0.98	0.96	0.94		
140			1.11	1.11	1.08	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.96	0.91	
130			1.10	1.10	1.07	1.00	1.00	1.00	1.00	0.99	0.99	0.99	1.00	0.96	0.93	
120			1.09	1.07	1.01	1.01	1.00	1.00	1.00	0.99	0.99	1.00	1.00	0.98	0.95	0.93
110		1.09	1.09	1.06	1.01	1.01	1.01	1.00	1.00	0.99	1.00	1.00	1.00	1.00	0.96	0.95
100		1.03	1.08	1.01	1.02	1.01	1.01	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.95
90		1.02	1.05	1.02	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	1.00
80		1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00
70		1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00
60		1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00
50		1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
40	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
30	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
20	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
10	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.01	1.01	1.00
5	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	1.00	1.00
2	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01				

Figure 11-13 Ford Fox Lambda

AFRINCYL

	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		13.76	13.70	13.78	13.90	14.10	14.08	14.33	13.42	13.60	14.06	13.91	13.36	13.35	13.02	13.10
200						14.10	14.05	14.33	13.78	14.39						
190						14.07	14.12	14.31	13.38	13.85						
180					13.88	14.07	14.18	14.29	13.89	13.65	14.03					
170				13.77	13.72	14.08	14.18	14.27	14.32	13.49	14.22	13.92				
160				13.81	13.81	14.10	14.17	14.21	14.30	14.32	14.37	13.97	13.54			
150				13.85	13.93	14.03	14.10	14.09	14.24	14.30	14.35	14.16	13.98	13.65		
140			13.74	13.88	13.97	13.93	14.03	14.04	14.21	14.27	14.33	14.38	14.34	13.94	13.25	
130			13.83	13.98	14.09	13.91	13.96	14.02	14.22	14.23	14.29	14.33	14.42	13.99	13.55	
120			13.98	14.01	13.58	13.87	13.93	13.97	14.20	14.21	14.29	14.35	14.36	14.18	13.70	13.47
110		13.71	14.13	14.10	13.61	13.92	14.02	14.00	14.20	14.23	14.28	14.34	14.32	14.36	13.85	13.74
100		13.34	14.33	13.74	13.93	14.16	14.20	14.09	14.17	14.32	14.31	14.36	14.34	14.38	14.29	13.71
90		14.04	14.57	14.21	14.31	14.53	14.49	14.30	14.37	14.44	14.40	14.40	14.36	14.40	14.44	14.48
80		14.46	14.56	14.55	14.62	14.62	14.63	14.54	14.58	14.62	14.53	14.47	14.36	14.43	14.45	14.48
70		14.59	14.65	14.61	14.59	14.63	14.60	14.56	14.59	14.65	14.62	14.56	14.39	14.39	14.43	14.46
60		14.65	14.66	14.66	14.65	14.69	14.66	14.53	14.63	14.67	14.68	14.65	14.49	14.42	14.42	14.42
50		14.66	14.64	14.64	14.67	14.68	14.66	14.64	14.64	14.69	14.69	14.67	14.65	14.57	14.48	14.45
40	14.54	14.62	14.66	14.69	14.68	14.64	14.62	14.67	14.67	14.66	14.67	14.65	14.65	14.59	14.59	14.54
30	14.56	14.59	14.60	14.67	14.68	14.62	14.61	14.64	14.66	14.66	14.66	14.65	14.64	14.61	14.63	14.60
20	14.63	14.57	14.50	14.59	14.62	14.56	14.65	14.67	14.68	14.69	14.68	14.65	14.62	14.58	14.59	14.57
10	14.65	14.61	14.55	14.60	14.57	14.64	14.68	14.66	14.69	14.68	14.67	14.67	14.58	14.59	14.59	14.56
5	14.62	14.57	14.60	14.58	14.59	14.66	14.67	14.64	14.67	14.67	14.68	14.66	14.58	14.55	14.58	14.55
2	14.70	14.56	14.58	14.58	14.67	14.69	14.62	14.60	14.66	14.65	14.68	14.63				

Figure 11-14 Ford Fox A/F Ratio

FUELMASS kg/h																
	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		3.24	5.22	7.52	9.39	11.35	12.92	14.34	18.08	18.92	21.54	22.34	25.55	26.61	27.62	25.11
200						10.77	12.04	13.39	16.91	18.46						
190						10.05	11.26	12.52	15.24	17.76	20.61					
180					9.11	10.05	11.26	12.52	15.24	17.76	20.61					
170				7.51	8.77	9.38	10.52	11.72	14.06	17.14	18.91	21.41				
160				7.10	8.08	8.74	9.77	10.88	13.05	15.06	17.46	19.80	23.68			
150				6.52	7.46	8.17	9.12	10.19	11.98	14.00	16.18	18.15	20.99	24.47		
140			5.19	6.04	6.84	7.63	8.45	9.44	11.01	12.93	14.87	16.65	18.92	21.63	25.58	
130			4.73	5.46	6.16	6.96	7.73	8.55	10.05	11.89	13.84	15.40	17.30	19.71	22.93	
120			4.35	4.93	5.75	6.39	7.07	7.79	9.15	10.95	12.86	14.24	15.88	18.00	20.45	23.30
110		3.22	3.91	4.52	5.24	5.78	6.43	7.13	8.42	9.97	11.65	13.06	14.58	16.31	18.66	20.90
100		2.97	3.43	4.13	4.66	5.20	5.78	6.48	7.71	9.03	10.53	11.88	13.38	15.00	16.78	19.21
90		2.56	3.00	3.60	4.11	4.55	5.13	5.77	6.90	8.05	9.36	10.70	12.11	13.59	15.15	16.95
80		2.20	2.66	3.15	3.59	4.05	4.55	5.13	6.11	7.13	8.39	9.56	10.95	12.32	13.64	15.25
70		1.89	2.33	2.77	3.21	3.60	4.07	4.56	5.40	6.32	7.45	8.44	9.71	10.92	12.18	13.69
60		1.63	2.02	2.42	2.78	3.12	3.54	4.02	4.75	5.54	6.50	7.39	8.51	9.60	10.76	12.04
50		1.38	1.73	2.08	2.38	2.70	3.03	3.41	4.09	4.80	5.60	6.41	7.31	8.25	9.33	10.42
40	1.04	1.16	1.46	1.76	2.01	2.28	2.57	2.87	3.46	4.10	4.77	5.48	6.27	7.10	7.94	8.92
30	0.89	0.95	1.19	1.42	1.67	1.88	2.13	2.36	2.85	3.41	3.94	4.55	5.21	5.94	6.62	7.51
20	0.51	0.73	0.93	1.10	1.30	1.48	1.65	1.84	2.21	2.67	3.13	3.64	4.18	4.76	5.37	6.08
10	0.44	0.51	0.65	0.78	0.93	1.05	1.16	1.29	1.63	1.92	2.38	2.72	3.18	3.64	4.18	4.79
5	0.36	0.42	0.53	0.63	0.79	0.88	0.98	1.09	1.32	1.60	1.99	2.33	2.73	3.14	3.56	4.08
2	0.32	0.39	0.46	0.56	0.66	0.78	0.86	0.98	1.22	1.44	1.83	2.09				

Figure 11-15 Ford Fox Fuel Mass Kg/h

11.8 Ford Sigma Data Sheet

BLOW_VAL l/min												
	0	1000	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000
FL			46.760	55.220	52.713	47.897	54.906	50.939	51.026	58.077	53.600	54.745
1.5			44.229	52.120	50.070	49.025				55.365		
1.4			38.631	48.973	47.862	33.950	48.909	50.497	49.412	49.736	51.819	51.591
1.3			36.758	46.459	42.056	35.166	44.931	48.062	45.329	44.525	47.566	47.040
1.2			38.488	41.117	42.203	27.919	39.236	43.743	39.957	39.251	24.537	35.840
1.1			39.561	37.549	36.318	20.027	33.651	35.224	26.944	28.145	33.637	10.156
1		28.400	33.134	36.718	34.418	11.690	25.133	28.724	20.117	9.687	33.149	4.148
0.9		25.029	28.777	29.025	28.447	15.504	20.202	24.739	21.053	0.768	28.273	5.392
0.8		17.728	24.610	26.073	23.416	11.041	13.071	0.574	0.575	29.703	0.581	0.582
0.7		0.579	15.690	10.616	0.586	4.177	7.042	11.651	10.188	7.265	5.940	4.833
0.6		0.579	0.581	0.585	10.178	8.617	8.713	13.281	10.165	10.316	4.731	7.793
0.5		0.578	0.637	0.584	11.071	8.943	0.574	1.263	11.209	12.019	9.655	11.311
0.4		0.579	0.581	0.585	3.209	10.327	12.801	0.574	3.776	3.675	11.500	
0.3		7.224	10.754	1.538	0.585	2.023	4.294	10.531	9.301	0.583	6.862	
0.2		9.175	0.581	3.917	0.587	0.635	2.819	4.310	0.580	0.583	0.583	

Figure 11-16 Ford Sigma Blowby l/min

AIRMASS kg/h (kg/hr)												
	0	1000	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000
FL			152.378	198.515	243.789	282.000	308.799	357.423	386.916	440.617	467.935	483.478
1.5			143.961	192.111	235.237	272.923				436.388		
1.4			132.614	175.543	211.264	247.218	294.725	338.216	364.343	404.358	441.306	482.934
1.3			121.690	160.788	183.978	235.801	270.069	310.149	337.571	372.091	407.886	441.037
1.2			101.352	133.739	178.050	213.193	247.833	286.229	308.786	333.768	365.903	396.685
1.1			94.461	123.826	158.626	192.860	225.339	252.874	277.047	301.948	336.622	365.241
1		46.522	84.677	122.871	149.241	175.251	196.819	223.907	250.371	286.340	314.582	340.200
0.9		43.524	79.359	107.285	133.968	159.422	176.666	203.362	223.423	261.292	284.816	308.818
0.8		40.090	68.345	96.160	118.872	143.102	159.400	180.901	202.424	238.171	258.741	278.575
0.7		37.704	60.784	82.314	103.990	125.420	142.519	163.810	186.305	210.230	227.012	245.177
0.6		32.397	52.152	69.427	89.290	107.130	123.307	143.003	160.670	180.389	196.665	209.856
0.5		28.933	43.860	58.221	74.423	89.665	103.988	120.053	134.562	149.504	166.329	174.313
0.4		23.034	35.835	47.279	58.801	73.165	84.536	95.475	109.917	119.670	133.579	
0.3		17.210	26.670	35.516	44.187	53.115	61.572	70.945	80.640	86.993	97.764	
0.2		11.473	17.765	24.059	29.828	36.932	42.422	47.466	52.640	57.174	63.171	

Figure 11-17 Ford Sigma Airmass Kg/h

LAMBDA (Dyno)

	0	1000	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000
FL			1.011	0.987	0.914	0.896	0.842	0.813	0.808	0.810	0.810	0.807
1.5			0.999	0.990	0.994	0.870				0.899		
1.4			1.003	1.000	0.996	0.985	0.975	0.978	0.958	0.930	0.916	0.810
1.3			1.006	0.996	0.991	0.985	0.985	0.974	0.965	0.943	0.931	0.924
1.2			1.003	0.999	0.991	0.987	0.988	0.988	0.977	0.964	0.945	0.932
1.1			1.003	1.001	0.996	0.990	0.990	0.993	0.991	0.976	0.970	0.947
1	1.004	1.007	1.004	1.001	0.995	0.993	0.991	0.991	0.995	0.994	0.975	0.963
0.9	1.005	1.007	1.002	1.002	0.998	0.994	0.996	0.996	0.995	0.995	0.992	0.976
0.8	1.005	1.003	0.999	1.001	0.998	0.995	0.996	0.996	0.995	0.995	0.994	0.993
0.7	1.004	1.001	0.999	1.000	1.000	0.999	0.998	0.998	0.997	0.997	0.997	0.995
0.6	1.003	1.000	1.000	1.000	1.001	1.002	1.002	1.000	0.999	0.999	0.999	0.999
0.5	1.001	1.000	1.002	1.001	1.002	1.005	1.005	1.005	1.005	1.004	1.001	0.999
0.4	0.998	1.000	1.003	1.002	1.003	1.005	1.007	1.005	1.005	1.005	1.005	
0.3	0.997	0.999	1.002	1.002	1.005	1.008	1.008	1.006	1.005	1.005	1.005	
0.2	0.994	0.999	1.001	1.002	1.005	1.008	1.010	1.011	1.008	1.006		

Figure 11-18 Ford Sigma Lambda

AFR CALC (Dyno)

	0	1000	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000
FL			14.712	14.354	13.304	13.039	12.255	11.826	11.761	11.782	11.783	11.748
1.5			14.531	14.408	14.464	12.656				13.087		
1.4			14.596	14.552	14.490	14.327	14.182	14.228	13.933	13.525	13.327	11.782
1.3			14.631	14.493	14.421	14.327	14.338	14.171	14.041	13.722	13.548	13.445
1.2			14.597	14.531	14.421	14.361	14.372	14.378	14.210	14.020	13.756	13.568
1.1			14.595	14.568	14.485	14.398	14.410	14.451	14.422	14.199	14.116	13.779
1	14.609	14.650	14.611	14.570	14.481	14.445	14.425	14.484	14.460	14.188	14.017	
0.9	14.617	14.656	14.582	14.578	14.523	14.461	14.489	14.481	14.473	14.439	14.194	
0.8	14.630	14.592	14.536	14.564	14.515	14.482	14.488	14.484	14.478	14.457	14.447	
0.7	14.615	14.558	14.530	14.552	14.552	14.537	14.521	14.517	14.510	14.503	14.471	
0.6	14.590	14.548	14.552	14.548	14.560	14.581	14.584	14.556	14.537	14.534	14.537	
0.5	14.564	14.551	14.582	14.567	14.583	14.620	14.624	14.619	14.603	14.565	14.540	
0.4	14.525	14.554	14.592	14.575	14.591	14.621	14.647	14.624	14.629	14.628		
0.3	14.510	14.532	14.576	14.586	14.630	14.670	14.667	14.636	14.616	14.626		
0.2	14.467	14.529	14.562	14.579	14.620	14.665	14.689	14.715	14.664	14.632		

Figure 11-19 Ford Sigma A/F Ratio

11.9 Stoichiometric Oxygen Values

	10 bar		20 bar		25 bar		30 bar		35 bar		40 bar		45 bar		50 bar		55 bar		60 bar
Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.001704	1500	0.001352	1500	0.001255	1500	0.001181	1500	0.001122	1500	0.001073	1500	0.001032	1500	0.000996	1500	0.000965	1500	0.000938
2000	0.064366	2000	0.05116	2000	0.047512	2000	0.044724	2000	0.042494	2000	0.040652	2000	0.039094	2000	0.03775	2000	0.036574	2000	0.035533
2100	0.107736	2100	0.08572	2100	0.079629	2100	0.074973	2100	0.071247	2100	0.068169	2100	0.065563	2100	0.063317	2100	0.06135	2100	0.059608
2200	0.171534	2200	0.136691	2200	0.127032	2200	0.119643	2200	0.113727	2200	0.108837	2200	0.104696	2200	0.101124	2200	0.097997	2200	0.095225
2300	0.261381	2300	0.20875	2300	0.194119	2300	0.182913	2300	0.173934	2300	0.166506	2300	0.160213	2300	0.154782	2300	0.150025	2300	0.145808
2400	0.38219	2400	0.306161	2400	0.284943	2400	0.268668	2400	0.255612	2400	0.244801	2400	0.235635	2400	0.227718	2400	0.22078	2400	0.214626
2500	0.537987	2500	0.432692	2500	0.403156	2500	0.380454	2500	0.362214	2500	0.347092	2500	0.334257	2500	0.323162	2500	0.31343	2500	0.304793
2700	0.96636	2700	0.788121	2700	0.734812	2700	0.695149	2700	0.663139	2700	0.636503	2700	0.613824	2700	0.594168	2700	0.576889	2700	0.56152
3000	1.874165	3000	1.563741	3000	1.472447	3000	1.400946	3000	1.34264	3000	1.293704	3000	1.251738	3000	1.21514	3000	1.18279	3000	1.153879
	65 bar		70 bar		75 bar		80 bar		85 bar		90 bar		95 bar		100 bar		105 bar		110 bar
Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.000913	1500	0.000891	1500	0.00087	1500	0.000852	1500	0.000835	1500	0.000819	1500	0.000804	1500	0.000791	1500	0.000778	1500	0.000766
2000	0.034601	2000	0.033759	2000	0.032995	2000	0.032295	2000	0.031651	2000	0.031056	2000	0.030503	2000	0.029987	2000	0.029505	2000	0.029053
2100	0.058048	2100	0.056641	2100	0.055361	2100	0.05419	2100	0.053112	2100	0.052115	2100	0.05119	2100	0.050327	2100	0.049519	2100	0.048762
2200	0.092744	2200	0.090504	2200	0.088467	2200	0.086602	2200	0.084886	2200	0.083299	2200	0.081825	2200	0.080451	2200	0.079164	2200	0.077957
2300	0.142032	2300	0.138621	2300	0.135518	2300	0.132678	2300	0.130063	2300	0.127644	2300	0.125397	2300	0.123301	2300	0.12134	2300	0.119498
2400	0.209113	2400	0.204132	2400	0.199598	2400	0.195447	2400	0.191624	2400	0.188087	2400	0.184799	2400	0.181733	2400	0.178862	2400	0.176166
2500	0.297049	2500	0.290049	2500	0.283676	2500	0.277836	2500	0.272457	2500	0.267477	2500	0.262848	2500	0.258527	2500	0.254482	2500	0.250682
2700	0.547718	2700	0.535221	2700	0.523825	2700	0.51337	2700	0.503727	2700	0.49479	2700	0.486473	2700	0.478704	2700	0.471422	2700	0.464576
3000	1.127803	3000	1.104099	3000	1.082407	3000	1.062441	3000	1.04397	3000	1.026805	3000	1.010789	3000	0.995793	3000	0.981705	3000	0.968432

Figure 11-20 n5 Values at Stoichiometric at 5 bar intervals

11.10 Excel Coding for Macro's

Goal seek required the use of macro's and coding which evolved over time as the author became more familiar with excel. To begin with the author just created macro's by recording their input actions resulting in this example at 1000 RPM:

```
Sub Error_1000()  
' Error_1000 Macro  
Range("BB377").Select  
    Application.CutCopyMode = False  
    Application.CutCopyMode = False  
    Range("BB377").GoalSeek Goal:=0, ChangingCell:=Range("AP377")  
    Range("BB378").Select  
    Application.CutCopyMode = False  
    Application.CutCopyMode = False  
    Range("BB378").GoalSeek Goal:=0, ChangingCell:=Range("AP378")  
    Range("BB379").Select  
(Keeps repeating this step until final cell)  
    Range("BB412").Select  
    Application.CutCopyMode = False  
    Application.CutCopyMode = False  
    Range("BB412").GoalSeek Goal:=0, ChangingCell:=Range("AP412")  
End Sub
```

As this was carried out for each RPM it was seen that this method was overly inefficient as such a new method was sought after:

```
Sub Error_1000_0_3()  
' Error 1000 0.3 RPM Macro  
Dim i As Long  
For i = 357 To 393  
    Worksheets("1000RPM 0.3").Range("BC" & i).GoalSeek Goal:=0.0000001,  
    ChangingCell:=Worksheets("1000RPM 0.3").Range("AQ" & i)  
Next i  
End Sub
```

Which reset the n5/nt guess and then recalculated all the values. This type of coding then quickly evolved into:

```
Sub goalseekCOMP()  
    ' goalseekCOMP Macro  
  
    Dim i As Long  
  
    For i = 377 To 402  
        Worksheets("1000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 376 To 403  
        Worksheets("1250").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 377 To 412  
        Worksheets("1500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 377 To 412  
        Worksheets("1750").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 378 To 420  
        Worksheets("2000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 379 To 422  
        Worksheets("2500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 375 To 426  
        Worksheets("3000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 373 To 422  
        Worksheets("3500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 364 To 417  
        Worksheets("4000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 364 To 426  
        Worksheets("4500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 364 To 421  
        Worksheets("5000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 363 To 424  
        Worksheets("5500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 365 To 417  
        Worksheets("6000").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i  
    For i = 359 To 418  
        Worksheets("6500").Range("AP" & i).FormulaR1C1 = "0.0000001"  
    Next i
```

```

For i = 377 To 402
    Worksheets("1000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("1000").Range("AP" & i)
Next i
For i = 376 To 402
    Worksheets("1250").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("1250").Range("AP" & i)
Next i
    For i = 377 To 412
        Worksheets("1500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("1500").Range("AP" & i)
    Next i
For i = 377 To 412
    Worksheets("1750").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("1750").Range("AP" & i)
Next i
    For i = 379 To 420
        Worksheets("2000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("2000").Range("AP" & i)
    Next i
    For i = 379 To 422
        Worksheets("2500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("2500").Range("AP" & i)
    Next i
    For i = 375 To 426
        Worksheets("3000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("3000").Range("AP" & i)
    Next i
    For i = 373 To 422
        Worksheets("3500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("3500").Range("AP" & i)
    Next i
    For i = 364 To 417
        Worksheets("4000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("4000").Range("AP" & i)
    Next i
    For i = 364 To 426
        Worksheets("4500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("4500").Range("AP" & i)
    Next i
    For i = 364 To 421
        Worksheets("5000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("5000").Range("AP" & i)
    Next i
    For i = 363 To 424
        Worksheets("5500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("5500").Range("AP" & i)
    Next i
    For i = 365 To 417
        Worksheets("6000").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("6000").Range("AP" & i)
    Next i
    For i = 359 To 418
        Worksheets("6500").Range("BB" & i).GoalSeek Goal:=0.0000001, ChangingCell:=Worksheets("6500").Range("AP" & i)
    Next i
MsgBox ("Calculations Complete")

End Sub

```

Figure 11-21 Full Code for Excel

When running this code, it takes around 15 minutes to finish calculations but is much more efficient compared to going onto each RPM sheet and running each code individually.

11.11 Oxygen Values for Ford Sigma FER

100 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050094346	1500	-4.34752E-09	1500	1.47E-08	1500	-9.66462E-08
2000	0.068828034	2000	1.48398E-05	2000	1.91E-06	2000	1.73934E-06
2100	0.086526686	2100	7.02376E-05	2100	8.89E-06	2100	8.08067E-06
2200	0.114269425	2200	0.000287762	2200	3.6E-05	2200	3.26713E-05
2300	0.154812599	2300	0.001042495	2300	0.000129	2300	0.000116961
2400	0.21079869	2400	0.003372314	2400	0.000414	2400	0.000375897
2500	0.284834527	2500	0.00980367	2500	0.001208	2500	0.001095283
2700	0.498079315	2700	0.06054261	2700	0.008075	2700	0.007319833
3000	1.001202637	3000	0.374391947	3000	0.080753	3000	0.073727741
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137556521	1500	8.47188E-09	1500	-9.3E-08		
2000	0.150166538	2000	9.39196E-06	2000	1.76E-06		
2100	0.163891025	2100	4.41144E-05	2100	8.17E-06		
2200	0.187435151	2200	0.000180455	2200	3.3E-05		
2300	0.224221679	2300	0.000652356	2300	0.000118		
2400	0.277201356	2400	0.00211152	2400	0.00038		
2500	0.34895976	2500	0.006167769	2500	0.001107		
2700	0.559194603	2700	0.039733148	2700	0.007399		
3000	1.05971927	3000	0.289787173	3000	0.074471		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	1.80091E-07	1500	-2.63911E-09	1500	8.34E-10		
2000	0.000903692	2000	3.09666E-06	2000	1.82E-06		
2100	0.0041267	2100	1.44772E-05	2100	8.43E-06		
2200	0.014948479	2200	5.88308E-05	2200	3.42E-05		
2300	0.041095702	2300	0.000211611	2300	0.000122		
2400	0.087563273	2400	0.000682589	2400	0.000392		
2500	0.155917825	2500	0.001994651	2500	0.001144		
2700	0.363892195	2700	0.013318609	2700	0.007644		
3000	0.865503392	3000	0.126235489	3000	0.076756		

Figure 11-22 Oxygen for each Sigma FER at 100 Bar

90 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050104293	1500	-4.27977E-09	1500	1.47E-08	1500	-9.66383E-08
2000	0.070553292	2000	1.81519E-05	2000	2.34E-06	2000	2.12631E-06
2100	0.089651197	2100	8.58556E-05	2100	1.09E-05	2100	9.87793E-06
2200	0.119437231	2200	0.000351657	2200	4.4E-05	2200	3.99305E-05
2300	0.162828574	2300	0.001273558	2300	0.000157	2300	0.000142955
2400	0.222620596	2400	0.004115393	2400	0.000506	2400	0.000459389
2500	0.301550951	2500	0.011929838	2500	0.001476	2500	0.001338331
2700	0.528231325	2700	0.072279177	2700	0.00985	2700	0.008930768
3000	1.059502314	3000	0.422102612	3000	0.096941	3000	0.088659015
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137562485	1500	8.51295E-09	1500	-9.3E-08		
2000	0.15144141	2000	1.14752E-05	2000	2.15E-06		
2100	0.166439755	2100	5.39165E-05	2100	9.98E-06		
2200	0.192002191	2200	0.000220496	2200	4.04E-05		
2300	0.231692587	2300	0.000797119	2300	0.000144		
2400	0.288565826	2400	0.002578635	2400	0.000464		
2500	0.365303664	2500	0.007520462	2500	0.001353		
2700	0.589091786	2700	0.047882094	2700	0.009027		
3000	1.117818256	3000	0.331767847	3000	0.089536		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	2.11327E-08	1500	-2.62491E-09	1500	8.43E-10		
2000	0.001101694	2000	3.78627E-06	2000	2.22E-06		
2100	0.004990228	2100	1.76975E-05	2100	1.03E-05		
2200	0.017700085	2200	7.19015E-05	2200	4.17E-05		
2300	0.047231418	2300	0.000258627	2300	0.000149		
2400	0.098141646	2400	0.000834119	2400	0.00048		
2500	0.171845123	2500	0.002436574	2500	0.001397		
2700	0.39375238	2700	0.016219176	2700	0.009325		
3000	0.923879056	3000	0.149857578	3000	0.092232		

Figure 11-23 Oxygen for each Sigma FER at 90 Bar

80 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050110613	1500	-4.23319E-09	1500	1.47E-08	1500	-9.66329E-08
2000	0.071631557	2000	2.04289E-05	2000	2.63E-06	2000	2.39236E-06
2100	0.091594451	2100	9.65923E-05	2100	1.22E-05	2100	1.11136E-05
2200	0.122641239	2200	0.000395576	2200	4.95E-05	2200	4.49211E-05
2300	0.16778861	2300	0.001432286	2300	0.000177	2300	0.000160826
2400	0.229925004	2400	0.004624946	2400	0.00057	2400	0.000516781
2500	0.311865568	2500	0.013381007	2500	0.00166	2500	0.001505354
2700	0.546775757	2700	0.080065233	2700	0.011066	2700	0.010035176
3000	1.095094461	3000	0.451898513	3000	0.107759	3000	0.098663122
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137566275	1500	8.54119E-09	1500	-9.3E-08		
2000	0.152246029	2000	1.29074E-05	2000	2.42E-06		
2100	0.168040496	2100	6.06553E-05	2100	1.12E-05		
2200	0.194855435	2200	0.000248021	2200	4.54E-05		
2300	0.236338809	2300	0.000896601	2300	0.000163		
2400	0.295609137	2400	0.002899336	2400	0.000522		
2500	0.375406457	2500	0.008446762	2500	0.001522		
2700	0.607490598	2700	0.053360311	2700	0.010143		
3000	1.153292209	3000	0.358310698	3000	0.099628		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	2.25299E-08	1500	-2.61515E-09	1500	8.49E-10		
2000	0.001237258	2000	4.26037E-06	2000	2.5E-06		
2100	0.005573892	2100	1.99115E-05	2100	1.16E-05		
2200	0.019507156	2200	8.08874E-05	2200	4.69E-05		
2300	0.051139565	2300	0.000290948	2300	0.000168		
2400	0.10476111	2400	0.000938262	2400	0.000539		
2500	0.181728581	2500	0.002740115	2500	0.001572		
2700	0.412143043	2700	0.018201358	2700	0.010477		
3000	0.959529242	3000	0.165402046	3000	0.10259		

Figure 11-24 Oxygen for each Sigma FER at 80 Bar

70 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050118241	1500	-4.17331E-09	1500	1.47E-08	1500	-9.6626E-08
2000	0.072915782	2000	2.33566E-05	2000	3.01E-06	2000	2.73441E-06
2100	0.093900141	2100	0.000110396	2100	1.4E-05	2100	1.27022E-05
2200	0.126433623	2200	0.000452031	2200	5.66E-05	2200	5.13376E-05
2300	0.173650861	2300	0.001636213	2300	0.000202	2300	0.000183802
2400	0.238548227	2400	0.005278524	2400	0.000651	2400	0.000590561
2500	0.324029207	2500	0.015233835	2500	0.001897	2500	0.001720009
2700	0.568586082	2700	0.089764805	2700	0.012625	2700	0.011451181
3000	1.136700502	3000	0.487301738	3000	0.12132	3000	0.111231044
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137570849	1500	8.57749E-09	1500	-9.3E-08		
2000	0.153211914	2000	1.47488E-05	2000	2.76E-06		
2100	0.169954387	2100	6.93192E-05	2100	1.28E-05		
2200	0.198252529	2200	0.000283407	2200	5.19E-05		
2300	0.241851023	2300	0.001024455	2300	0.000186		
2400	0.303942967	2400	0.003311138	2400	0.000597		
2500	0.387335908	2500	0.00963336	2500	0.001739		
2700	0.629139129	2700	0.060262963	2700	0.011574		
3000	1.194763628	3000	0.390137198	3000	0.112302		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	2.58173E-08	1500	-2.6026E-09	1500	8.56E-10		
2000	0.001410888	2000	4.86994E-06	2000	2.85E-06		
2100	0.006312847	2100	2.27581E-05	2100	1.33E-05		
2200	0.021740221	2200	9.24403E-05	2200	5.36E-05		
2300	0.055855973	2300	0.0003325	2300	0.000192		
2400	0.112646411	2400	0.001072122	2400	0.000616		
2500	0.193430629	2500	0.003130045	2500	0.001796		
2700	0.43379416	2700	0.020735649	2700	0.011955		
3000	1.001213219	3000	0.184634409	3000	0.11559		

Figure 11-25 Oxygen for each Sigma FER at 70 Bar

60 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050127702	1500	-4.09346E-09	1500	1.47E-08	1500	-9.66167E-08
2000	0.074483724	2000	2.726E-05	2000	3.51E-06	2000	3.19049E-06
2100	0.096703406	2100	0.0001288	2100	1.63E-05	2100	1.48204E-05
2200	0.131032411	2200	0.000527283	2200	6.6E-05	2200	5.98928E-05
2300	0.180747587	2300	0.001907849	2300	0.000236	2300	0.000214434
2400	0.248973805	2400	0.006147247	2400	0.000759	2400	0.000688915
2500	0.338716496	2500	0.017684188	2500	0.002212	2500	0.002006062
2700	0.594838203	2700	0.102199233	2700	0.014695	2700	0.013332418
3000	1.186419239	3000	0.530337701	3000	0.138832	3000	0.127503583
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137576524	1500	8.62589E-09	1500	-9.3E-08		
2000	0.154401983	2000	1.7204E-05	2000	3.22E-06		
2100	0.172301458	2100	8.08707E-05	2100	1.5E-05		
2200	0.202398473	2200	0.000330581	2200	6.05E-05		
2300	0.248551516	2300	0.00119484	2300	0.000217		
2400	0.314043175	2400	0.00385929	2400	0.000696		
2500	0.401760525	2500	0.011207941	2500	0.002028		
2700	0.655208539	2700	0.069233619	2700	0.013476		
3000	1.244325811	3000	0.42920282	3000	0.128708		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	2.94494E-08	1500	-2.58586E-09	1500	8.66E-10		
2000	0.001641242	2000	5.68268E-06	2000	3.33E-06		
2100	0.007278946	2100	2.65534E-05	2100	1.55E-05		
2200	0.024576584	2200	0.000107844	2200	6.25E-05		
2300	0.061691559	2300	0.000387895	2300	0.000224		
2400	0.122269184	2400	0.001250533	2400	0.000719		
2500	0.207619408	2500	0.003649363	2500	0.002094		
2700	0.459881876	2700	0.024090349	2700	0.013917		
3000	1.051038138	3000	0.209085724	3000	0.132402		

Figure 11-26 Oxygen for each Sigma FER at 60 Bar

50 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050139874	1500	-3.98169E-09	1500	1.48E-08	1500	-9.66037E-08
2000	0.076462704	2000	3.27247E-05	2000	4.21E-06	2000	3.82899E-06
2100	0.100224722	2100	0.000154562	2100	1.96E-05	2100	1.77858E-05
2200	0.136792198	2200	0.000632598	2200	7.92E-05	2200	7.18697E-05
2300	0.189619108	2300	0.00228763	2300	0.000283	2300	0.000257316
2400	0.261986994	2400	0.007358295	2400	0.000911	2400	0.000826577
2500	0.357021251	2500	0.021074534	2500	0.002653	2500	0.002406242
2700	0.627430213	2700	0.118749964	2700	0.017578	2700	0.015953622
3000	1.247604066	3000	0.584261976	3000	0.162345	3000	0.149425485
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137583826	1500	8.69366E-09	1500	-9.3E-08		
2000	0.155920273	2000	2.06412E-05	2000	3.87E-06		
2100	0.175278997	2100	9.7042E-05	2100	1.8E-05		
2200	0.20762858	2200	0.000396611	2200	7.26E-05		
2300	0.256965625	2300	0.001433208	2300	0.00026		
2400	0.326683489	2400	0.004624947	2400	0.000835		
2500	0.41976489	2500	0.013398064	2500	0.002432		
2700	0.687589618	2700	0.081376817	2700	0.016124		
3000	1.305323372	3000	0.478665915	3000	0.150802		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	6.71118E-08	1500	-2.56243E-09	1500	8.81E-10		
2000	0.001961558	2000	6.82053E-06	2000	3.99E-06		
2100	0.008596797	2100	3.18668E-05	2100	1.86E-05		
2200	0.028312657	2200	0.000129408	2200	7.5E-05		
2300	0.069156222	2300	0.000465436	2300	0.000269		
2400	0.134397584	2400	0.001500175	2400	0.000863		
2500	0.225379634	2500	0.004375286	2500	0.002512		
2700	0.492305406	2700	0.02874074	2700	0.016651		
3000	1.112371319	3000	0.241301875	3000	0.155019		

Figure 11-27 Oxygen for each Sigma FER at 50 Bar

40 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050156358	1500	-3.81404E-09	1500	1.48E-08	1500	-9.65843E-08
2000	0.079080082	2000	4.09215E-05	2000	5.26E-06	2000	4.78674E-06
2100	0.104856357	2100	0.000193202	2100	2.45E-05	2100	2.2234E-05
2200	0.144342676	2200	0.000790485	2200	9.89E-05	2200	8.98346E-05
2300	0.201223133	2300	0.002856191	2300	0.000354	2300	0.000321631
2400	0.278977331	2400	0.009163718	2400	0.001138	2400	0.001032994
2500	0.380875159	2500	0.026074481	2500	0.003314	2500	0.00300587
2700	0.669695696	2700	0.141954345	2700	0.021869	2700	0.019858369
3000	1.32607104	3000	0.654760646	3000	0.19566	3000	0.180618356
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137593717	1500	8.7953E-09	1500	-9.3E-08		
2000	0.157954618	2000	2.5797E-05	2000	4.84E-06		
2100	0.179241045	2100	0.000121297	2100	2.25E-05		
2200	0.214541081	2200	0.000495629	2200	9.08E-05		
2300	0.2680269	2300	0.001790389	2300	0.000325		
2400	0.34323484	2400	0.00576962	2400	0.001044		
2500	0.443265692	2500	0.0166526	2500	0.003038		
2700	0.72960375	2700	0.098767442	2700	0.02007		
3000	1.383556946	3000	0.544066666	3000	0.182225		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	5.43459E-08	1500	-2.52729E-09	1500	9.02E-10		
2000	0.002437367	2000	8.52729E-06	2000	4.99E-06		
2100	0.010503619	2100	3.98368E-05	2100	2.32E-05		
2200	0.033487274	2200	0.000161751	2200	9.38E-05		
2300	0.079159586	2300	0.000581719	2300	0.000336		
2400	0.150395029	2400	0.00187435	2400	0.001078		
2500	0.248629587	2500	0.005461722	2500	0.003138		
2700	0.534401685	2700	0.035618261	2700	0.020721		
3000	1.19105399	3000	0.285888572	3000	0.187141		

Figure 11-28 Oxygen for each Sigma FER at 40 Bar

30 bar:

0.996		1.094		1.23		1.239	
Temp	n5	Temp	n5	Temp	n5	Temp	n5
1500	0.050180502	1500	-3.53466E-09	1500	1.48E-08	1500	-9.65518E-08
2000	0.082796659	2000	5.45822E-05	2000	7.01E-06	2000	6.38299E-06
2100	0.11138998	2100	0.000257587	2100	3.26E-05	2100	2.96474E-05
2200	0.154951406	2200	0.001053403	2200	0.000132	2200	0.000119775
2300	0.217483659	2300	0.003800852	2300	0.000472	2300	0.000428804
2400	0.302730375	2400	0.012143623	2400	0.001517	2400	0.001376821
2500	0.414140584	2500	0.03419569	2500	0.004413	2500	0.004003543
2700	0.728252149	2700	0.177093783	2700	0.028931	2700	0.026293469
3000	1.433179016	3000	0.753020098	3000	0.246762	3000	0.228738242
0.989		1.116		1.238			
Temp	n5	Temp	n5	Temp	n5		
1500	0.137608209	1500	8.96471E-09	1500	-9.2E-08		
2000	0.160891171	2000	3.43898E-05	2000	6.45E-06		
2100	0.18490882	2100	0.000161718	2100	3E-05		
2200	0.224346859	2200	0.000660582	2200	0.000121		
2300	0.283616132	2300	0.002384705	2300	0.000433		
2400	0.366449445	2400	0.007667354	2400	0.001392		
2500	0.47609815	2500	0.021997543	2500	0.004047		
2700	0.787845556	2700	0.125843616	2700	0.026571		
3000	1.490355833	3000	0.636357014	3000	0.23067		
1.013		1.188		1.235			
Temp	n5	Temp	n5	Temp	n5		
1500	-3.64359E-07	1500	-2.46871E-09	1500	9.38E-10		
2000	0.00321835	2000	1.13719E-05	2000	6.66E-06		
2100	0.013515887	2100	5.31198E-05	2100	3.09E-05		
2200	0.041216794	2200	0.000215652	2200	0.000125		
2300	0.093546563	2300	0.000775451	2300	0.000447		
2400	0.173003675	2400	0.002497207	2400	0.001437		
2500	0.281210543	2500	0.007265971	2500	0.004179		
2700	0.592797915	2700	0.046832885	2700	0.027427		
3000	1.298497785	3000	0.352255362	3000	0.236571		

Figure 11-29 Oxygen for each Sigma FER at 30 Bar

20 bar:

0.996				1.094				1.23				1.239	
Temp	n5			Temp	n5			Temp	n5			Temp	n5
1500	0.050220979			1500	-2.97602E-09			1500	1.49E-08			1500	-9.6487E-08
2000	0.088757622			2000	8.19014E-05			2000	1.05E-05			2000	9.57548E-06
2100	0.121782431			2100	0.000386305			2100	4.89E-05			2100	4.4474E-05
2200	0.1717424			2200	0.001578389			2200	0.000198			2200	0.000179649
2300	0.243129859			2300	0.005679269			2300	0.000708			2300	0.000643078
2400	0.340072627			2400	0.017998021			2400	0.002274			2400	0.002063721
2500	0.466248208			2500	0.049710171			2500	0.006604			2500	0.005992523
2700	0.819092642			2700	0.23760004			2700	0.042741			2700	0.038906252
3000	1.595766754			3000	0.905692711			3000	0.336134			3000	0.313574456
0.989				1.116				1.238					
Temp	n5			Temp	n5			Temp	n5				
1500	0.137632516			1500	9.30354E-09			1500	-9.2E-08				
2000	0.165706618			2000	5.15745E-05			2000	9.67E-06				
2100	0.19408683			2100	0.000242543			2100	4.49E-05				
2200	0.240049526			2200	0.000990206			2200	0.000182				
2300	0.308371345			2300	0.003569663			2300	0.00065				
2400	0.403083094			2400	0.011425839			2400	0.002086				
2500	0.527634479			2500	0.032405465			2500	0.006057				
2700	0.878256334			2700	0.17427545			2700	0.03931				
3000	1.652486812			3000	0.781766181			3000	0.316005				
1.013				1.188				1.235					
Temp	n5			Temp	n5			Temp	n5				
1500	8.75872E-08			1500	-2.35156E-09			1500	1.01E-09				
2000	0.004737735			2000	1.7061E-05			2000	9.98E-06				
2100	0.019026513			2100	7.96846E-05			2100	4.64E-05				
2200	0.054329627			2200	0.000323431			2200	0.000187				
2300	0.11689075			2300	0.001162637			2300	0.000671				
2400	0.208966849			2400	0.00374005			2400	0.002154				
2500	0.332517255			2500	0.010850495			2500	0.006255				
2700	0.683519236			2700	0.0683947			2700	0.040555				
3000	1.461674125			3000	0.463745037			3000	0.323409				

Figure 11-30 Oxygen for each Sigma FER at 20 Bar

10 bar:

0.996				1.094				1.23				1.239	
Temp	n5			Temp	n5			Temp	n5			Temp	n5
1500	0.050312224			1500	-1.30108E-09			1500	1.51E-08			1500	-9.62924E-08
2000	0.10122187			2000	0.000163841			2000	2.1E-05			2000	1.91528E-05
2100	0.143260713			2100	0.000772054			2100	9.78E-05			2100	8.8951E-05
2200	0.206198433			2200	0.003146606			2200	0.000395			2200	0.000359227
2300	0.295470158			2300	0.011229731			2300	0.001415			2300	0.001285316
2400	0.415863397			2400	0.034786564			2400	0.004537			2400	0.004118419
2500	0.57132524			2500	0.091505563			2500	0.013114			2500	0.011908904
2700	0.999087526			2700	0.374058254			2700	0.081882			2700	0.074858985
3000	1.905775988			3000	1.205057154			3000	0.541119			3000	0.510603768
0.989				1.116				1.238					
Temp	n5			Temp	n5			Temp	n5				
1500	0.137687367			1500	1.032E-08			1500	-9.2E-08				
2000	0.176126208			2000	0.000103123			2000	1.94E-05				
2100	0.213543443			2100	0.000484882			2100	8.99E-05				
2200	0.272780104			2200	0.001976819			2200	0.000363				
2300	0.359335922			2300	0.007095587			2300	0.001299				
2400	0.47778664			2400	0.022419045			2400	0.004162				
2500	0.631824488			2500	0.061634989			2500	0.012036				
2700	1.05753624			2700	0.289909362			2700	0.075602				
3000	1.961637038			3000	1.071647271			3000	0.513917				
1.013				1.188				1.235					
Temp	n5			Temp	n5			Temp	n5				
1500	1.71922E-07			1500	-2.00011E-09			1500	1.22E-09				
2000	0.008997895			2000	3.41279E-05			2000	2E-05				
2100	0.032743576			2100	0.000159369			2100	9.28E-05				
2200	0.083545997			2200	0.000646599			2200	0.000375				
2300	0.166100498			2300	0.002321987			2300	0.001341				
2400	0.282944623			2400	0.007445876			2400	0.004298				
2500	0.436614727			2500	0.021418222			2500	0.012426				
2700	0.863590114			2700	0.127242608			2700	0.077886				
3000	1.773029183			3000	0.704942122			3000	0.523973				

Figure 11-31 Oxygen for each Sigma FER at 10 Bar

11.12 Excel Sheets

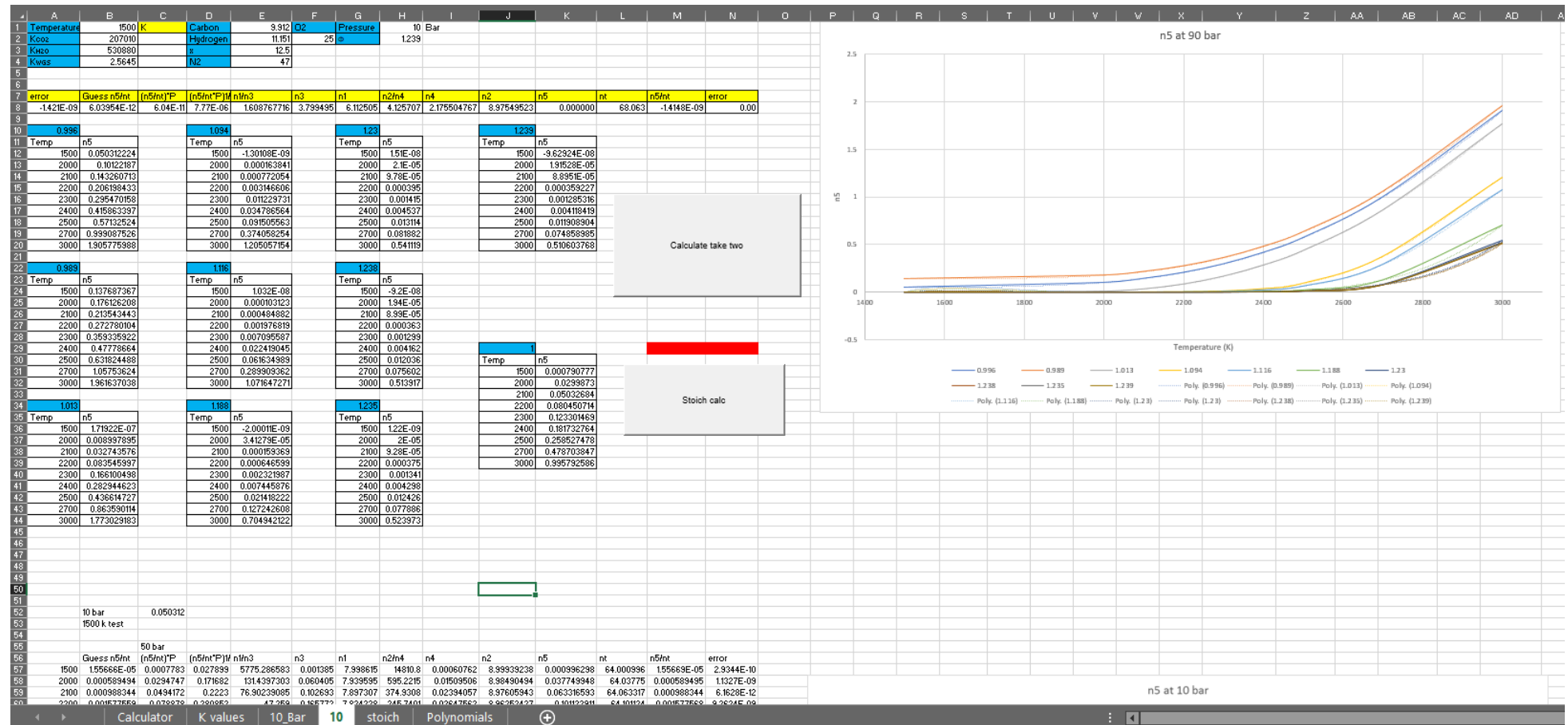
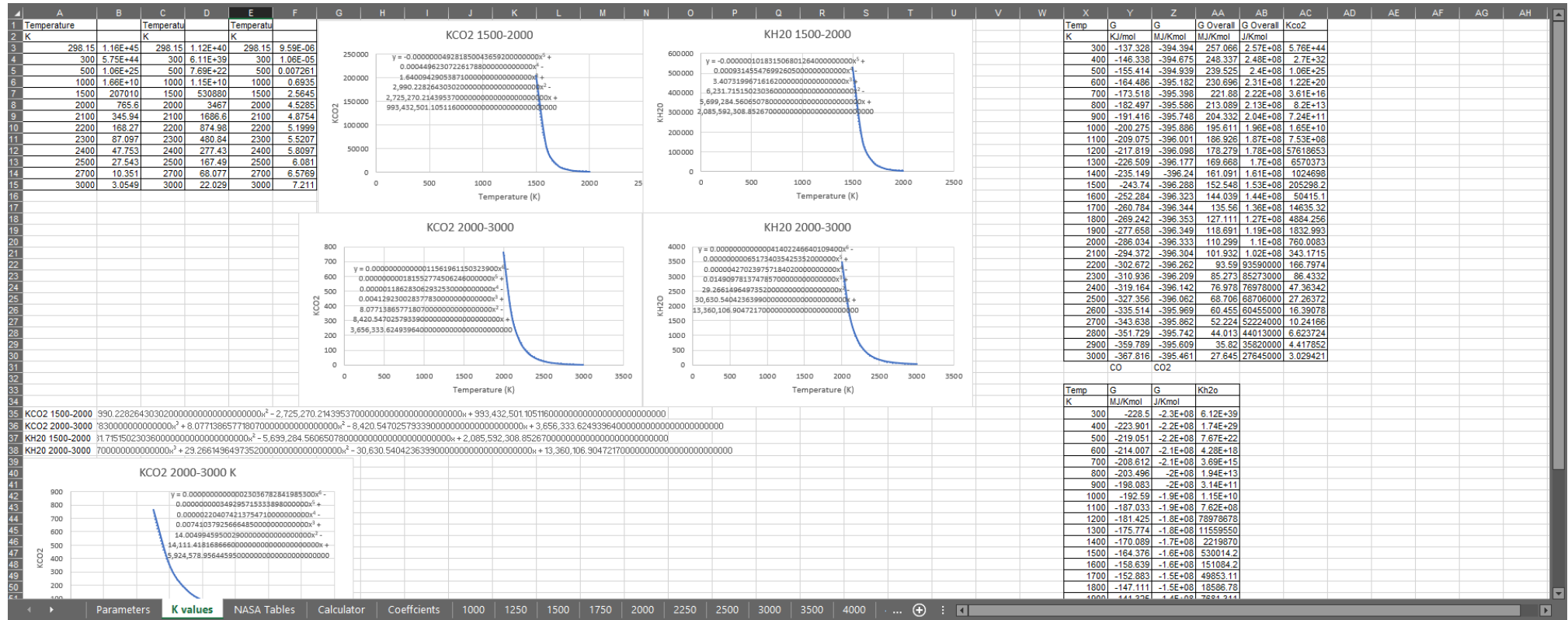


Figure 11-32 Original Dissociation Model

This is the original calculator to determine the oxygen content, used to gather the polynomials for the linear interpolation but development was scrapped due to using the other method. However, it still proved a useful tool in determining how dissociation works at different pressures and FER. The next few pages are from the Ford Fox Excel sheet which is similar to the Sigma except the Fox has the water injection included.

Figure 11-33 Constant Values for CO₂ and H₂O

Where the original constant values from the JANAF tables were held with the inclusion of the calculated constants from the Gibbs function.

Figure 11-34 Ford Fox Chemical Equilibrium Calculator

Where relevant data sheet information is held as well as the calculator for the chemical equilibrium and water injection reductions.

Figure 11-35 Ford Fox Mass Calculator

Where the masses of the A/F mixture for each FER were calculated.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	CO2	T range (K)	ai1	ai2	ai3	ai4	ai5									
2		1000-5000	4.4608	0.003098	-1.2E-06	2.27E-10	-1.6E-14									
3		300-1000	2.4008	0.008735	-6.6E-06	2E-09	6.33E-16									
4																
5	H2O	1000-5000	2.7168	0.002945	-8E-07	1.02E-10	-4.8E-15									
6		300-1000	4.0701	-0.00111	4.15E-06	-3E-09	8.07E-13									
7																
8	CO	1000-5000	2.9841	0.001489	-5.8E-07	1.04E-10	-6.9E-15									
9		300-1000	3.7101	-0.00162	3.69E-06	-2E-09	2.4E-13									
10																
11	O2	1000-5000	3.622	0.000736	-2E-07	3.62E-11	-2.9E-15									
12		300-1000	3.6256	-0.00188	7.06E-06	-6.8E-09	2.16E-12									
13																
14	N2	1000-5000	2.8963	0.001516	-5.7E-07	9.98E-11	-6.5E-15									
15		300-1000	3.6748	-0.00121	2.32E-06	-6.3E-10	-2.3E-13									
16																
17		Af1	Af2	Af3	Af4	Af5										
18	C8H18	-0.55313	181.62	-97.787	20.402	-0.03095										
19																
20																
21																
22																
23																
24																
25																
26																
27																
28																
29																
30																
31																
32																
33																
34																
35																
36																
37																
38																
39																
40																
41																
42																
		Parameters	K values	NASA Tables	Calculator	Coefficients	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000

Figure 11-36 Ford Fox Coefficients

Polynomial coefficients for calculating the specific heat values.

Haydn Jones

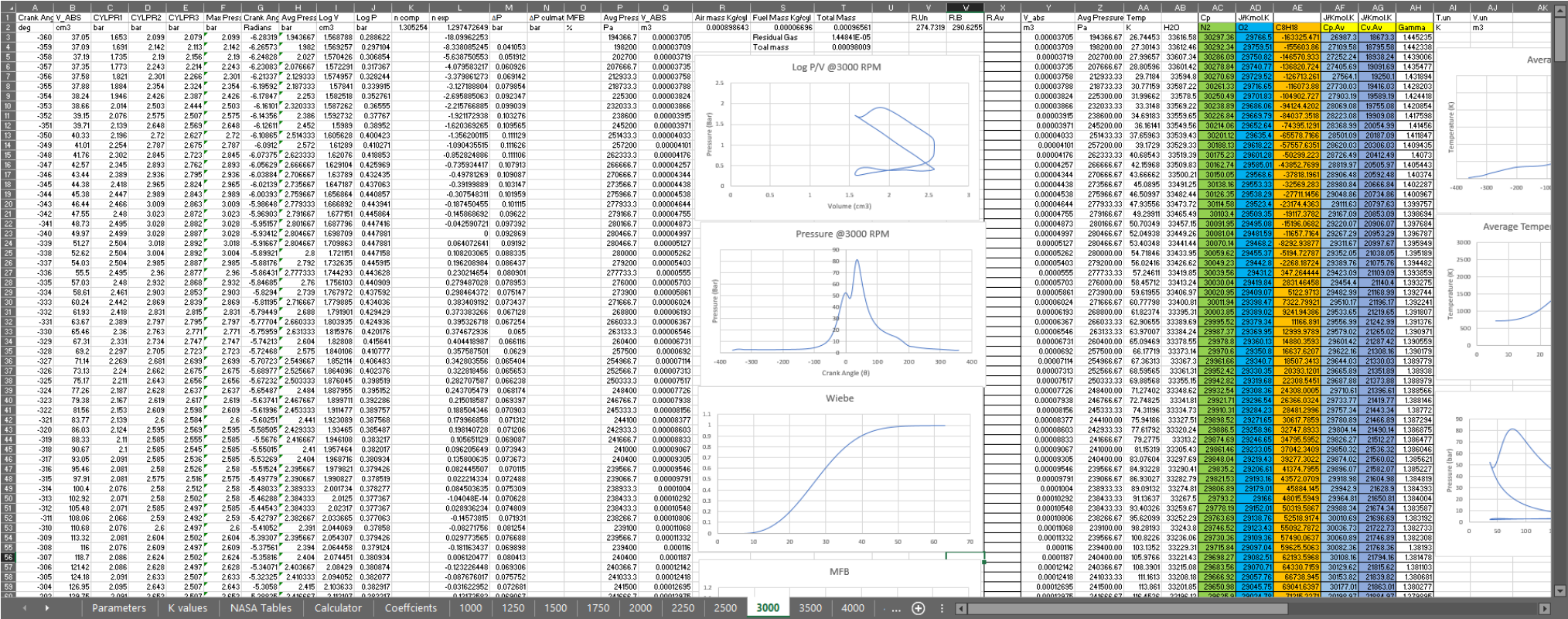


Figure 11-37 Ford Fox Example Worksheet at 3000 RPM

Main calculations set out in order of this report.

[illegible]

[illegible]



Figure 11-40 Ford Fox Results Page

11.3 Ford Sigma Part Load Combustion Comparison

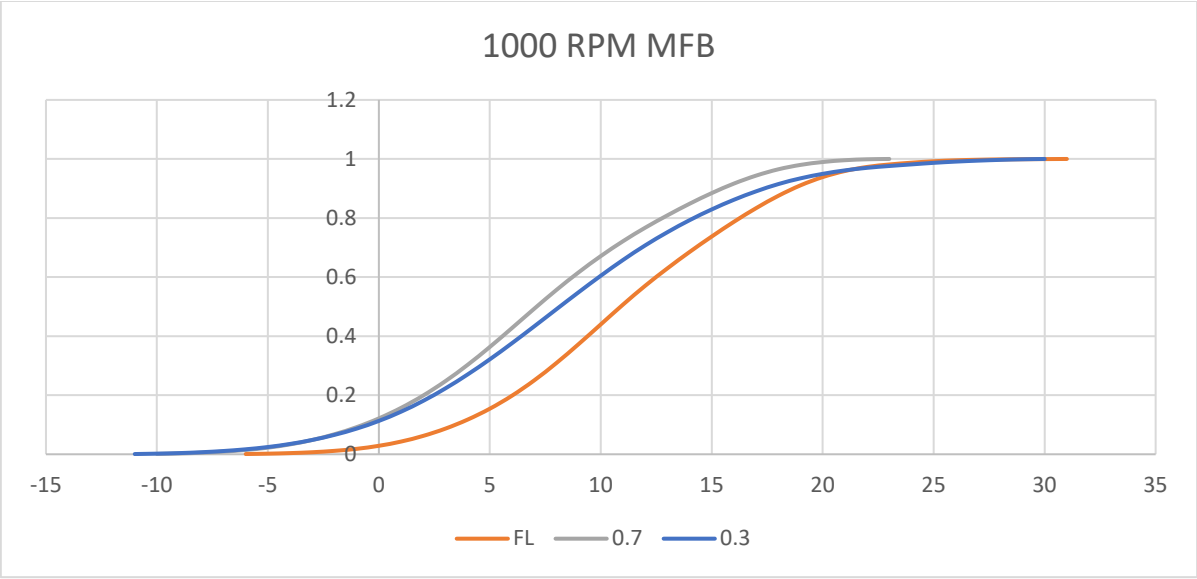


Figure 11-41 Ford Sigma Part Load MFB at 1000 RPM

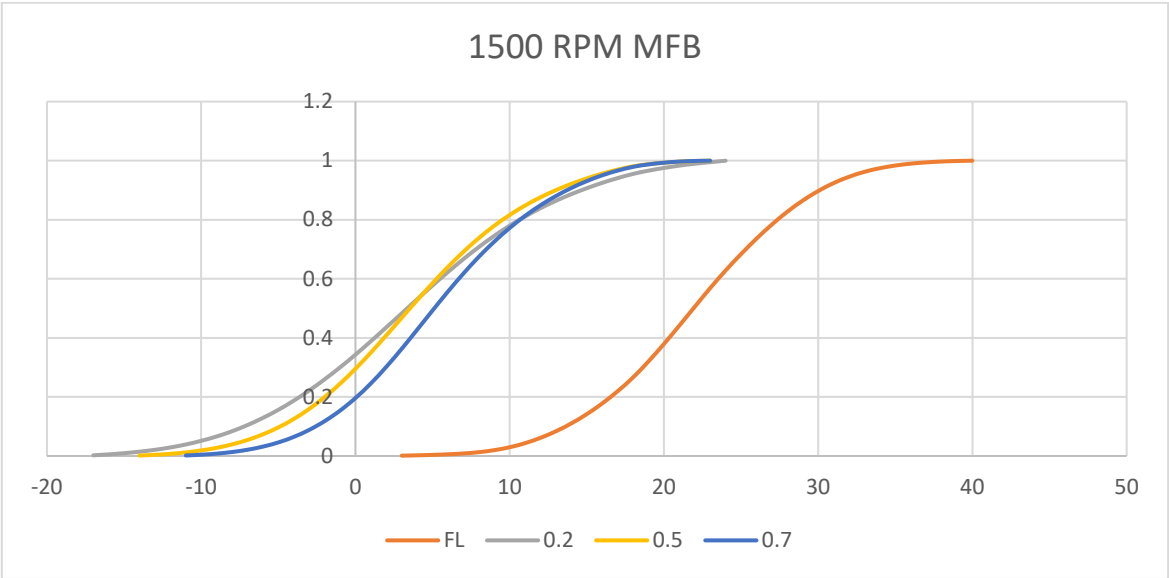


Figure 11-42 Ford Sigma Part Load MFB at 1500 RPM

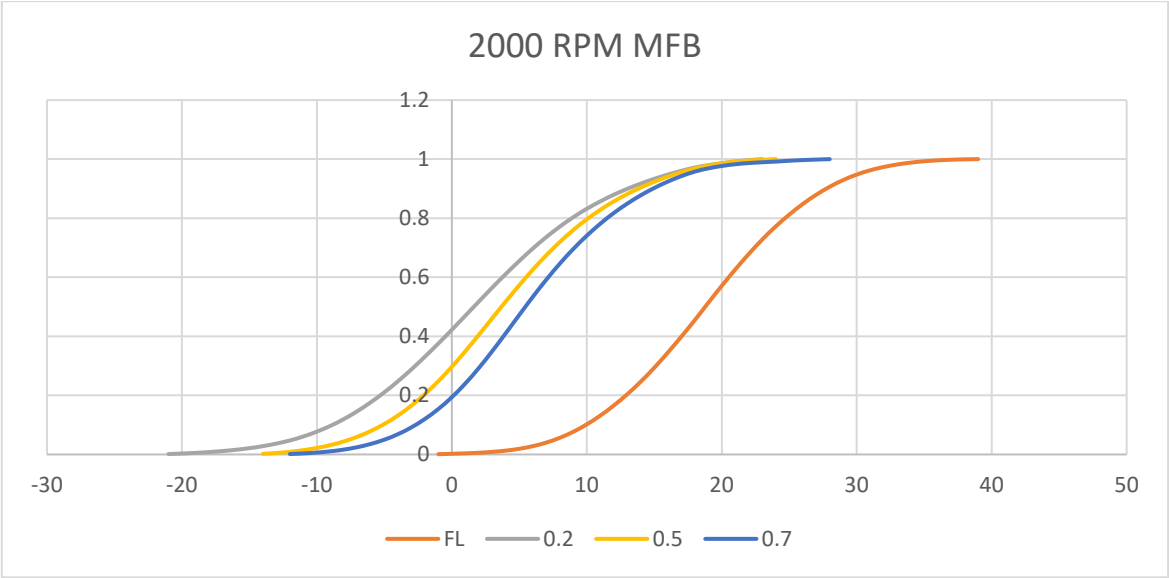


Figure 11-43 Ford Sigma Part Load MFB at 2000 RPM

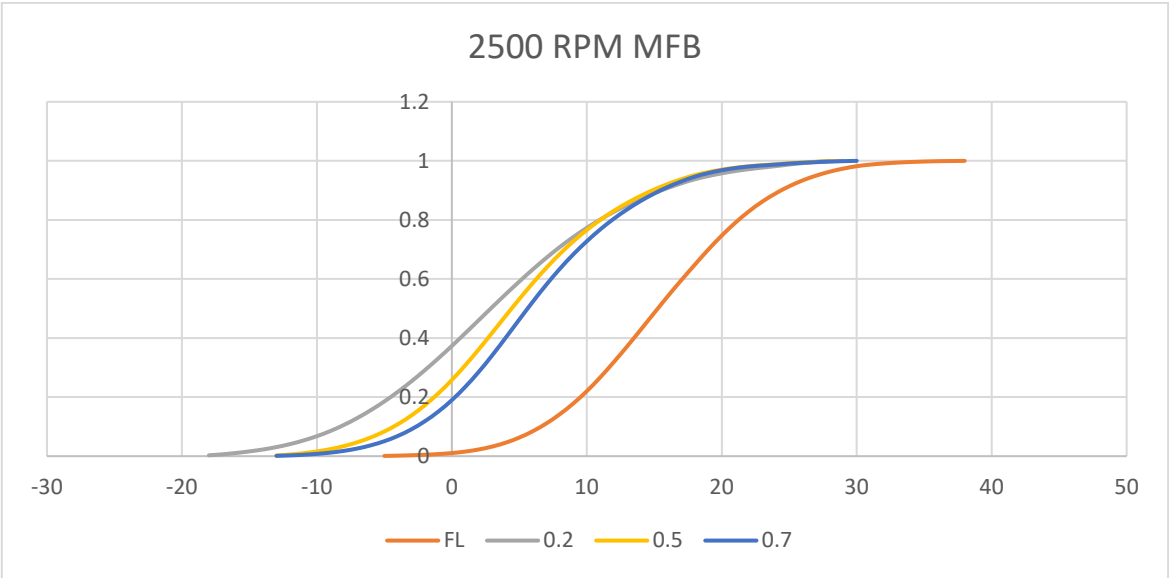


Figure 11-44 Ford Sigma Part Load MFB at 2500 RPM

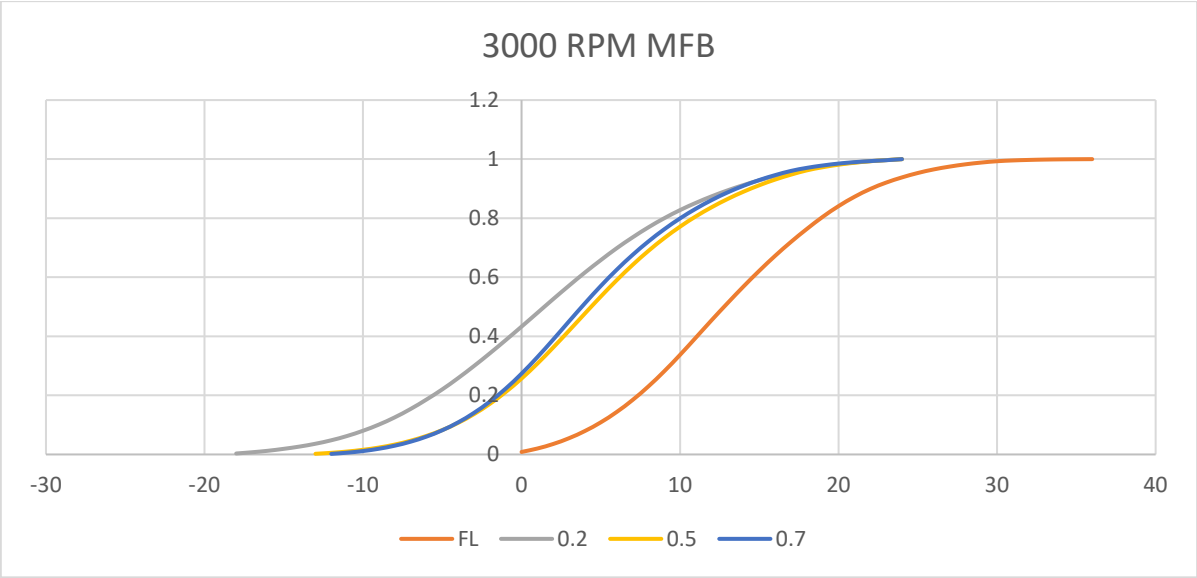


Figure 11-45 Ford Sigma Part Load MFB at 3000 RPM

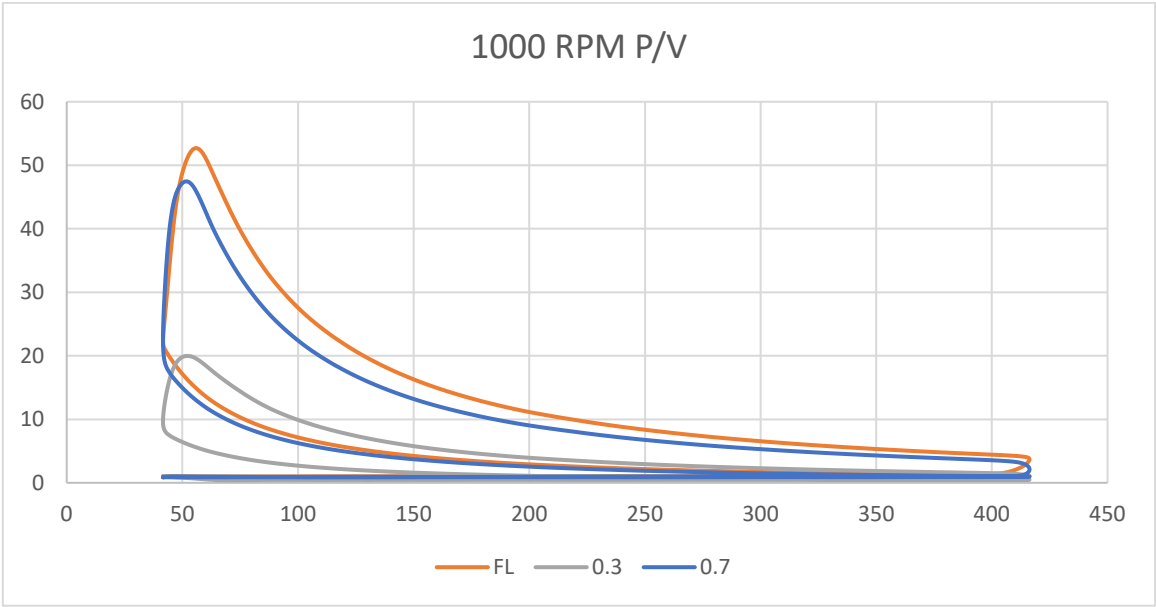


Figure 11-46 Ford Sigma Part Load PV at 1000 RPM

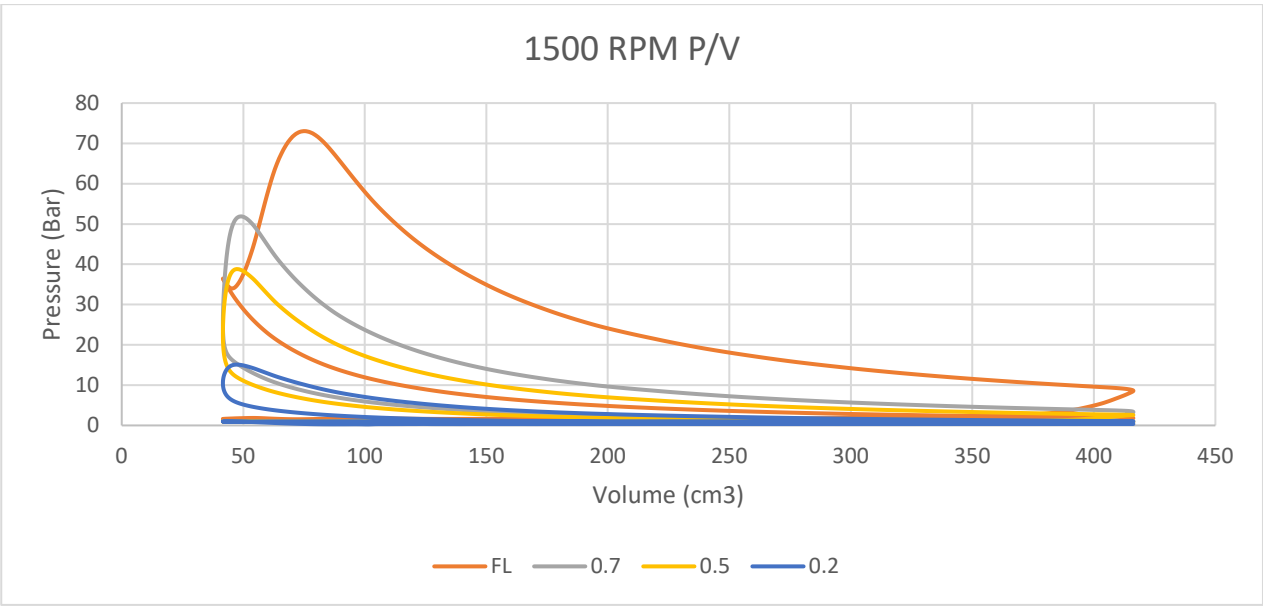


Figure 11-47 Ford Sigma PV at Part Load at 1500 RPM

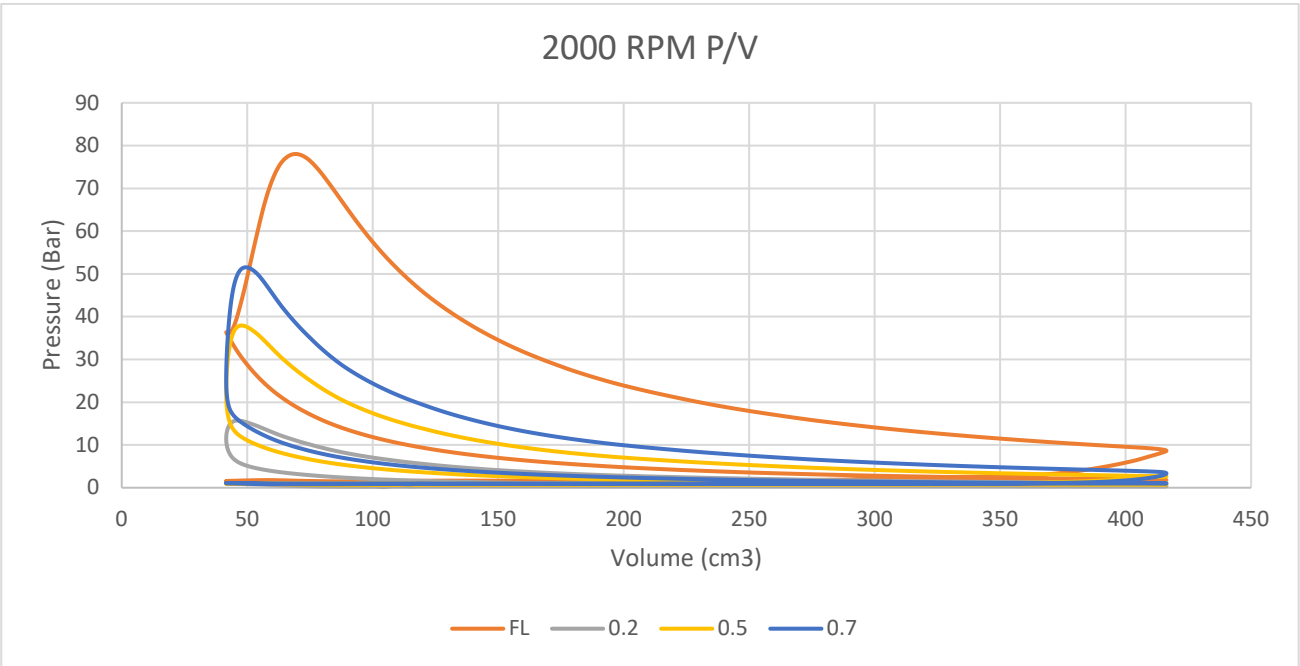


Figure 11-48 Ford Sigma PV at Part Load at 2000 RPM

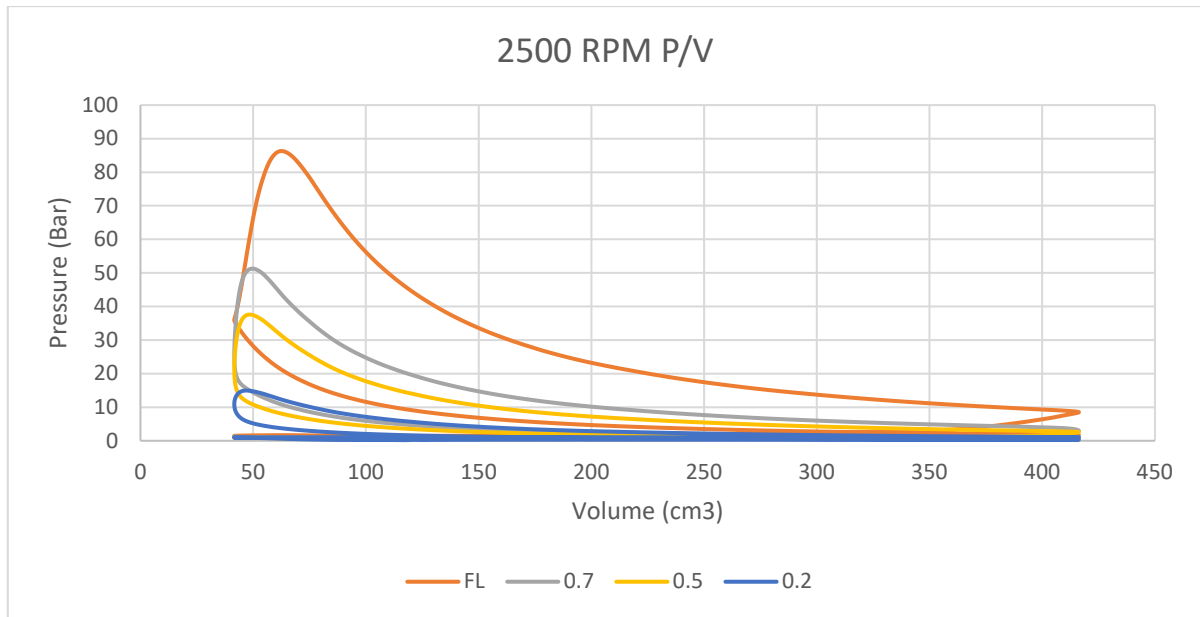


Figure 11-49 Ford Sigma PV at Part Load at 2500 RPM

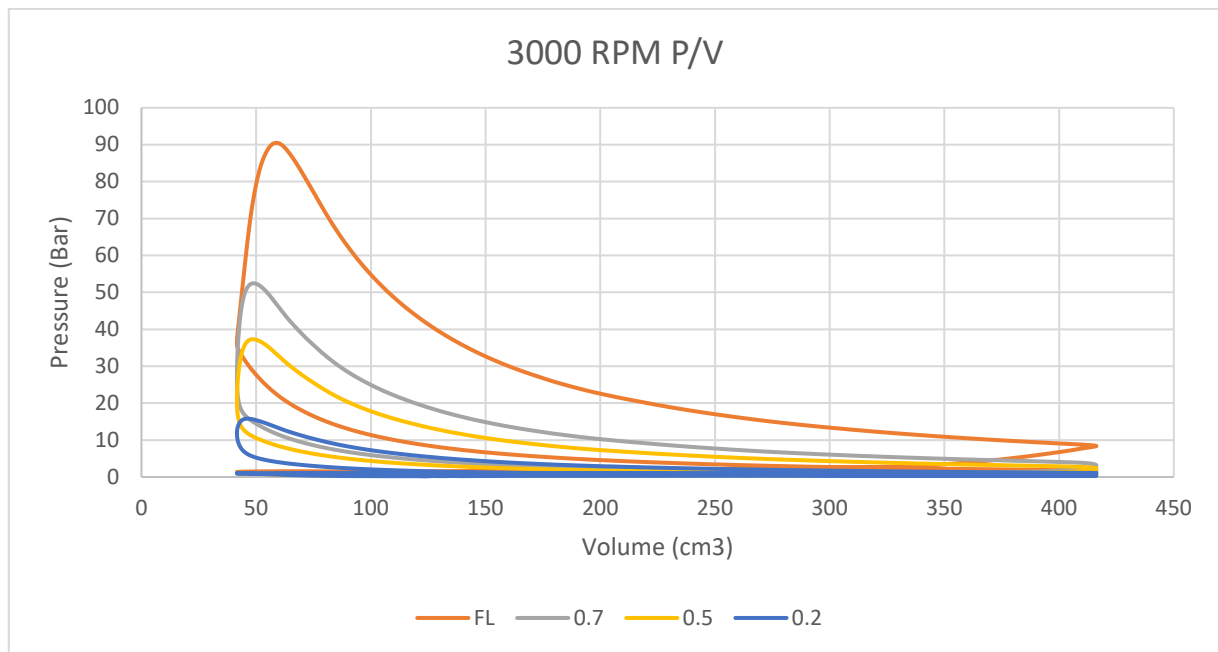


Figure 11-50 Ford Sigma PV at Part Load at 3000 RPM

At part load timing is heavily advanced due to the reduced pressures and temperatures experienced by the engine. Whilst FL is heavily retarded to help reduce the risk of auto-ignition from occurring. It can be seen that as the RPM increases even though the pressure rises the chance of auto-ignition decreases due to less time for heat transfer to occur allowing FL at higher RPM to be advanced coupled with the fact there is less time for combustion to occur so SOC needs to occur earlier.

11.14 Ford Fox 1l Specifications

Ford Fox 1.0-litre EcoBoost (125PS)		
Type		Inline three cylinder turbo petrol, direct fuel injection and Ti VCT, transverse
Displacement	cm ³	999
Bore	mm	71.9
Stroke	mm	82
Compression ratio		10.0:1
Max power	PS (kW)	125 (92)
at rpm		6000
Max torque	Nm	170 (up to 200 with transient overboost)
	at rpm	1400-4500
Valve gear		DOHC with 4 valves per cylinder, twin independent variable cam timing
Cylinders		3 in line
Cylinder head		Cast aluminium
Cylinder block		Cast iron
Camshaft drive		Low friction Belt-in-Oil with dynamic tensioner
Crankshaft		Cast iron, 6 counterweights, 4 main bearings
Engine management		Bosch MED17 with CAN-Bus and individual cylinder knock control
Fuel injection		High pressure direct fuel injection with 6 hole injectors
Emission control		Close coupled three-way catalyst system with heated universal oxygen sensor and catalyst monitor sensor post catalyst
Emission level		Euro Stage 5
Turbocharger		Continental low inertia turbo
Lubrication system		Electronically controlled variable displacement oil pump for improved fuel economy
System capacity with filter	litres	4.1
Cooling system		Split cooling system with 2 thermostats
Transmission		Durashift 6- speed (B6) manual
Gear Ratios		
		6th 0.690
		5th 0.821
		4th 1.032
		3rd 1.357
		2nd 2.048
		1st 3.727
		Reverse
		3.82
		FDR 4.07

Figure 11-51 Ford Fox Specifications (Ford, 2013)

Exact specification for the 1.5l Ford Sigma engine were not produced in this report due to conflicting specifications between reports.