

Combustion Modelling for NOx Production Analysis

BEng – Advanced Engine Design

Major project - 2017

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By use of a mathematical presented model to show a two zone representation of in cylinder dynamics under combustion, with analyses on the sensitivity giving a large effect. Resulting in how the formation of NOx production is present at high cylinder temperatures with comparative results, giving a new method of parametrization of pressures to give greater accuracy with NOx prediction.



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1. Introduction

The use of mathematical models for engine simulations is becoming more popular due to the advantage of increased computational power for some complex models. This saves manufacturers time and cost as a model will be able to compute a prediction within a few seconds where as a dynamometer run will take a considerably longer time to carry out.

By started with equations used day to day such as the ideal gas law, adiabatic relationships and relatable equations to give the simple combustion model. Where supplied engine data from a secondary source Ford Motor Company is used. Where the base data is pressure and volume values, with a data sheet giving details of each parameter necessary for input data. The model will evolve into a two zone model where combustion temperatures and pressures will help give a prediction of Nitrogen Oxides (NOx) formation.

Each NOx formation will be looked at and from the Extended Zeldovich Mechanism (EZM), to the Super Extended Zeldovich Mechanism (SEZM) and the suitability of results towards the engine data given. Chemical formations will be divulged leading onto reaction rates of the engine out emissions to find equilibrium. The use of Microsoft Excel will be used to provide a platform for the extensive amount of calculations where some limitations are made for calculation quantities.

From the use of the SEZM, the use of the empirical parametrization will be used to further increase the accuracy of the NOx predictions. As the pressure data is averaged over 300 cycles it will be used to best fit the parametrization.

As the engine manufacturers are under EU regulations for tailpipe emissions, there is the use of aftermarket available to combat the engine out emissions. The use of the model is important as it predicts the engine out emissions so combating the problem in cylinder rather than adding more and more after treatment devices. The New European Drive Cycle (NEDC) cycle is now in force and soon to come is the Real Driving Emissions (RDE) and Worldwide harmonized Light vehicles Test Procedure (WLTP). These models can be used in the ECU to actively change the engines parameters to tackle the future strict regulations.

2. Two zone model

With engine data from a 1.0L turbocharged direct injection engine, showing the pressure and volume at each interval of crank angle. A piezoelectric pressure transducer is used to measure the in cylinder pressure. A model is used for analytical work and prediction before any dynamometer work is done as the calculations can take a matter of seconds where a simple engine run on the dyno can take considerably longer.

The need for direct injection came from the need of lowering specific fuel consumption and as a result lowering CO₂ emissions. The greater efficiency of the engine is made by the charge drawn in consisting wholly of air with or without the addition of exhaust gas recirculation (EGR), with the use of fuel stratification before combustion.

2.1. Polytropic Index

By taking logarithms of the pressure and volume to result in the Log PV loop in Figure 1. It can be used to narrow down the start of combustion (SOC) and end of combustion (EOC), from workings it can be found within ± 10 degrees. This isn't ideal for following calculations so it was necessary to narrow down by an alternative method. (Tazerout, Le corre, & Ramesh, 2000)

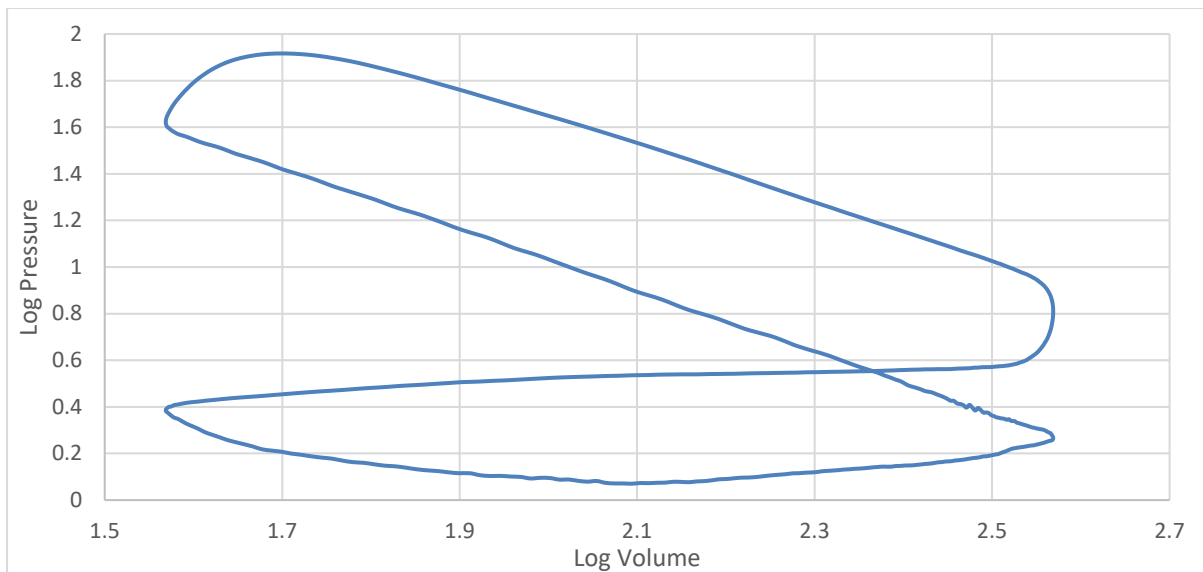


Figure 1 Log PV loop – Expansion and compression are assumed to be straight lines

From the Log PV loop diagrams, it is possible to find the relation between the pressure and volume. It is known that the compression and expansion processes are assumed to be adiabatic thus, can be fitted well with a polytropic relation; where ' η ' is the Polytropic index,

$$pV^\eta = \text{constant}$$

Equation 1

Where it is seen that a suitable for the index is of the order of 1.3 (± 0.05). To gain a value it is achieved by;

$$\text{Polytropic index } (\eta) \approx \frac{-(\text{Log}P_2 - \text{Log}P_1)}{(\text{Log}V_2 - \text{Log}V_1)}$$

Equation 2

It is seen that it is analogous to the average value of ' γ_{unb} ' over compression process, but it is larger than ' γ_b ' for the burned gas during expansion; as a result of the heat loss to the walls. (Heywood, 1988). The SOC and EOC were found by an immediate increase/decrease in the polytropic index. The delay from spark to a noticeable change in pressure is, the ignition delay is approximately 9 degrees.

2.2. Pressure without combustion

From the polytropic relation equation, to find the resultant pressure after 1 degree if the EOC stopped at ' P_1 ' (Bar). Where ' η ' value is used appropriately for compression and expansion.

$$P_{2\eta} = P_1 \left(\frac{V_1}{V_2} \right)^\eta$$

Equation 3

This value is dependent on the correct calculation of the polytropic index due to the power mathematic function.

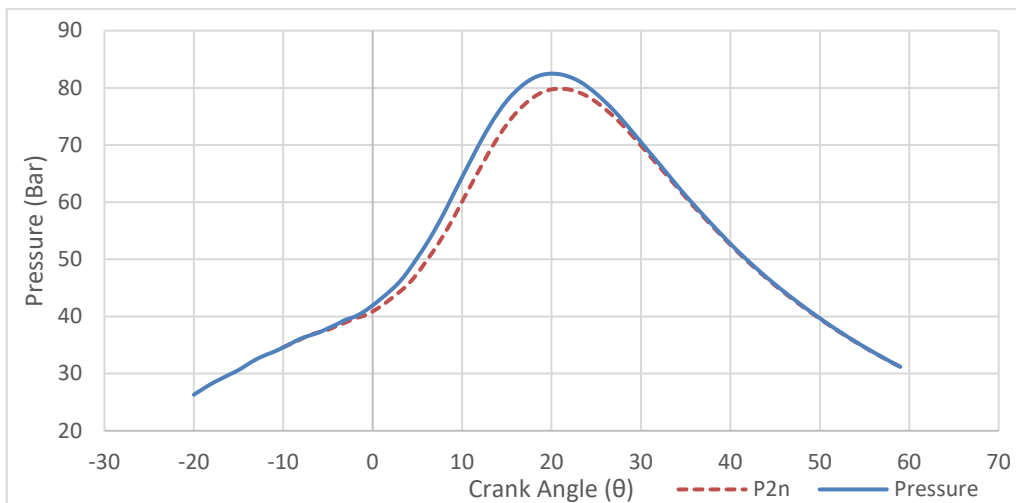


Figure 2 Pressure added from combustion at 6500RPM

The maximum pressure added to the combustion is at 12 degrees ATDC with an additional 4.52Bar. This pressure is at 38% MFB, where the maximum flame speed is produced as this intersects with the steepest part of the slope from the MFB trace.

Pressure rise due to combustion is the measured by pressure minus calculated pressure (Bar) in Equation 3;

$$\Delta P = P_1 - P_{2\eta_1}$$

Equation 4

2.3. Mass fraction burned (MFB)

By calculating the MFB, it will show the percentage of the total mass in cylinder that has been burned at each crank angle. The determined SOC and EOC are sensitive towards the polytropic index. As the MFB is imperative for later calculations, it is crucial that it is close as possible to a representative of the real engine data. A simple MFB is a summation of the pressure differences (from Equation 4) from SOC to EOC, as follows;

$$MFB_{simple} = \frac{\sum_{SOC \rightarrow \theta} \Delta P}{\sum_{SOC \rightarrow EOC} \Delta P}$$

Equation 5

From these values a simple two zone model can be calculated.

2.3.1. Heat release

By approaching the MFB in a different way to gain a higher accuracy, as the values given are used in later calculations. By assuming that the heat release in 1 degree is proportional to the pressure rise the transposition steps are given in Appendix A, (Merket, Schwarz, stiesch, & Otto, 2006) resulting in;

$$MFB_{dQ} = \frac{\sum_{SOC \rightarrow \theta} V_2 \times \Delta P}{\sum_{SOC \rightarrow EOC} V_2 \times \Delta P}$$

Equation 6

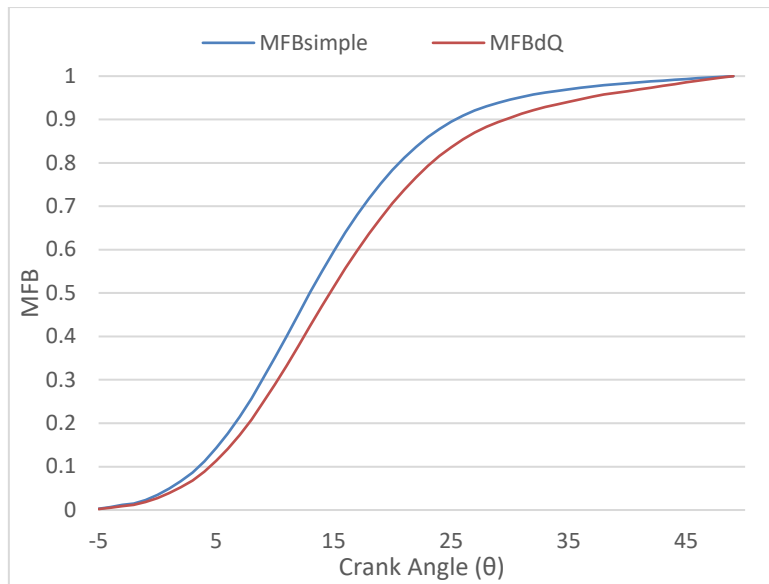


Figure 3 MFB comparison at 6500RPM

The accuracy is higher due to taking into account the change in volume, as a result of the heat released in that 1 CA. It assumes a homogeneous charge with addition of a complete 100% burn; the model also assumes a 'normal' combustion where the maximum pressure increase 2 bar per CA, this has a soft pressure path where the flame propagation spreads steadily across the combustion chamber up to 25m/s. (Merket, Schwarz, stiesch, & Otto, 2006).

The crevice volume can be defined as small regions that the mixture can pass into but the flame cannot penetrate in the combustion chamber. These are known to be the valve seat area, piston land/ring area, sparkplug thread and head gasket. As the cylinder pressure increases the mixture is forced into these regions and are known to escape combustion; this results in lower combustion efficiency and higher hydrocarbon emissions as some are seen to escape when scavenging is in effect when exhaust valve open. The crevice volume have been found to be 1-2% of the cylinder clearance volume and up to 4-6% of the mixture at peak pressure; where 2% flows back at EOC. (McGrath, 1996) (Merket, Schwarz, stiesch, & Otto, 2006)

In reality 100% MFB strictly isn't true as you have a percentage of crevice volume. As a result you get a residual gas fraction from the mass unburned left in the cylinder, this will get taken into account with the EGR in the model.

2.4. In-cylinder mass calculations

Producing base data of the mass going into the engine is needed for future calculations, the input data used is from Ford's data sheets. The Airflow (KG/H), RPM and Air/fuel ratio are used. As the two cylinders are drawing in air, this needs to be factored in with addition to the conversion for KG/Hour to KG/rev. This follows as;

$$\text{Air mass per cylinder (Kg)} = \frac{\text{Airflow}}{2 \times 60 \times \text{RPM}}$$

Equation 7

With the addition of the air/fuel ratio (AFR), to provide the fuel mass;

$$\text{Fuel mass per cylinder (Kg)} = \frac{\text{Airflow}}{2 \times 60 \times \text{RPM} \times \text{AFR}}$$

Equation 8

To gain total mass incoming to the cylinder;

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

Equation 9

2.4.1. EGR addition

By recirculating a measured percentage of the exhaust gas back into the plenum, the intake charge is contaminated with post burn mixture. As more mass is introduced in the cylinder from EGR, like CO₂, H₂O and N₂, therefore the space for the molecules to interact (degrees of freedom) is lessened due to the denser mixture. This lowers the flame temperature as it introduces inert gas between the homogeneous mixture as a result reduces NOx emissions; adding too much EGR can result in slow burn rates so this need to be considered.

New total mass including EGR% is found by;

$$M_{\text{totalEGR}} (\text{Kg}) = M_{\text{total}} + \left((n_T \times \alpha) \times \left(\frac{\text{EGR}\%}{100} \right) \right)$$

Equation 10

In the real engine, EGR levels are seen to use up to 33.3% seen in Appendix B, although EGR is used throughout the whole map, it is substantially increased load whilst in the typical 'drive cycle'. Using EGR and burning lean to counter NOx emissions and passing the legislation it's possible in a theoretical model and real world by the data found from Ford. (Ford, 2012)

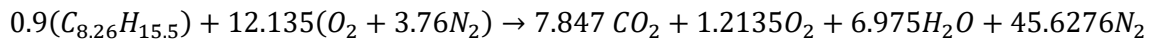
2.5. Fuel molecule calculator

Fuel equivalence ratio is seen to be opposite to lambda, and is usually used when discussing fuel-in situations. It is found by;

$$FER(\varphi) = \frac{1}{\text{Lambda}}$$

Equation 11

By balancing the chemical equation of the mixture in (reactants) to mixture out (products out) for each FER, producing an accurate value for each element. Values from 0.8-1.3 was calculated in 0.001 steps to ensure accuracy. Giving a global stoichiometric reaction of combustion;



Equation 12

To find the molecular weight of the reactants, the equation was used with the molecular weight of each element and the quantity used;

$$\text{Mol. Wt reactants (Kg)} = \frac{(114.62 \times \varphi) + (\text{air} \times (32 + (3.76 \times 28)))}{(\varphi + (\text{air} \times 4.76))}$$

Equation 13

Following the same approach for the products (in Kg);

$$\text{Mol. Wt products} = \frac{(CO_2 \times (12 + (32))) + (H_2O \times ((2) + 16)) + (O_2 \times (32)) + (N_2 \times (28))}{(CO_2 + H_2O + O_2 + N_2)}$$

Equation 14

To gain the gas constant for the reactants or products, by using the universal gas constant (J/Kmol.K) and using the appropriate molecular weight thus;

$$R_{unburned}/R_{burned} = \frac{8314}{\text{Mol. Wt}}$$

Equation 15

Tabulating all this data in a suitable form for ease of lookup function.

Table 1 Fuel calculator lookup table

<i>FER (ϕ)</i>	<i>CO₂</i>	<i>CO</i>	<i>H₂O</i>	<i>O₂</i>	<i>N₂</i>	<i>MolWt.Rea</i>	<i>MolWt.Pro</i>	<i>R.unb</i>	<i>R.b</i>
0.8	6.61	0.00	6.20	2.43	45.63	30.01	28.88	277.02	287.90
0.85	7.02	0.00	6.59	1.82	45.63	30.08	28.88	276.36	287.88
0.9	7.43	0.00	6.98	1.21	45.63	30.16	28.88	275.70	287.86
0.95	7.85	0.00	7.36	0.61	45.63	30.23	28.88	275.04	287.83
1	8.26	0.00	7.75	0.00	45.63	30.30	28.89	274.39	287.81
1.05	7.48	1.19	8.13	0.00	45.63	30.37	28.61	273.75	290.56
1.1	6.68	2.40	8.52	0.00	45.63	30.44	28.34	273.11	293.34
1.15	5.87	3.62	8.90	0.00	45.63	30.51	28.08	272.47	296.11
1.2	5.07	4.83	9.29	0.00	45.63	30.58	27.82	271.84	298.86
1.25	4.27	6.04	9.68	0.00	45.63	30.66	27.57	271.20	301.59
1.3	3.47	7.26	10.07	0.00	45.63	30.73	27.32	270.58	304.31

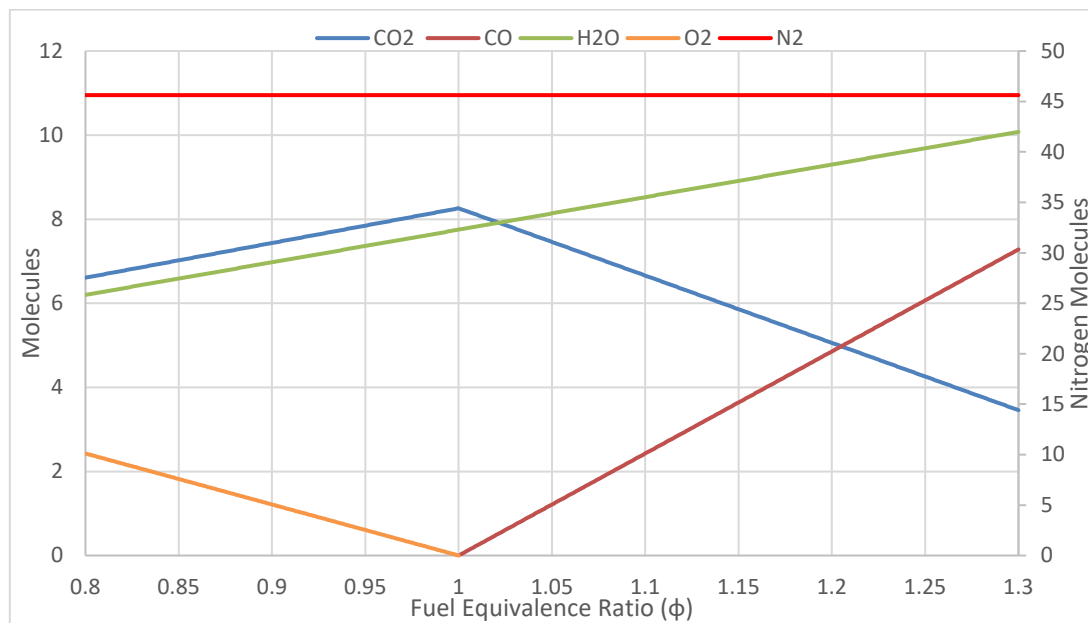


Figure 4 Calculated combustion products

The nitrogen stays constant throughout FER. The content of oxygen lessens with the rise of FER until stoichiometric. CO starts to rise when there isn't enough oxygen to support full combustion and fuel droplets don't get a complete burn as, the outer layer of fuel is burnt locally, whereas in the centre of the droplet there is still fuel molecules so it doesn't burn globally; thus producing CO. As the reason for CO, the resultant is that CO₂ decreases, as the hydrogen excess is burnt off to H₂O.

Due to the greater fuel the flame temperature will greaten until stoichiometric where it is highest thus, encouraging the O₂ dissociation from CO₂ and H₂O; creating NO_x. As the FER

greatens so does the CO_2 and H_2O molecules, further exacerbating the dissociation into NO_x , until there isn't enough O_2 .

2.6. Average temperature

To gain the average temperature that is in the cylinder the ideal gas law is used;

$$T_{AVG}(K) = \frac{PV}{MR} = \frac{P_1 \times V_1}{M_{total/cyl} \times R}$$

Equation 16

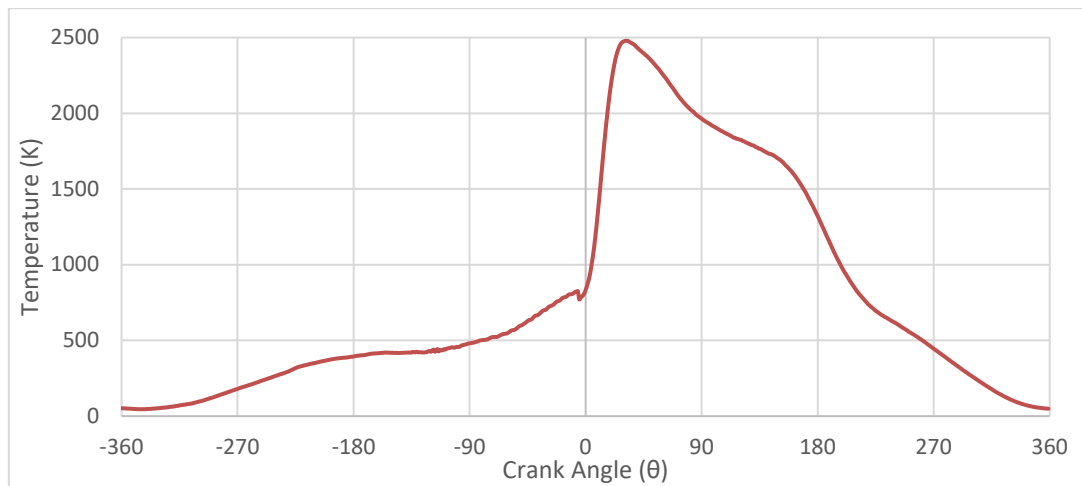


Figure 5 Average in-cylinder temperature

The dip in the trace is due to the gas constant changing at the SOC from ' $R_{unburned}$ ' to ' R_{burned} ', this results in a lower temperature value, due to the lower molecular weight of the products from combustion. So the dip in temperatures should be disregarded. It is clear to see where the exhaust valve opens from the rapid loss in heat after combustion. This could also be used as a basic single zone model.

2.7. Unburned zone

Up until SOC the same temperature from Equation 16 is used. After SOC Equation 17 should be employed to the temperature of the unburned zone. Where Gamma is variable to each previous temperature and the FER used at that RPM. From the adiabatic relation (Merket, Schwarz, stiesch, & Otto, 2006);

$$T_{unburned}(K) = T_1 \left(\frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}}$$

Equation 17

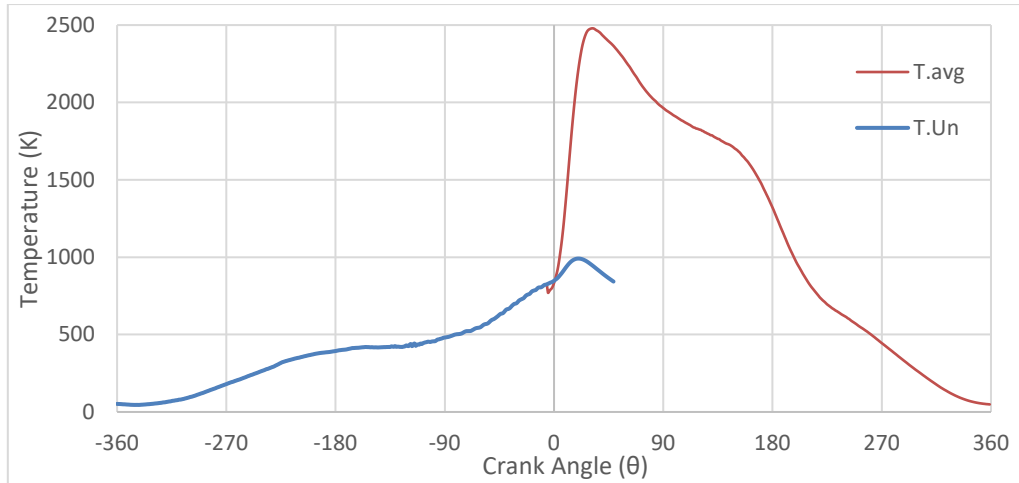


Figure 6 Temperature unburned against temperature average

The temperatures also need to be relative to a real engine where they need to be less than 1200K to prevent auto ignition of the unburned zone (Merket, Schwarz, stiesch, & Otto, 2006). Whilst the model assumes a rapid rise in temperature. Shown in the unburned zone as it gains temperature with the flame front until after the peak temperature from the burned zone, it starts cooling as the volume of unburned gets smaller whilst the piston motion downwards is increasing volume, until the rapid decrease of when the exhaust valve is opened.

The unburned volume uses MFB which is sensitive to the polytropic index for precision. By finding the unburned mass in the zone, using the MFB for the mass left in the cylinder. By continuing to use the ideal gas law;

$$V_{unburned}(cc) = \left(\frac{(1 - MFB) \times M \times R_{un} \times T_{un}}{P} \right)$$

Equation 18

2.8. Burned zone

As the flame front is propagating, burning the mass of the mixture in the cylinder, the volume of which is found by;

$$V_{burned}(cc) = V - V_{unburned}$$

Equation 19

The temperature of the mixture propagating over the burned volume is gained by;

$$T_{burned}(K) = \frac{P \times V_{burned}}{MFB \times M \times R_{burned}}$$

Equation 20

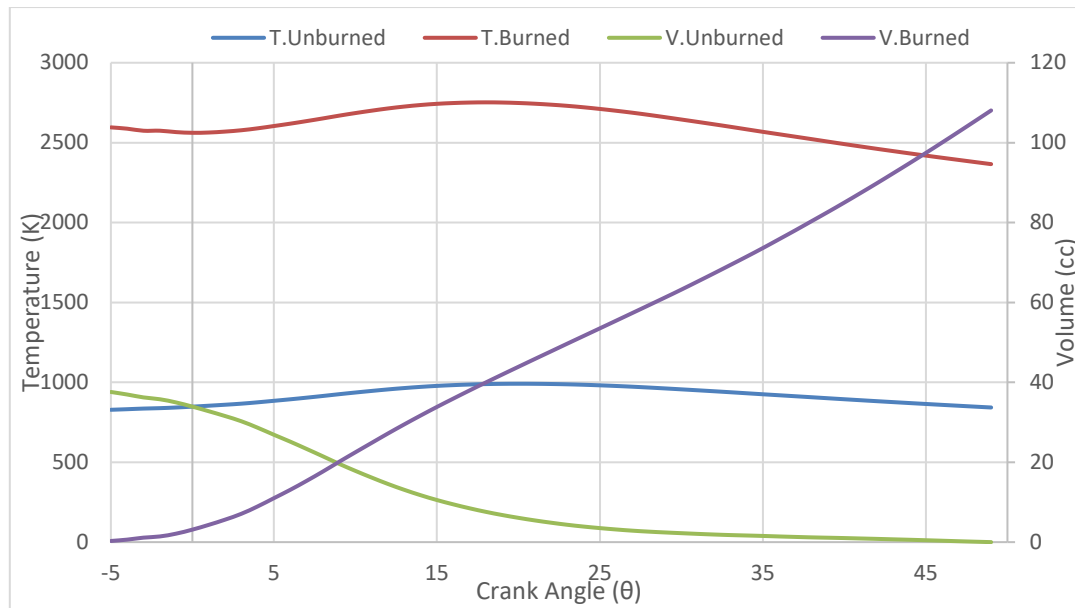


Figure 7 Two zone temperatures and volumes

The peak temperature of the burned zone is 2752.2K, 18 degrees ATDC whilst unburned zone is 991.2K at 15 degrees ATDC, the delay between the two zones is due to the internal heat transfer. Whilst the unburned temperature is peak when the pressure is highest in the cylinder. The volume of the unburned zone is the volume of the mixture at the point of SOC (seen at 37.6cc), whereas the volume of the burned zone continues to increase past this volume as the piston moves down increasing overall volume until EOC (seen at 108.1cc).

The model assumes rapid rise in pressure from SOC, this increases the unburned zone temperature by an adiabatic compression; in the burned zone it is similar from adiabatic expansion.

2.9. Burned temperature correction

When carrying out the calculations for burned temperatures from Equation 20, it's shown that up to the first 12 degrees of combustion are not realistic; at lower RPM's this is intensified. This is a calculation error from MFB, this could be a result of the determination of SOC. As in the equation the denominator has two constants of the mass and gas, so this changes with the MFB, whereas the numerator changes with the cylinder pressure and burned volume. As the values are so small at SOC, this exacerbates the problem and results in a high temperature value, only until the values start to get larger does it begin to result in realistic temperatures. This is shown in Figure 8, where varying RPM's of the FOX engine, however as the RPM increases there is a larger mass at the start hence the lower first few degrees.

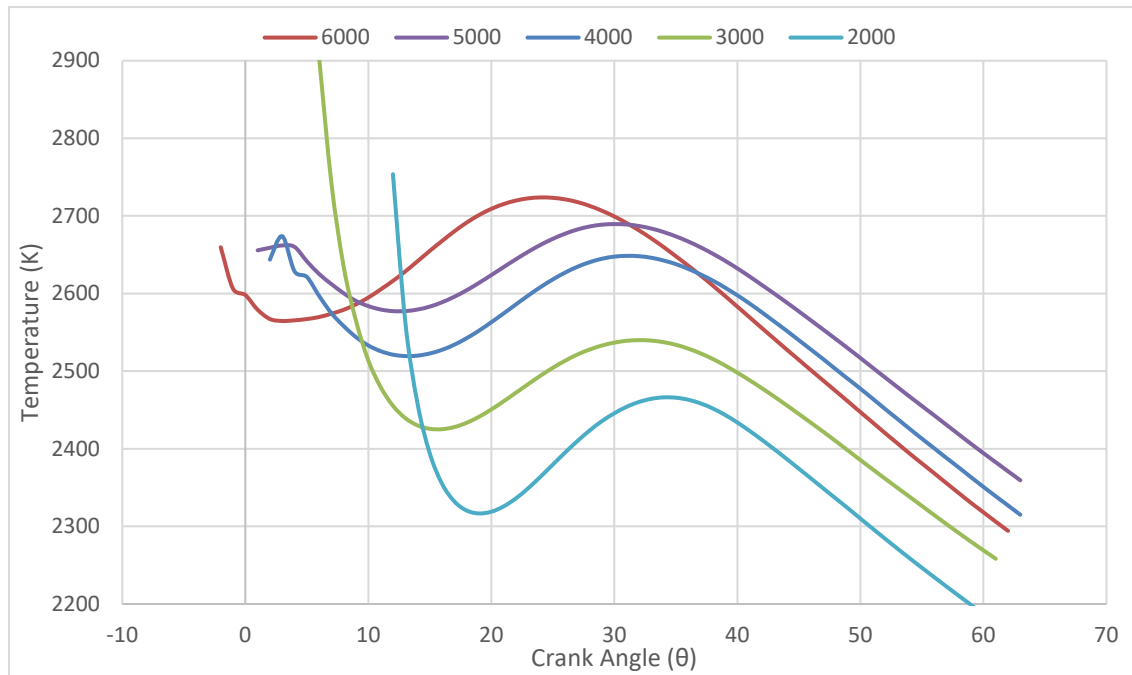


Figure 8 SOC burned temperatures for varying RPM's

Whilst the author tried the Rassweiler and Withrow, Isermann and Muller methods, they showed slightly varying results but would still result in a discrepancy in the SOC temperature. An alternative method was used to change the immediate temperature by means of a trend line fitting too the slope of the curve.

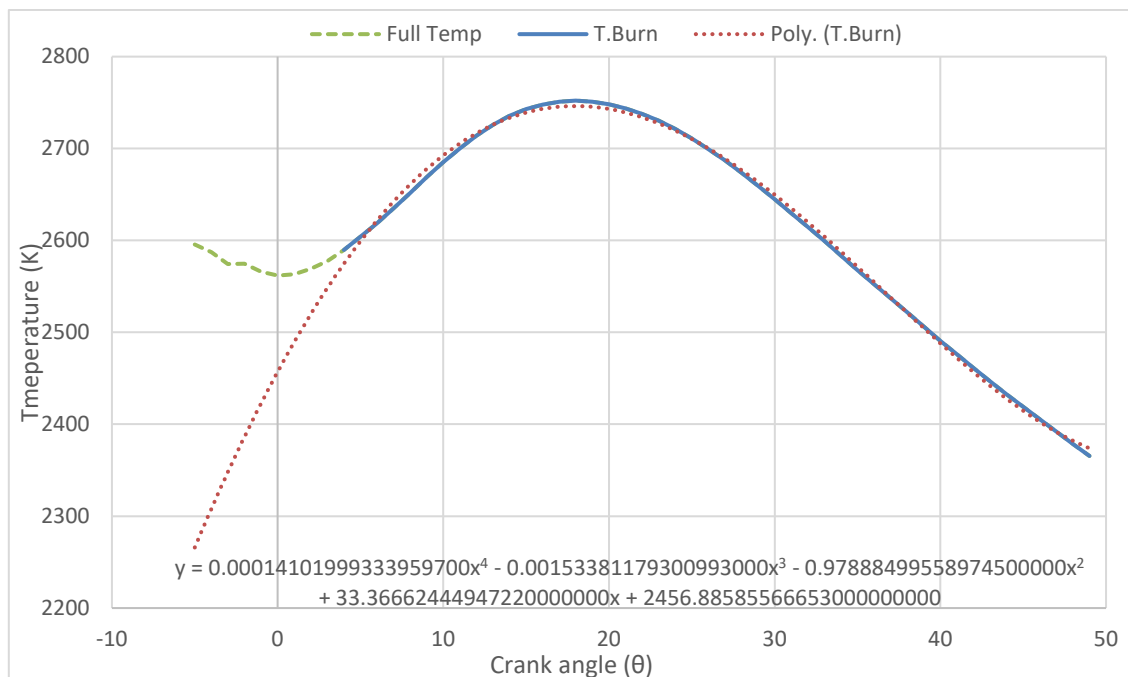


Figure 9 Polynomial temperature curve fitting for burned correction

Using a fourth order polynomial to fit the curve by taking the temperature values until greater realism shown as the blue trace (T.Burn), where the green dashes are the full calculated

burned zone temperatures. The polynomial trace is shown to represent the rapid rise in temperature and showing rapid flame propagation through the burned zone.

The polynomial is seen to result in less peak temperature by 6 Kelvin at 6500RPM which is negligible and slight variation in later temperatures as the volume is expanding, the values will be averaged out as it is the variation is seen to be less than 0.0022%. This method gives a greater realism for the models NOx production as the temperatures are critical for accuracy. Both methods results will be compared to show the accuracy to the engine data provided.

2.10. Variable gamma

The variable gamma is dependent on temperature and FER. As used for the unburned temperature calculation, the gamma changes as the temperature does and, the FER will stay constant for each RPM. The gamma will change from each degree, and will be used for the next temperature calculation as used in Equation 17.

2.10.1. Molar specific heat of species

Using the polynomial that was used by Heywood and NASA plotted against temperature; so that by using a lookup function can easily be used to find the correct value needed. This would be used to find the value of the specific heat at a constant pressure of the products of combustion.

Table 2 Molar specific heat for species, polynomial values. (Heywood, 1988)

Species	Temperature (K)	a_{i1}	a_{i2}	a_{i3}	a_{i4}	a_{i5}
CO2	1000-5000	4.46E+00	3.10E-03	-1.24E-06	2.27E-10	-1.55E-14
H2O	1000-5000	2.72E+00	2.95E-03	-8.02E-07	1.02E-10	-4.85E-15
CO	1000-5000	2.98E+00	1.49E-03	-5.79E-07	1.04E-10	-6.94E-15
H2	1000-5000	3.10E+00	5.11E-04	5.26E-08	-3.49E-11	3.69E-15
O2	1000-5000	3.62E+00	7.38E-04	-1.97E-07	3.62E-11	-2.89E-15
N2	1000-5000	2.90E+00	1.52E-03	-5.72E-07	9.98E-11	-6.52E-15

$$\hat{C}_{pi} = (a_{i1} + (a_{i2} \times T) + (a_{i3} \times T^2) + (a_{i4} \times T^3) + (a_{i5} \times T^4)) \times Ru$$

Equation 21

2.10.2. Molar specific heat of Gasoline

Using the specific heat for the fuel (vapour phase), and fitting to a polynomial for temperature.

Table 3 Molar specific heat of Gasoline, polynomial values. (Heywood, 1988)

Fuel	Formula	Af1	Af2	Af3	Af4	Af5
Gasoline	C8.26H15.5	-24.078	256.63	-201.68	64.75	0.5808

Where; T = Temperature (Kelvin)

$$t = \frac{T}{1000}$$

$$\hat{C}_{p fuel} = \left(A_{f1} + (A_{f2} \times t) + (A_{f3} \times t^2) + (A_{f4} \times t^3) + \left(\frac{A_{f5}}{t^2} \right) \right) \times 4180$$

Equation 22

Where the result polynomial value is in cal/gmol.K it is multiplied by 4180, to be used in the model to J/Kmol.K. The results are tabulated to enable easy lookup.

2.10.3. Specific heats of mixture

$$C_{p \text{ mixture}} = \frac{\hat{C}_{p fuel} + 12.135 \times (\hat{C}_{p iO_2} + (3.76 \times \hat{C}_{p iN_2}))}{1 + (12.135 \times 4.76)}$$

Equation 23

To find the specific heat ratio (γ), the following was used (Ferguson & Kirkpatrick, 2001);

$$C_{v \text{ mixture}} = C_{p \text{ mixture}} - Ru$$

$$\text{Specific heat ratio } (\gamma) = \frac{c_p}{c_v}$$

Equation 24

As the heat increases, gamma increases as it is proportional to heat; due to the increased mass and having more molecules and increased density so that the modes of freedom are of greater difficulty. As the variable gamma changes with the FER, resulting in a change to the equation shown also in Appendix C;

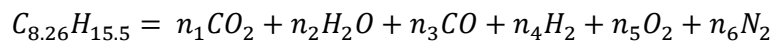
$$\gamma_{variable} = \frac{\left(\frac{(\hat{C}_{p fuel} \times \varphi) + 12.135 \times (\hat{C}_{p iO_2} + (3.76 \times \hat{C}_{p iN_2}))}{\varphi + (12.135 \times 4.76)} \right)}{\left(\frac{(\hat{C}_{p fuel} \times \varphi) + 12.135 \times (\hat{C}_{p iO_2} + (3.76 \times \hat{C}_{p iN_2}))}{\varphi + (12.135 \times 4.76)} \right) - 8314}$$

Equation 25

3. Oxygen content

The oxygen content is variable to the temperature and pressure. As the pressure increases the O_2 molecules decrease furthermore, it is seen that the oxygen molecules increase as the temperature rises. This is a result of the reaction rate constant of CO_2 and H_2O , and the resultant of a greater disassociation at increased temperatures.

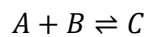
The products of combustion are given 'n' values. As the values for O_2 are of particular interest, these are noted as ' n_5 ' and used further more in this report. As the Gasoline equation becomes;



Equation 26

3.1. Reaction rate constants

As temperatures increase in the combustion chamber above 2000K, the thermal agitation of the products increases the rate of dissociation back to the original reactant state. "Increasing the temperature from 1473K to 2273K increases the rate of this reaction by a factor of 10,000", (P.G. Boulter, 2012). By considering a simple equation for reversibility from combustion;



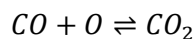
Equation 27

At these higher temperatures a dynamic equilibrium is present with the equivalent rates of combustion and dissociation. This means that the reactant and product materials coexist in proportions that remain constant. (Goodger, 2000) The constant can be defined as;

$$K_c = \frac{[C]}{[A][B]}$$

Equation 28

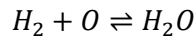
Following this for the oxidation of CO_2 ;



$$K_{CO_2} = \frac{[CO_2]}{[CO][O]}$$

Equation 29

With the same process for H_2O ;



$$K_{H_2O} = \frac{[H_2O]}{[H_2][O]}$$

Equation 30

As the oxygen is proportional;

$$[O] \propto [O_2]^{0.5}$$

Equation 31

It is logical that the dissociation is of a wider scale with different radicals such as O, H, OH, and NOx. Although computational time and complexity in greatly increased, for simplicity the first calculation it is kept to only CO, H₂ and O₂. This allows calculations to continue for Equation 29 and, deriving the equations further to give the tabulated results of the constants in Appendix D. The resultant equation for CO₂;

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

Equation 32

For H₂O;

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

Equation 33

3.2. Goal seek

By using the goal seek method in excel to find the correct value on the 'n₅' values, the computing time was less than a second per temperature as the method uses a guess cell. Using reaction rate constant of CO₂ and H₂O. The calculation steps are as follows; an assumed value is used to start calculations i.e. 0.001;

$$\text{Assumed value} = \frac{n_5}{n_{Total}}$$

Equation 34

By adding pressure and evaluating;

$$\left(P \times \frac{n_5}{n_{Total}} \right)^{0.5}$$

Equation 35

Multiply by the reaction rate constant of CO₂/ H₂O to gain the carbon/hydrogen balance;

$$\text{Carbon balance} = \frac{n_1}{n_3} = K_{CO_2} \times (P \times \frac{n_5}{n_{Total}})^{0.5}$$

Equation 36

$$\text{Hydrogen balance} = \frac{n_2}{n_4} = K_{H_2O} \times (P \times \frac{n_5}{n_{Total}})^{0.5}$$

Equation 37

To find CO or H₂ in the exhaust;

$$n_3 = \frac{\text{Total Carbon in mixture}}{\text{Carbon balance} + 1}$$

Equation 38

$$n_4 = \frac{\text{Total Hydrogen in mixture}}{\text{Hydrogen balance} + 1}$$

Equation 39

To find the CO₂ or H₂O in the exhaust;

$$n_1 = \text{Total carbon in mixture} - n_3$$

Equation 40

$$n_2 = \text{Total carbon in mixture} - n_4$$

Equation 41

To find the total O₂ (n₅) in the exhaust;

$$n_5 = \frac{(\text{Total Oxygen} - (2 \times n_1) - n_2 - n_3)}{2}$$

Equation 42

Then a summation of the 'n' values gives the total in the exhaust; 'n₆' stays constant from the mixture that is in cylinder;

$$n_T = n_1 + n_2 + n_3 + n_4 + n_5 + n_6$$

Equation 43

To find the correct values for all the 'n' values a check column was used; it should represent the total molecules in the exhaust dependant on FER;

$$\text{Check value} = \frac{n_5}{n_T}$$

Equation 44

The goal seek method was used in an ERROR column to gain zero, the parameter was that the assumed value should be the same;

$$\text{Assumed value} - \text{Check value} = 0$$

$$\therefore \text{Assumed value} = \text{Check value}$$

With this understood, the ERROR column would find zero by means of the goal seek function and, go under many iteration calculations whilst the linked cells would change the value of each 'n' value simultaneously. Excel uses a standard iteration count of 100, with a maximum change 0.001 from the guess cell. This provided usable results. To ensure further accuracy was gained, the maximum iteration count raised can be raised to 32,767 and a maximum change of 1×10^{-10} .

	Pressure	10		[Equ.7] C bal	[n3]	[n1]	H2O balance	[n4]	[n2]	[n5]	[n6]	[nT]	CHECK	
	Guess (n5/nT)	P.n5/nT	(P.n5/nT)*0.5	kcO2*(P.n5/nT)*0.5 + [n3]=T.C/([7]+1)	[n1] = T.C - [n3]	kh2O*(P.n5/nT)	[n4]=T.H/([n2]/[n4])	[n2]=T.H-[n4]	[n5]=[O-2]/[n6]	[nTotal]	[n5]/[nT]	ERROR		
2000	0.001028995	0.01028995	0.0101439375	77.66198575	0.105006248	8.154993752	351.6903143	0.021973952	7.728026048	0.0634901	45.6276	61.70109	0.001029	-1E-10
2100	0.001723333	0.01723333	0.0131275762	45.41353706	0.177965321	8.082034679	221.4097	0.034845603	7.715154397	0.1064055	45.6276	61.74401	0.001723	-1E-10
2200	0.002743873	0.02743873	0.0165646413	27.87332193	0.286077231	7.973922769	144.9372985	0.053104998	7.696895002	0.1695911	45.6276	61.80719	0.002744	-1E-10
2300	0.004178824	0.04178824	0.0204421713	17.80451798	0.439256141	7.820743859	98.29413669	0.078050933	7.671949067	0.2586535	45.6276	61.89625	0.004179	-1E-10
2400	0.006102703	0.06102703	0.0247036502	11.7967341	0.645477193	7.614522807	68.53533685	0.111454123	7.638545877	0.3784657	45.6276	62.01607	0.006103	-1E-10
2500	0.008573795	0.08573795	0.0292810428	8.064877622	0.911209213	7.348790787	49.04281861	0.154867376	7.595132624	0.5330383	45.6276	62.17064	0.008574	-1E-10
2700	0.015306255	0.15306255	0.0391232089	4.049643352	1.635759087	6.624240913	26.63390691	0.280452562	7.469547438	0.9581058	45.6276	62.59571	0.015306	-1E-10
3000	0.029250485	0.29250485	0.0540837176	1.652203489	3.1143915	5.1456085	11.91410215	0.60011915	7.14988085	1.8572553	45.6276	63.49486	0.02925	-1E-10

Figure 10 A visual representation of the n5 calculation with goal seek

The calculations shown that the 'n5' levels are dependent on pressure. Where oxygen content post combustion is greater at lower pressures than at high pressures. At lower pressures the NOx productions is greater given the same temperature as the higher pressure as N₂ levels stay constant due to higher oxygen present. As engine functions main use of the negative work done is to compress a volume, as a result increase pressure which is proportional to the increase in heat. This meaning that it will never stay at a constant pressure or volume, whereas this model will assume at a specified degree this is the case as calculations will be made at each degree interval.

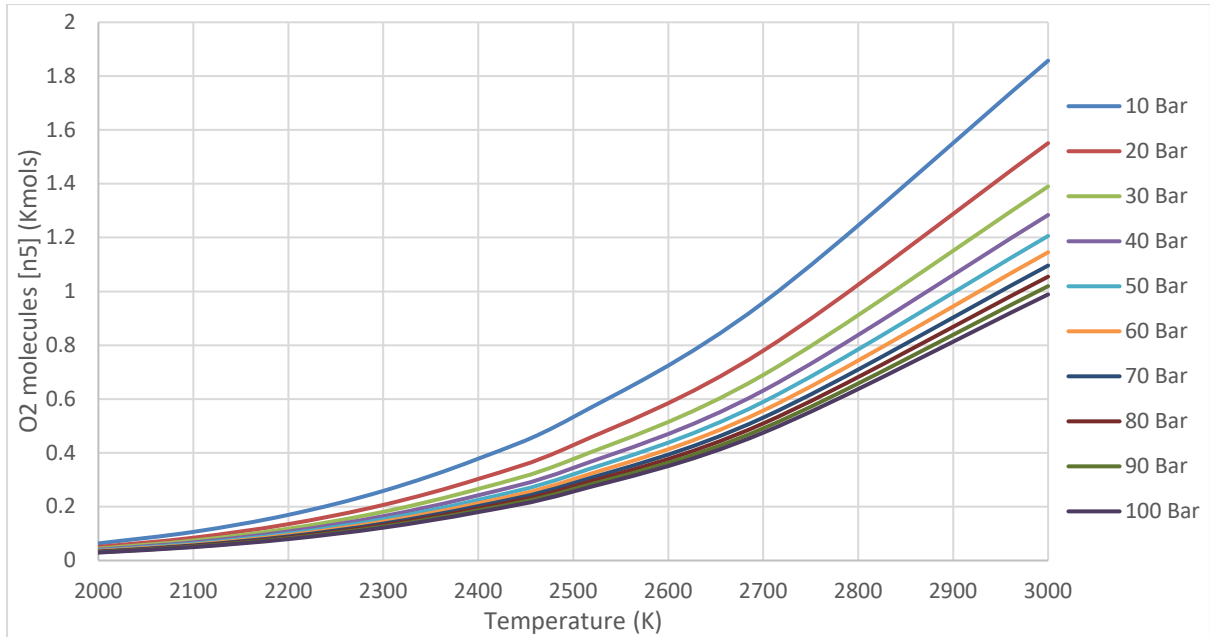


Figure 11 O₂/n₅ values shown at 10 bar intervals after combustion at FER 1.00

The values can be tabulated further at each 5 bar interval, this is seen to have the best medium of calculation time versus accuracy rather than 10 bar intervals. These are further tabulated and shown in Appendix E.

	Fuel Equivalence ratio - 1.00										
	10	20	30	35	40	45	50	55	60	65	
2000	0.0634901	0.050465244	0.044116576	0.041917205	0.040100456	0.038563159	0.037237799	0.036077992	0.035050619	0.034131284	0.033301545
2100	0.106405462	0.084663957	0.074050243	0.070370835	0.067330558	0.064757253	0.062538208	0.060595964	0.058875199	0.057335151	0.055944999
2200	0.169591115	0.135148417	0.118295299	0.112446932	0.107612132	0.103518292	0.099986832	0.096894961	0.094154947	0.091702123	0.089487572
2300	0.258653537	0.206583727	0.181020184	0.172136002	0.164786409	0.158559563	0.153185448	0.148478265	0.14430518	0.140568227	0.137193269
2400	0.378465658	0.303203703	0.266083596	0.253156788	0.242452585	0.233376307	0.225537597	0.218667584	0.212573878	0.207114479	0.202181853
2500	0.533038294	0.428766344	0.377023995	0.358956134	0.343975678	0.331259896	0.320267891	0.310626666	0.302068789	0.294396989	0.287461548
2600	0.718105825	0.579619518	0.506848348	0.477605569	0.4531360382	0.4328881182	0.415397309	0.399978841	0.386203123	0.373844789	0.362695825
2700	0.958105825	0.779619518	0.68483348	0.637760569	0.600881182	0.572267841	0.546334879	0.52267841	0.500958425	0.480869846	0.46195263
2800	1.257255325	1.00921762	0.889969841	0.822279759	0.76845707	0.72298418	0.68456819	0.651740162	0.623177127	0.598541974	0.576558357
2900	1.657255325	1.350921762	1.189969841	1.102279759	1.03845707	0.98456819	0.939740162	0.89456819	0.858541974	0.821541974	0.784541974
3000	2.157255325	1.750921762	1.549969841	1.422279759	1.33845707	1.27456819	1.220740162	1.17656819	1.141541974	1.11541974	1.096054495

Figure 12 n₅ values at each 5 bar intervals up to peak pressure

3.3. Bilinear interpolation

A polynomial was thought to be used as the pressure and temperature is so variable from each degree to degree. As an automatic model for calculating the 'n₅' levels, the two polynomials took too much processing time and, would process a slower result. A 6th order polynomial wasn't seen to always follow the graph trace and as a result provide incorrect values. This hindered the sensitivity analysis of adjusting the polytropic index and MFB. The model needed to use a different method that pinpointed with use of the two variables. So bilinear interpolation was used, which used four 'n₅' sites and interpolated four ways to ensure an accurate value.

Using bilinear interpolation, it uses four directions of linear interpolation to gain the end result of 'n₅' denoted 'P' in Equation 45. This method uses the temperature range given by the

constants for CO₂ and H₂O, with 5 BAR intervals. A lookup function can be used with the higher and lower values for each X and Y axis.

$$P = \frac{(x_2 - x)(y_2 - y)}{(x_2 - x_1)(y_2 - y_1)} Q_{11} + \frac{(x - x_1)(y_2 - y)}{(x_2 - x_1)(y_2 - y_1)} Q_{21} \\ + \frac{(x_2 - x)(y - y_1)}{(x_2 - x_1)(y_2 - y_1)} Q_{12} + \frac{(x - x_1)(y - y_1)}{(x_2 - x_1)(y_2 - y_1)} Q_{22}$$

Equation 45

As a visual aid, where each 'Q' value will be used from the 'n₅' table, and the lookup code in Appendix F, will follow and calculate the P value, to give a precise 'n₅' value at each pressure and temperature target.

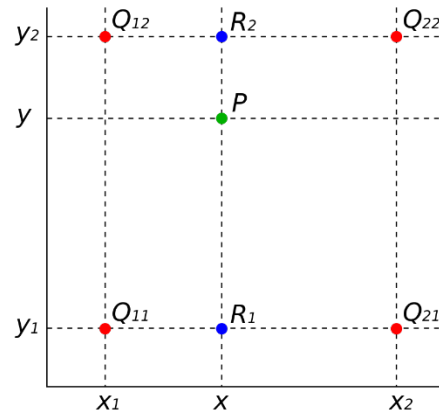


Figure 13 Bilinear interpolation representation (Supercomputing, 2017)

4. Extended Zeldovich mechanism (EZM)

To find the amount of Kmols in the cylinder, as the fuel mass is known and the FER, it can be found by alpha as;

$$\alpha = \frac{\text{Fuel mass in cylinder}}{\phi * ((8.26 * 12) + 15.5)}$$

Equation 46

Total Kmols of mass in the exhaust including EGR is found by;

$$\text{Total in exhaust} = (n_T \times \alpha) \times \left(1 + \left(\frac{\text{EGR}\%}{100} \right) \right)$$

Equation 47

Concentration of O₂ molecules (Kmols/m³) are found by;

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

Equation 48

Concentration of N₂ molecules (Kmols/m³) are found by;

$$[N_2] = \frac{(45.6276 \times \alpha \times MFB)}{V_b}$$

Equation 49

To find the rate of NOx production (Kmols) per second, it is found by;

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

Equation 50

Converting to per degree, then per volume that has been burned thus, giving the NOx concentration in the cylinder for each degree (Kmols/m³/degree);

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

$$NOx \text{ Kmols/degree} = \frac{d[NO]}{d\theta} \times V_b$$

Equation 51

To get the total NOx production (PPM) over combustion. It is a summation of the NOx production from SOC to EOC thus;

$$NOx \text{ PPM} = \left(\frac{NOx \sum SOC \rightarrow EOC}{Total \text{ Kmols in exhaust inc EGR}} \right) \times 10^6$$

Equation 52

For later calculations, where NOx up to peak temperature is compared;

$$NOx \text{ PPM} = \left(\frac{NOx \sum SOC \rightarrow T_{peak}}{Total \text{ Kmols in exhaust inc EGR}} \right) \times 10^6$$

Equation 53

4.1. Super Extended Zeldovich Mechanism (SEZM)

A variation on the reaction scheme was researched by Ford Motor Company, resulting in the 'Super Extended Zeldovich Mechanism'. It consisted of 67 reaction kinetics and 13 chemical species (O, O₂, OH, H, N₂, N, NH, NH₂, NH₃, HNO, H₂O, NO₂ and NO). The results were seen to predict NOx emissions within 10% of engine data. By using the first three principle reactions that primarily control the production of thermal NOx; where 'K_f' the forward reaction rates.

Table 4 Zeldovich first three thermal NOx reaction rates

R1	$N_2 + O \leftrightarrow NO + N$	$k_{f1} = 1.8 \times 10^{14} \exp\left[-\frac{38370}{T}\right]$
R2	$N + O_2 \leftrightarrow NO + O$	$k_{f2} = 1.8 \times 10^{10} T \exp\left[-\frac{4680}{T}\right]$
R3	$N + OH \leftrightarrow NO + H$	$k_{f1} = 7.1 \times 10^{13} \exp\left[-\frac{450}{T}\right]$

As the Zeldovich takes the first reaction as the main reaction, as this is the most common element present in combustion. Ford Motor Company found that both SEZM and EZM assume a C-H-O radical pool whilst not factoring in reverse reactions with the effects of pressure on density. As this isn't modelled, a modified first reaction is used to introduce the effects of pressure. (Miller, Davis, Lavoie, Newman, & Gardner, 1998)

Table 5 Modified first reaction

R1M	$N_2 + O \leftrightarrow NO + N$	$k_{fR1M} = C_p \times 1.8 \times 10^{14} \exp\left[-\frac{38370}{T}\right]$
-----	----------------------------------	--

Where 'Cp' is a co-efficient for pressure and these values are found by empirical means. The in-cylinder pressure (BAR) denotes what value should be used for 'Cp';

Table 6 Pressure co-efficient for parametrization

Cp	In-cylinder pressure
1	<15
0.7	15-20
0.48	20-25
0.31	25-30
0.25	30-35
0.2	>35

As the pressure is the parameter that changes the co-efficient and whilst the effect it makes is still unclear. The author is concerned that the affect is a result from the oxygen constant. As the O2 is disassociated to O radicals this is a constant, where if the pressure is doubled therefore the reaction rate for O2 is doubled, but the O rate is quadrupled. So as the pressure gets considerably higher under compression and combustion,

the reverse reaction back to the left is far greater than that to the right. So meaning the probability of NOx production at higher pressures is lower with denser mixtures than that to a large volume with low density.

4.2. Reverse reactions

The thermal NOx has been shortly described before, as it is the formation of NOx that is a result of the flame front and temperatures found within combustion. There are three principle reactions, these are contained within TABLE4 as R1, R2 and R3. This giving the extended Zeldovich mechanism by (Baulch et al, 1994) also documented further by (Heywood, 1988).

Expanding on similar equations similar to Equation 28. Where the equation is fitted towards the first principle reaction 'R1'; where, 'r' denotes forward reaction and 'l' denotes reverse reaction;

$$k_{1,r}[O][N_2] = k_{1,l}[NO][O]$$

Equation 54

By changing to give the reaction rate constant;

$$\frac{k_{1,r}}{k_{1,l}} = \frac{[NO][N]}{[O][N_2]} = K_{C,1}$$

Equation 55

With this known, all three principle reactions can be included to give a NOx formation rate;

$$\frac{d[NO]}{dt} = k_{1,r}[O][N_2] + k_{2,r}[N][O_2] + k_{3,r}[N][OH] - k_{1,l}[ON][N] - k_{2,l}[NO][O] - k_{3,l}[NO][H]$$

Equation 56

The reverse reactions have been ignored from Equation 52, as the radical pool of O, H and C have greater reaction speeds, this would result in greater complexity of a model thus greater calculation times. So O radical have been used as below to result in the NOx formation rate given in Equation 52;

$$[O] = 0.13[O_2]^{0.5} \exp\left(\frac{-29,468}{T}\right)$$

Equation 57

As after the peak temperature the piston motion is lowering consequently increasing volume, hereby lessening the density and as a result the burned zone temperature is lowering. The reason for reverse reactions is that with longer period of higher temperatures (above 2000K) there is more time for a reverse reaction, hence lowering NOx values.

“This equation can, however, only be seen as a crude estimation, as it predicts an excessively high NO concentration. The reason for this is that the – no matter how minimal – reverse reactions of equations (1) to (3) slow down actual NO production and can even lead to a minor reduction of NO concentrations towards the end of the working cycle” (Merket, Schwarz, stiesch, & Otto, 2006)

The NOx predictions are seen to exhibit higher values of NOx production, these reverse reactions will need to be considered if the predictions are to be of greater accuracy. In real

engine, there would be freezing of the NO_x formation if there is rapid temperature loss, but also reverse reactions, this is one of the major indicators for accuracy that will need to be considered for future work. (Heywood, 1988)

4.2.1. Arrhenius equation

For a further understanding of Equation 52, it is explored further and derived. A reaction cannot start if the collision between 'N₂' molecule and 'O' atom doesn't provide enough activation energy, thus to atomise 'N₂' to start a reaction it needs a certain activation energy. To get the molecules/atoms to have a greater energy than that of the activation energy the Arrhenius function is used; Where k = rate constant, A = constant/pre-exponential factor, E_a = activation energy, R = gas constant, T = temperature (Merket, Schwarz, stiesch, & Otto, 2006);

$$k = Ae^{\left(\frac{-E_a}{Ru.T}\right)}$$

Equation 58

So the higher the temperature, the faster a given chemical reaction will proceed. This relationship between the rate a reaction proceeds and its temperature is determined by the Arrhenius Equation. At higher temperatures, the probability that two molecules will collide is higher. This higher collision rate results in a higher kinetic energy, which has an effect on the activation energy of the reaction. The activation energy is the amount of energy required to ensure that a reaction happens. The function is detailed greater in Appendix G. (Burton, 2017)

5. NOx predictions

Combustion emissions are oxygen, carbon dioxide, water/steam and nitrogen as detailed in Section 2.5. Where an incomplete combustion is present the added emissions are nitric oxides, carbon monoxide and unburnt hydrocarbons. All of these emissions are monitored for engine efficiency, as under the EU regulations NOx, CO, HC and CO₂ are monitored closely. As hydrocarbons and CO are mainly a result of FER greater than 1 ($\lambda < 1$). The NOx emissions are seen to be harmful to human health.

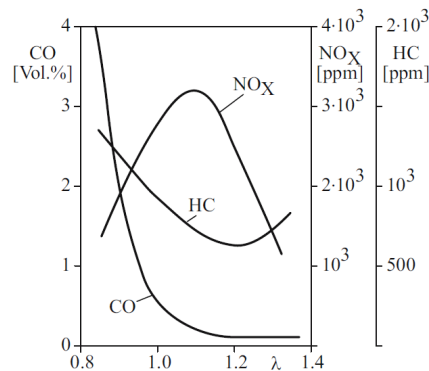


Figure 14 Engine out emissions shown over lambda (Merket, Schwarz, stiesch, & Otto, 2006)

In particular NOx has a greater chance of production in locally lean areas, and in a rich mixture where high temperatures are present with sufficient oxygen conversely due to the extended periods of high temperatures, the NOx may have a reverse reaction back to nitrogen and oxygen. From the two zone model, and the use of bilinear interpolation of the oxygen content and the EZM, producing a NOx prediction shown in Figure 15.

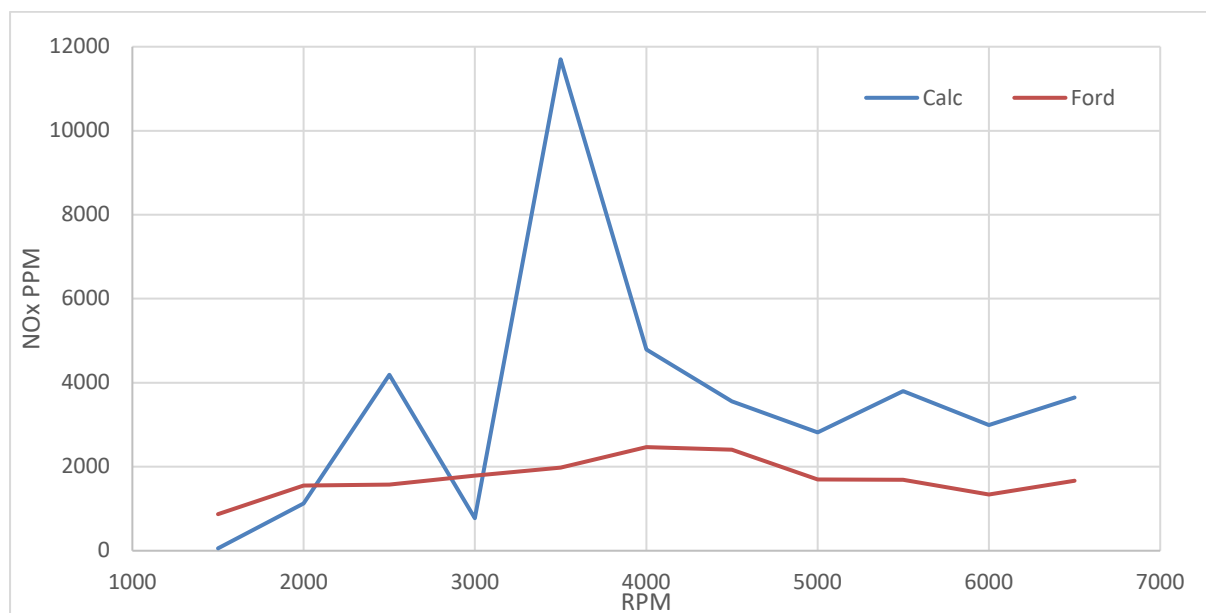


Figure 15 NOx prediction SOC to EOC

Using the EZM from SOC to EOC at each rpm and shown against Ford's engine data in Figure 15, the first thing seen is that the spike at 3500RPM and smaller spike 2500RPM; This is an error in the data that is to be explored further. The EZM is seen to over predict at higher RPM. At lower RPMs it is under predicting by 34% at 2000RPM, and 120% at 3000RPM. When over predicting at 2500, 4000 and above RPM, it is more than 55%. These results aren't ideal for tackling in cylinder NOx nor as an ideal model for NOx prediction.

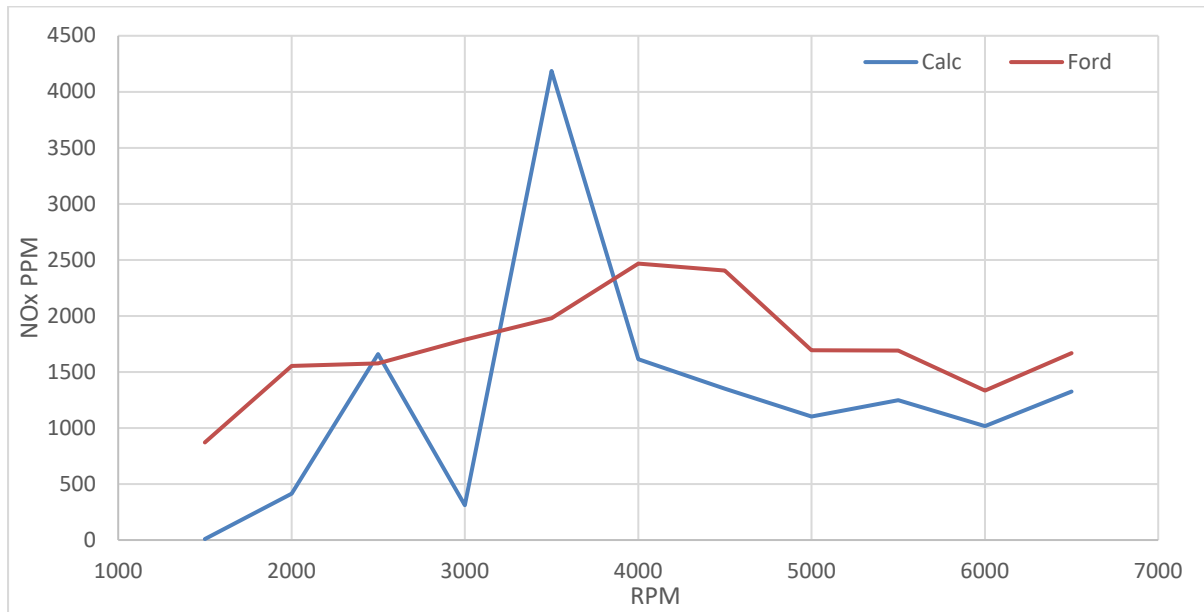


Figure 16 NOx prediction SOC to Peak temperature

This method is seen to under predict NOx up to 83%. As the engine is rich at FER of 1.087, 1.11 at 5000RPM and 6000RPM respectively, the under prediction is 35% and 24%; at 6500RPM the under prediction is 20.5%. This is a result of the rich mixture meaning a greater chance of a complete burn. As the engine is direction injection only some of the fuel is completely mixed homogeneously at all RPM's and especially at lower FER and RPM, this creates lean patches locally and globally thus increasing NOx. If the engine is running richer the local mixture has a greater chance to be homogeneous and burn stoichiometric. The mixing is intensified by the increasing RPM of the engine as the piston speed is higher causing more turbulence in the combustion chamber but on the other hand the time for mixture formation is too short to secure a sufficient mixture quality resulting in more NOx. (Miller, Davis, Lavoie, Newman, & Gardner, 1998)

A different method was taken to find the NOx prediction, from SOC up to peak burned temperature and the NOx results shown against Ford's measured data in Figure 15. As there is always a chance of NOx freeze discussed in Section 4.2. So the values above are the minimum predicted and may increase after "freeze" NOx formation takes place.

Upon further investigation for the 3500RPM anomaly, the engine data was examined. It was found there is a discrepancy in the recorded data shown in Figure 17. The data shows that all RPM are within 1 revolution of the target speed whereas at 3500RPM at full load, it is shown as 3251RPM, as reduction of 249RPM.

DYNO SPD rpm	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		997	1250	1500	1750	1999	2249	2500	3000	3251	3999	4500	5000	5500	6001	6500
200						2000	2250	2499	3000	3500						
190						1999	2250	2501	2999	3499						
180					1750	2000	2250	2499	3000	3500						
170				1500	1749	2000	2249	2499	3000	3499	4000	4500				
160				1500	1750	2000	2249	2500	3000	3499	3999	4501	5000			
150				1499	1750	2000	2251	2500	3001	3500	4000	4501	5000	5500		
140			1250	1500	1750	2000	2251	2500	3000	3499	4000	4500	5000	5500	6000	
130			1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	
120			1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
110		997	1250	1499	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
100		998	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
90		997	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
80		1000	1249	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
70		998	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
60		999	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
50		1001	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
40	878	1001	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
30	866	1001	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
20	802	1001	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	5999	6499
10	799	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
5	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5499	6000	6500
2	800	1000	1239	1500	1750	2000	2250	2499	3000	3501	4000	4485				

Figure 17 Ford engine data, showing error at 3500RPM at full load

The author thought this may just be a sole case, but through further analysis the reduction was validated at the crank position sensor on the engine which is used for the spark timing shown in Figure 18.

INRPMME_LMP rpm (Signal from CAC / CP In=830)	800	1000	1250	1500	1750	2000	2250	2500	3000	3500	4000	4500	5000	5500	6000	6500
FL		1000	1250	1500	1750	2000	2250	2500	3000	3249	4000	4500	5000	5500	6000	6500
200						2000	2249	2500	3000	3499						
190						2000	2249	2499	3000	3500						
180					1749	2000	2249	2499	3000	3499	4000					
170				1500	1749	2000	2249	2500	3000	3500	4000	4500				
160				1499	1750	2000	2250	2500	3000	3499	4000	4500	4999			
150				1500	1750	2000	2250	2500	3000	3499	4000	4499	5000	5499		
140			1250	1499	1749	2000	2250	2499	3000	3499	4000	4500	5000	5500	6000	
130			1249	1499	1750	2000	2250	2500	3000	3499	4000	4499	5000	5500	6000	
120			1250	1500	1749	2000	2250	2500	3000	3499	4000	4500	5000	5500	6000	6500
110		1000	1250	1500	1750	2000	2249	2500	3000	3500	4000	4500	5000	5499	6000	6500
100		1000	1250	1500	1750	2000	2249	2500	3000	3499	4000	4499	5000	5499	6000	6500
90		1000	1250	1500	1750	2000	2249	2500	3000	3499	4000	4500	4999	5500	6000	6499
80		999	1250	1500	1749	2000	2249	2500	3000	3499	4000	4500	5000	5500	6000	6500
70		1000	1249	1499	1750	2000	2250	2500	3000	3499	4000	4500	5000	5500	6000	6500
60		1000	1250	1500	1750	2000	2250	2500	3000	3499	4000	4500	5000	5500	6000	6500
50		1000	1250	1500	1750	2000	2249	2500	3000	3499	4000	4500	5000	5500	6000	6500
40	884	1000	1250	1500	1750	2000	2249	2500	3000	3500	4000	4500	5000	5500	6000	6500
30	871	999	1250	1499	1749	2000	2250	2500	3000	3499	4000	4500	5000	5500	6000	6500
20	800	1000	1250	1499	1750	2000	2249	2500	3000	3500	4000	4500	5000	5500	6000	6500
10	800	1000	1250	1500	1750	2000	2249	2500	3000	3500	4000	4500	5000	5500	6000	6501
5	800	1000	1250	1499	1750	2000	2249	2500	2999	3500	4000	4500	4999	5499	6000	6500
2	800	1000	1238	1500	1750	2000	2249	2500	3001	3501	3999	4491				

Figure 18 Crank position sensor on engine showing error at 3500RPM

With this information now known, the NOx predictions are adjusted accordingly. Shown below is one high prediction of 165% at 2500RPM and 4000RPM onwards is over predicting. The prediction of NOx up to peak temperature is generally showing a closer prediction; this is especially seen at 4000RPM onwards where the engine data and prediction, have very similar trends.

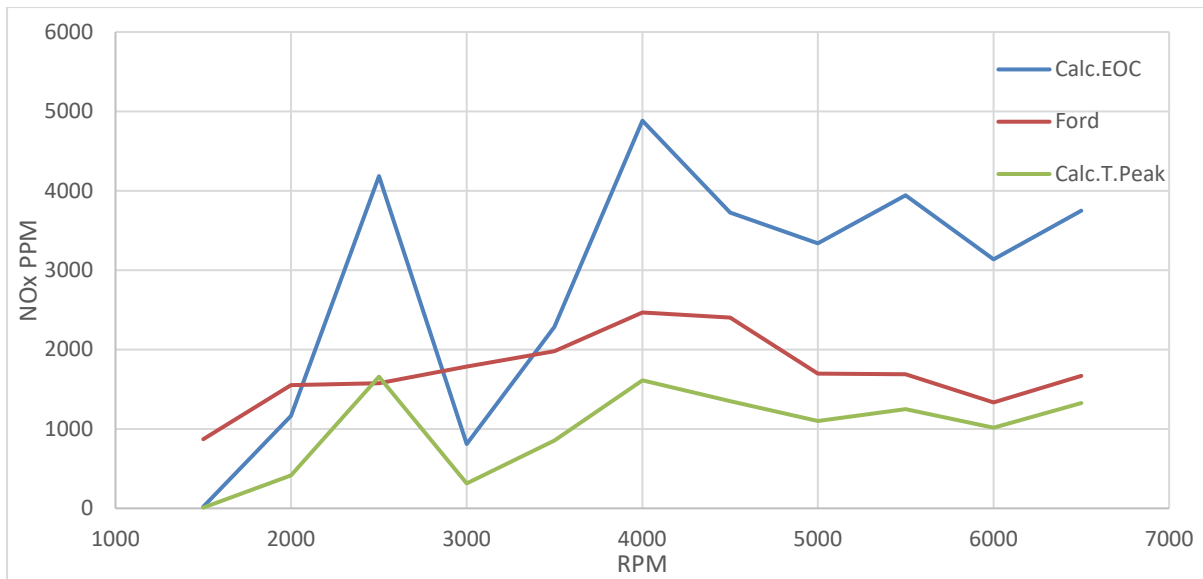


Figure 19 3500RPM fixed NOx prediction with prediction up to peak temperature

Where the under prediction at 3000 with FER is 1.075, it could be assumed where max torque is, there is more fuel to assist the engine produce and maintain peak torque by ensuring a greater change of homogeneous burn from the rich mixture resulting in lower NOx. This is now shown at 3500RPM where the NOx predictions are close to that of the data provided where the prediction is 2286PPM and the Ford data measured 1979PPM, thus the model predicting within 16%.

As the EZM can be seen as a crude estimation and predict high NOx, as stated in section 5.2. It is within a useable accuracy, where some variables have been taken into account at the stage of the values for Figure 19.

5.1. R1M predictions

Using the 'R1M' equation shown in Table 5 and Ford's pressure coefficient values. The results determine that the equation used isn't ideal for this engine as from SOC to EOC they are excessively over predicting at all RPMs, more so than EZM. This continues to the calculations used up to peak temperature. Where at 2500RPM it is over predicting up to 899% more than that of the EZM, and 787% more up to peak temperature.

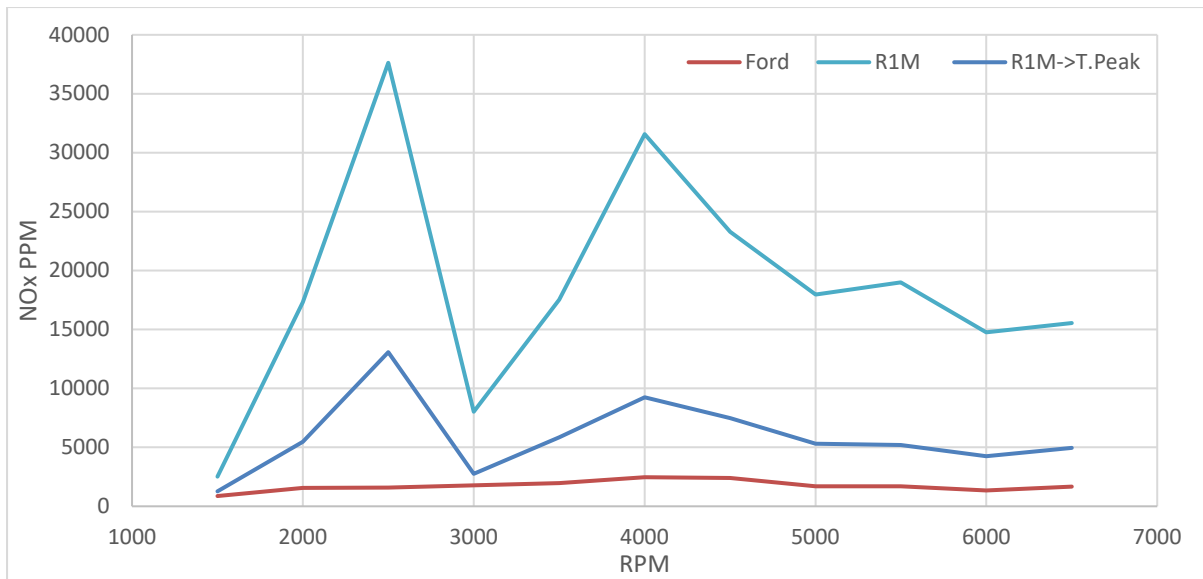


Figure 20 NOx values using R1M equation

As R1M equation uses a different empirical constant that is over three times larger and a smaller number on top of the exponent, which would give much larger values from this mathematic function. One of the main considerations is that the engine it was modelled on was port injection, this usually results in greater mixing time thus, on a real engine would mean less locally lean patches. Especially at lower rpm where piston speed is less and greater change of a completely global homogeneous burned mixture.

An interesting result for testing, but further workings will continue to gain greater accuracy for the direct injection. With this information, the pressure coefficient should be used and modified on the previous calculations for NOx for greater accuracy.

5.2. Pressure co-efficient

Using the values from Table 6 and Equation 52, where greater accuracy was achieved towards the engine data. At 2000RPM and 3000RPM, the prediction is within 85% and 91% respectively. Most of the other RPM sites are seen to be within 70% of the engine data supplied. The prediction of NOx up to peak temperature isn't seen to be greatly accurate with most RPMs showing a great under prediction at this calculation step. The values are seen to be more than 63-95% under predicting up to peak temperature.

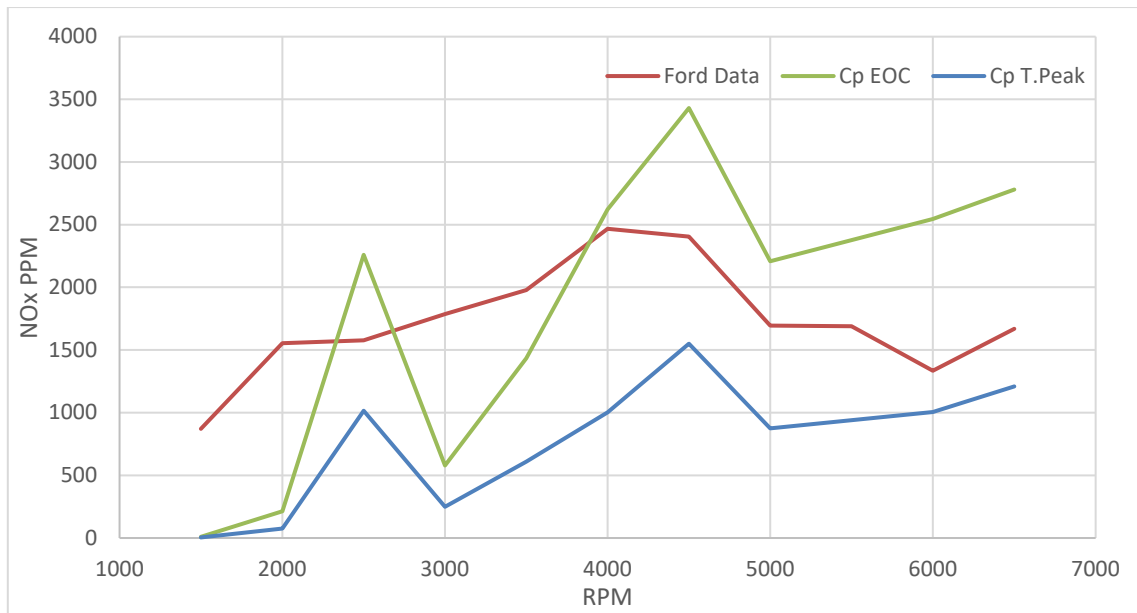


Figure 21 NOx values using given Co-efficient values from Table 6

With the pressure coefficient values being used, these are from various engine rigs that Ford have used and have data on to support these coefficient values. As discussed previously about the differences in engine geometry and the different types of injection. It would be ideal to gain custom values suitable for the FOX engine.

5.2.1. Custom pressure Co-efficient

Using different values for 'Cp' at each 5 Bar pressure until 35 bar, it was found to not have enough variable for the engine specification therefore the pressure was raised up to 110 Bar from 15 bar, in 10 Bar increments from 20 Bar. From various testing on the model, the values seen below are found to be the best medium without increasing other RPM values. The reason for the use of the greater values in Table 6, that are more than 1, is that the GDI engine isn't at completely homogeneous at lower RPM and engine pressure thus as a result a greater co-efficient is needed.

Table 7 Custom Cp Values. Pressure left and co-efficient right

<15	1.3
15.01-20	1.3
20.01-30	1.3
30.01-40	1.28
40.01-50	1.12
50.01-60	0.98
60.01-70	0.65
70.01-80	0.5
80.01-90	0.45
90.01-100	0.31
100.01-110	0.3

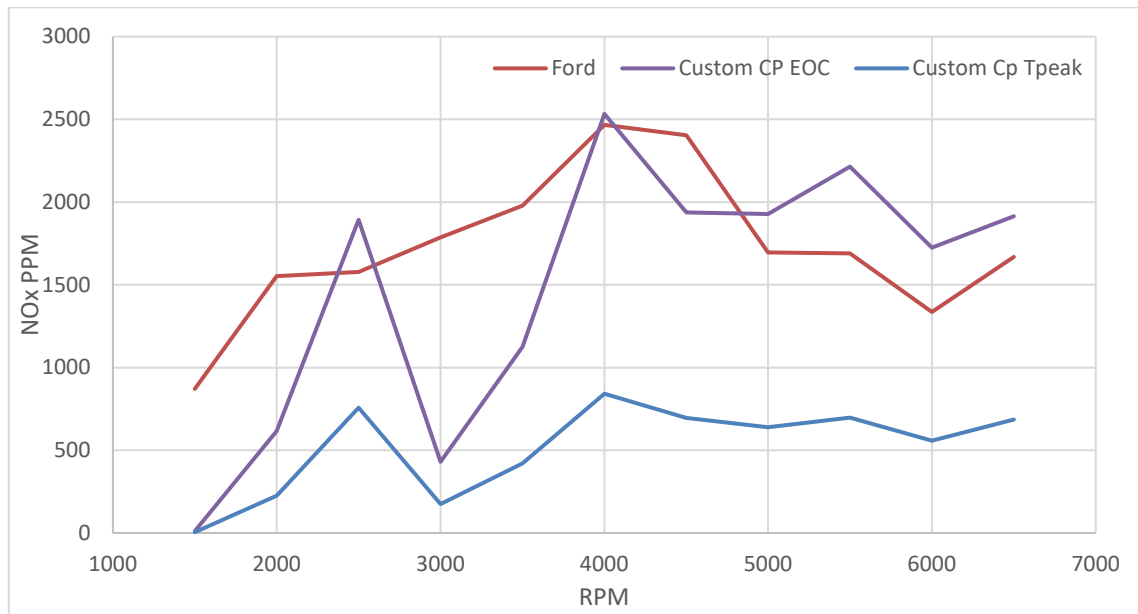


Figure 22 Custom pressure co-efficient for Zeldovich mechanism

At 3500RPM it has been found the 86.5 Bar is the highest peak pressure out of all the RPM's, hence the need for higher temperature range in Table 7. This is representative of the max torque that is produced. Whilst the prediction at 2000, 3000 and 3500RPM is still low. At the higher pressures the reverse reactions have a greater chance to return to their former element, as pressure is proportional the heat then the longer the element is subject to sustained temperatures, the greater probability it will return back to the left. So in a real engine these higher predictions may be lower as the Ford data suggests.

The overall accuracy is better than Figure 19, 20, 21 by using this method. At 4000RPM it predicts with 3% which is ideal whereas above 5000RPM the accuracy is within 34%, but the trend of NO_x production is close to that of the Ford data. A more viable option for modelling is NO_x prediction from SOC to EOC. Whereas for the prediction up to peak temperature (shown on the lower trace) the correlation is more than 52% than the engine data thus having no advantage other than in Figure 20.

5.2.2. Burn temperature corrected NO_x

Applying the polynomial burn temperatures to the Zeldovich mechanism used before in Figure 23. The temperatures have made a visual improvement. At 2500RPM the NO_x is seen to be lower by 45% from the previous prediction; the prediction is vastly improved showing it is 47% more than the measured engine data. It is still apparent that it is under predicting at lower RPM and over predicting with a corrected burn temperature. At higher RPMs the correction

has made on a majority of the points, others give negligible differences. At 4000RPM the reduction is 2%, 3500RPM a reduction by 4.4%, 5000 giving a considerable reduction of 15% and the higher RPMS showing greater than 3% reduction.

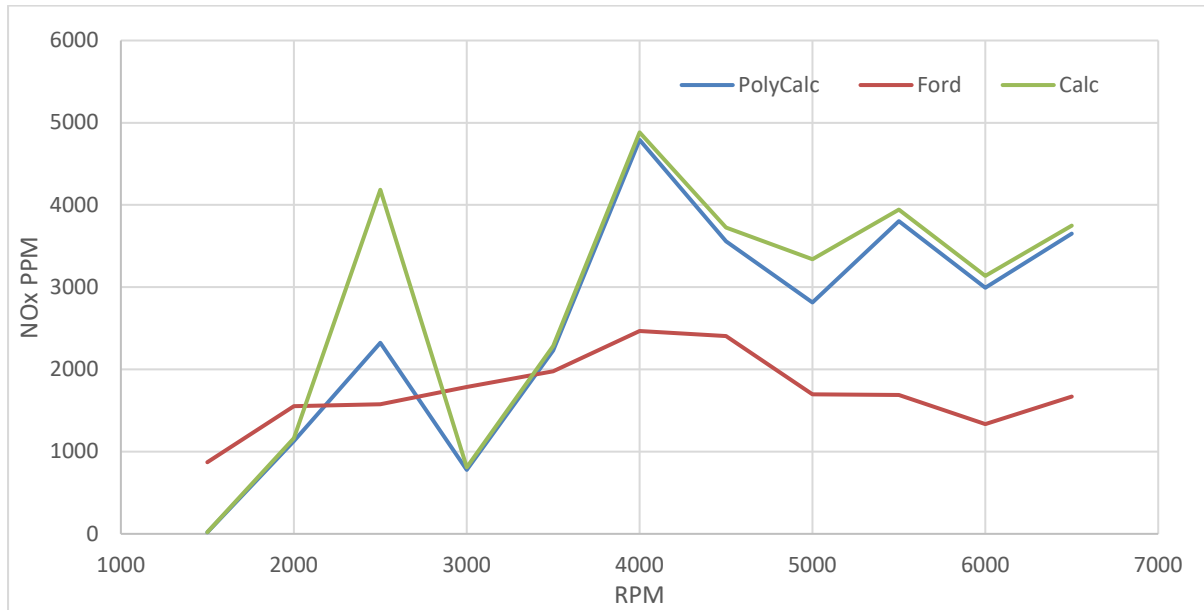


Figure 23 NOx prediction using EZM with old calculation vs polynomial calculation corrected burn temperatures

At peak temperature the predictions are now less than the real engine data and previous calculations; as NOx can still be created after peak temperature as discussed before. At 2500RPM the spike is eradicated, but also showing a closer trend to that of the engine data; this is due to the polynomial advancing the peak temperature by 10 degrees. As the trend follows that of the engine data, it would be easy to multiply the values but there would be no obvious reasoning why it they would need to be up to twice the values at the mid-high RPM unless from the data variable valve timing would occur, in which exhaust. In the model, fuel nitrogen hasn't been taken into account where as in a real engine, although a small percentage, it would account for some slight over 544prediction. Also GDI engines create

amass of NOx so up to peak temperature isn't a complete representation of the real engine. (P.G. Boulter, 2012)

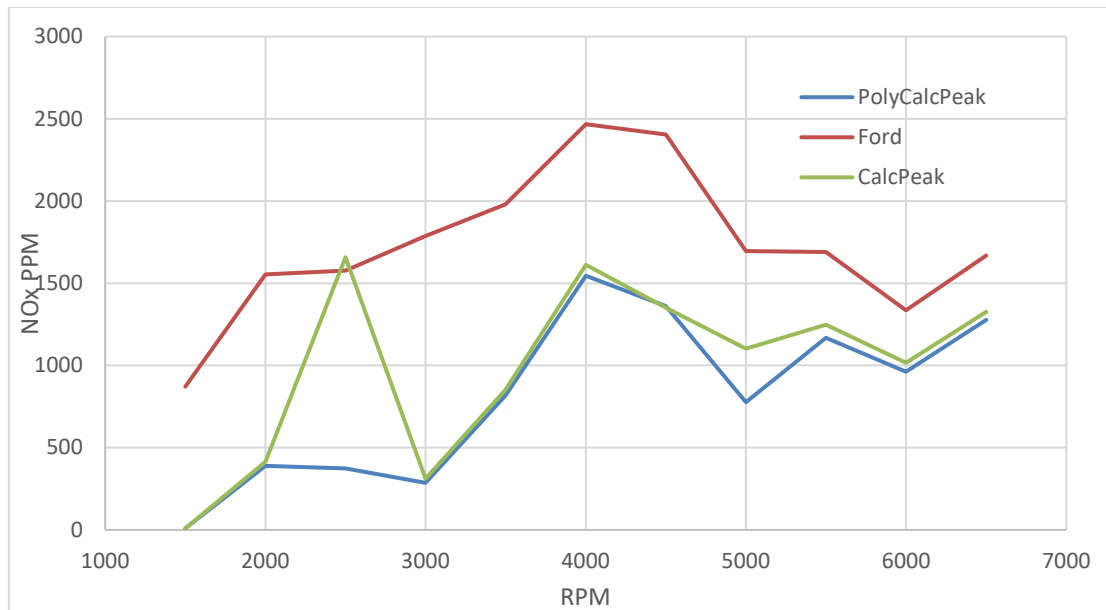


Figure 24 NOx prediction with corrected burn temperatures up to peak temperatures

At 1500RPM, there are limited values that are over 2000K in the burned zone. One of the limitations of the model is that it only models above 2000K due to the $\text{CO}_2/\text{H}_2\text{O}$ reaction rate constants. "According to the Zeldovich equations, NO is generated to the limit of available oxygen (about 200,000 ppm) in air at temperatures above 1600K". (EPA, 1999) One of the improvements for the model is that it needs to take reactions above 1600K, thus shown in Figure 24, at lower RPM, with a lower temperature it under predicts. In the model, fuel nitrogen hasn't been taken into account where as in a real engine, although a small percentage it would account for some slight under prediction.

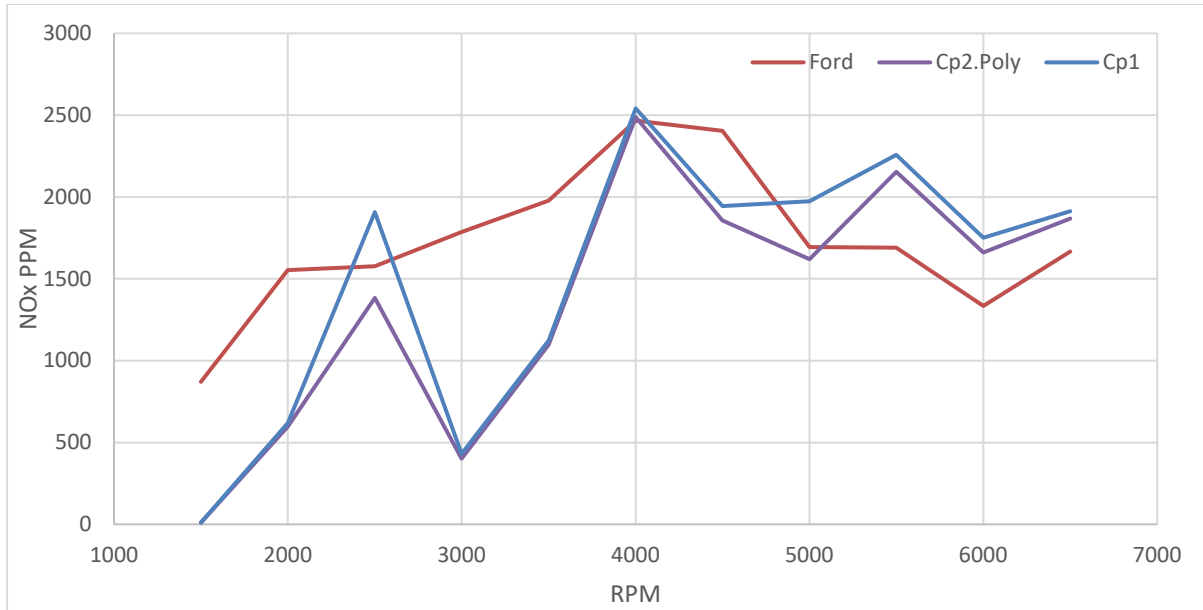


Figure 25 NOx prediction with custom coefficient with polynomial T.burned from SOC

As a final calculation towards increasing accuracy for NOx predictions. Where Cp1 is the closer trace from the polynomial burn temperatures, and Cp2 is adjusted to increase accuracy. The values from Table 7 have been adjusted further to give Table 8. It difficult to adjust the values for each RPM as the lower pressures also alter values for the higher RPM, as this is seen the increase in accuracy the most.

Table 8 Modified co-efficient values used for the NOx production

<15	1.3
15.01-20	1.3
20.01-30	1.3
30.01-40	1.28
40.01-50	1.21
50.01-60	0.95
60.01-70	0.6
70.01-80	0.5
80.01-90	0.46
90.01-100	0.35
100.01-110	0.3

At 2500RPM the NOx has predicted from within 21% above to 12% below. At 3500RPM the predicted is closer by 2%. At 4000RPM the accuracy of the prediction is within 1% of the engine data. Whilst at higher RPM it is now increase accuracy of 12% at 5000RPM, 7% at 5500RPM and 6000RPM and 3% at 6500RPM. It is still clear that the EZM under predicted at low rpm and over predicts at high rpm but it can be smoothed out with the co-efficient. Where the 3000-3500RPM values need to be inspected further. For values refer to Appendix H for NOx Prediction

5.3. Model validation

The previous equations and method were used on 1.5L turbo charged engine from Ford to validation the models results.

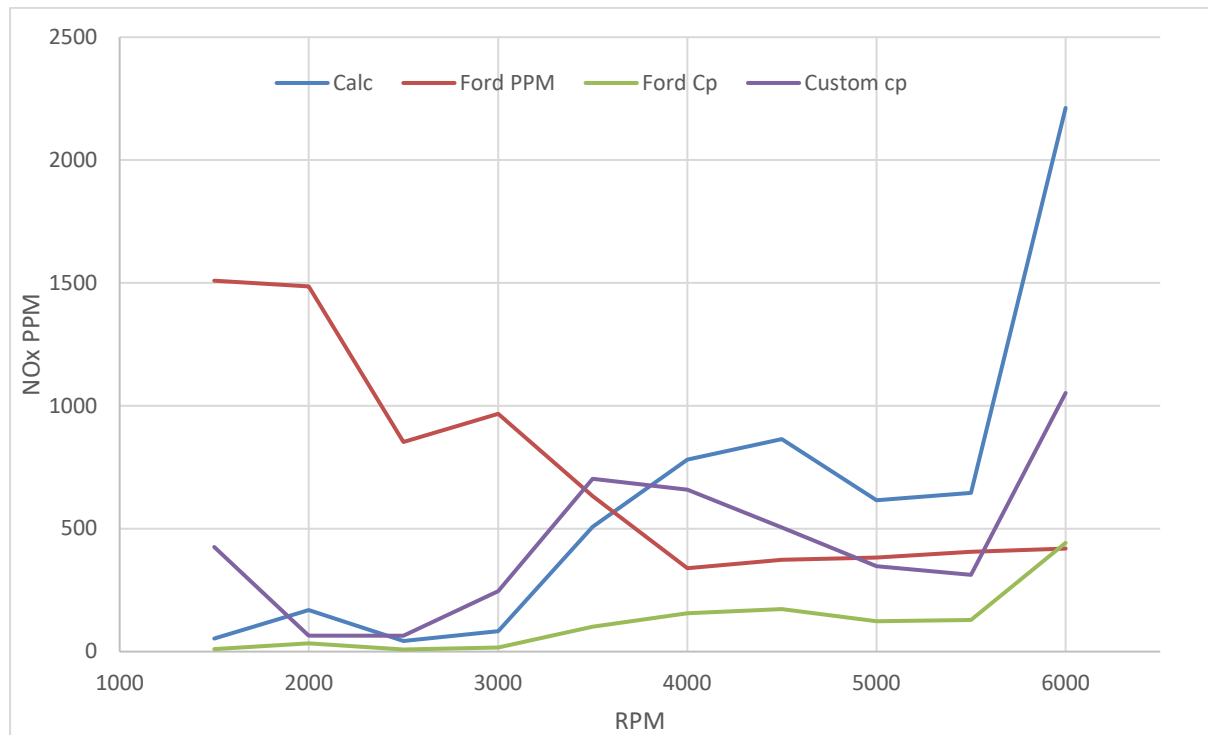


Figure 26 Ford 1.5L NO_x predictions with Cp – from SOC to EOC

Unfortunately as seen, the model doesn't follow any trend towards this engine even with the modified Cp values, although it shows some closer correlation at the higher rpm. With this in mind the Ford PPM data was retrieved from the data sheet supplied. Although the author is concerned that the 1.0L engine is seen to have a close link with values calculated on the other hand the values calculated are seen to be opposite to that of the 1.5L engine hence the suspicion and isn't discussed at great lengths. Although the model is predicts within 55% at the highest rpm but at the lower RPM predictions are more than 72% (although nitric oxides are highest at leaner mixtures).

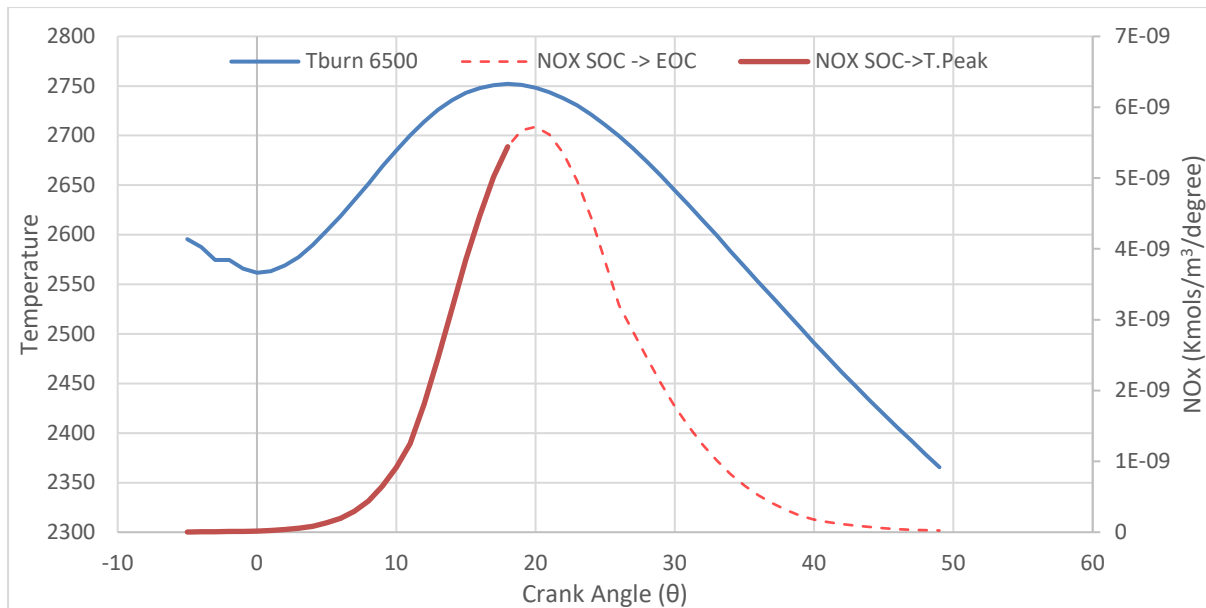


Figure 27 Burn temperatures vs NOx production 6500RPM

Above shown is the burn temperature against the NOx production. Where the peak temperature is the line is solid afterwards it is dashed. It is seen that up to peak temperature the greatest amount of NOx is produced as is evident from the slope of the trace. After peak temperature the NOx still increases until it starts to drop 3-4CA after, where sustained temperatures will be present. This is where more NOx could be formed although it is thought at least 60% of the fuel is burnt at this point so combustion will cool with the addition of the piston motion of expansion towards BDC.

The slope downwards is most important as if the slope is extreme and thermal runaway is present or if the exhaust valve opens early, this would cause NOx to freeze in their current state regardless of the equilibrium state thus greatly increasing engine out NOx levels; this isn't ideal for emission purposes so exhaust valve is best to open as late as possible. "The equilibrium approach usually gives higher concentrations of NOx but does not have the phenomenon called freezing, if the temperature is high and then rapidly drops." (Schwerdt, 2006)

The slowing of the slope of NOx, could be the result of the high RPM with less heat rejection enabled through the walls due to the higher piston speed resulting in higher friction.

Overall it is seen the use of the EZM combined with pressure co-efficient, it can give an insight into the production of NOx, albeit there are complexities in the simple model, the values are thought provoking for NOx formation.

6. Sensitivity analysis

The two zone model largely depends on the polytropic index from finding the values from Equation 2. This parameter can vary dependant on where it is taken on the trend of compression or expansion stroke. By changing this parameter, it will affect the resultant values for the rest of the model, from determining the SOC/EOC, burn temperatures and NO_x production. As the polytropic index is mostly seen at 1.3 (± 0.05) as mentioned by Heywood. These extremes were exercised on the model.

Table 9 Polytropic indices

	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000	6500
Ncomp	1.305	1.335	1.327	1.330	1.328	1.341	1.340	1.322	1.329	1.332	1.338
Nexp	1.275	1.257	1.247	1.248	1.260	1.263	1.239	1.255	1.256	1.265	1.264

As SOC is usually after TDC, this polytropic will be looked. 2000RPM will be taken in particular interest, as this has greater importance towards the NEDC cycle. To determine the SOC the polytropic index is a factor. By varying it, the SOC can be seen to change up to 1 degree from the values above. One way of correlating the model to the data is the MFB at 50%. The supplied data shows it at approximately 29CA. The original model data correlates to this; the value '1.35' presents at a degree later.

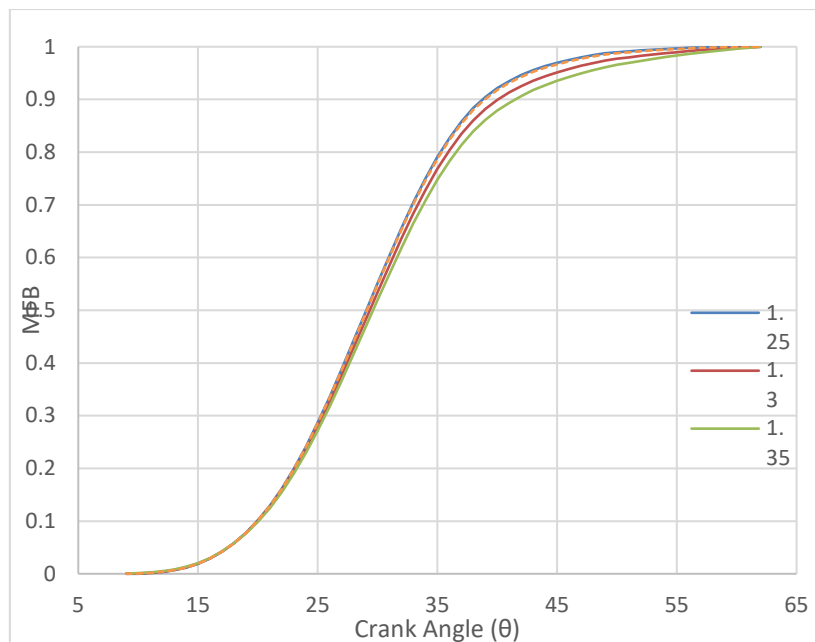


Figure 28 Varying polytropic indices for MFB

As the MFB is important to later calculations, it is shown above, where the calculation line is the value used in the original model in; hence the '1.25' trend follows closely. After 50% burned

the change in values becomes greater as the piston is travelling down and showing a greater decrease in burn rate. From the polytropic relation in Equation 3, as the larger the value of the polytropic index the smaller the number as a result of the mathematical function of square root. This lower number gives a bigger difference when using Equation 4, resulting in a larger end product for MFB. Overall the larger the polytropic index the slower the burn rate.

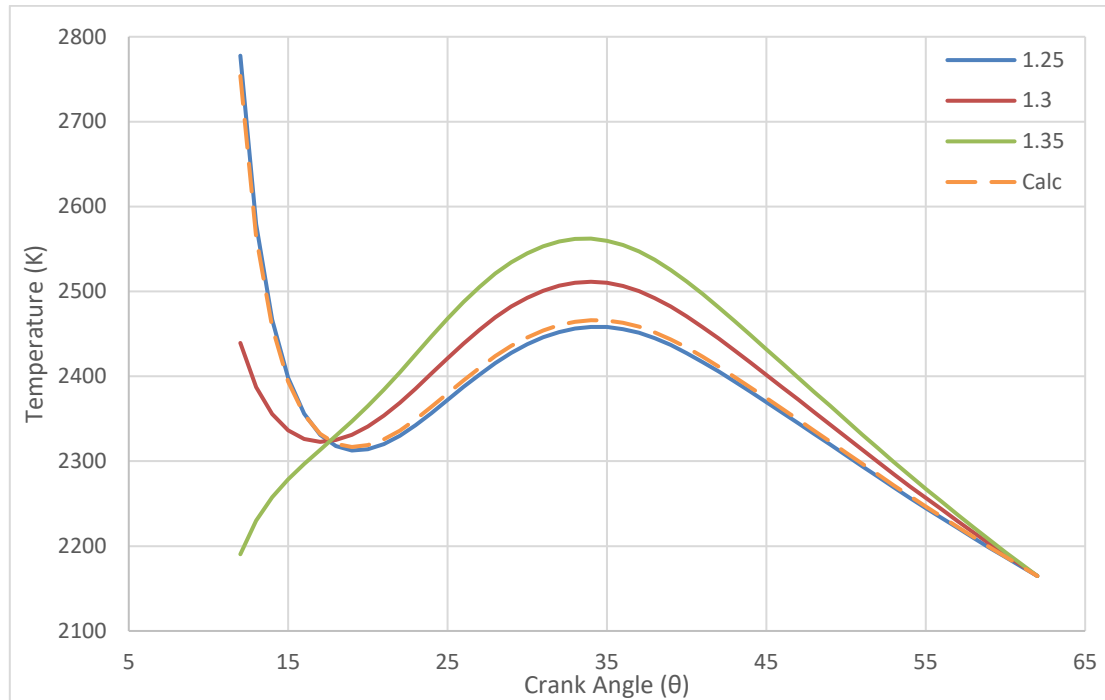


Figure 29 Varying polytropic indices for burned temperatures

At the start of the data trace, the spike in the initial starting temperature is as discussed in Section 2.9, but the higher polytropic index this follows the same development of larger MFB values. As at the start of '1.35' it begins lower as expected in a real engine, this is evident at the first few degrees of combustion the larger the number as a result of the larger MFB; resulting in higher temperatures throughout combustion.

As the tropic index is higher the burned temperature is higher this is proportional to the pressure rise. So as a result from the difference in pressures of Equation 4, the result of a higher pressure added from combustion is the greater temperature of the burned zone.

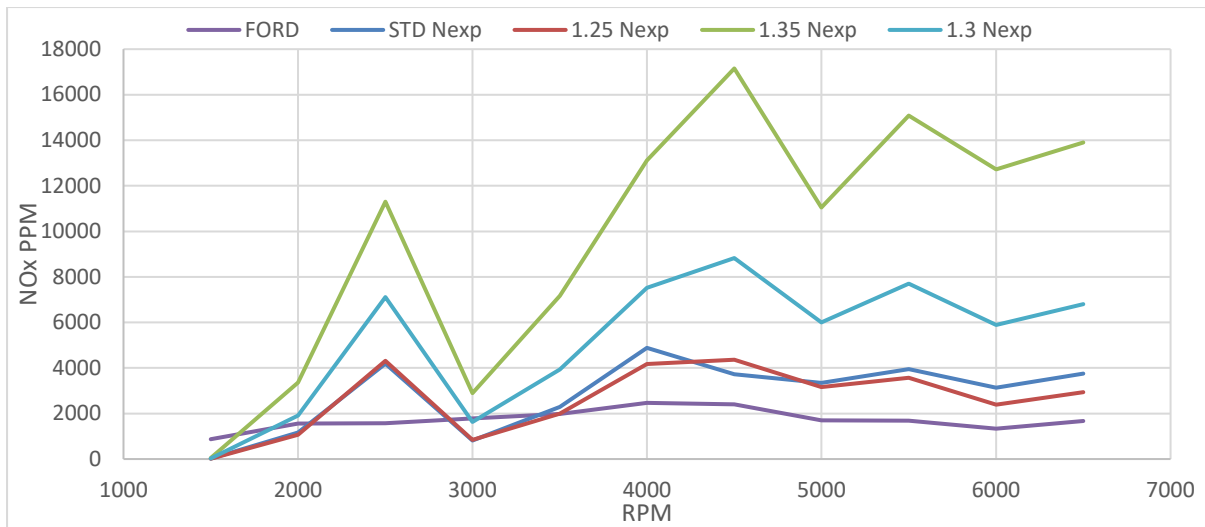


Figure 30 NOx predictions using EZM for varying polytropic indices

As a result of the higher burned temperatures from the higher polytropic index, the NOx PPM is greatly increased. The '1.25' trace is seen to be closest, whereas '1.3' is predicting twice than that of '1.25' and '1.35' is three times more than that of '1.25', thus showing no close correlation with the larger polytropic indices. At '1.25' the trace is close to that of the calculated data, as it is within 2% of that value of the polytropic index. If a simplified model was created it would be safe to assume the value of 1.25 for a polytropic index for expansion.

7. Conclusion

The final model gives a relatively accurate results based on the data provided. With mathematical models a small error can make a large difference in the end result or several calculations due to rounding errors which is a common problem in programming; this is seen in the MFB calculations resulting to the end NOx result. As experimented with the sensitivity analysis on how assumed values can make a difference to predictions to make a suitable empirical value but with the data this can be calculated. As the model is zero-dimensional where it has no real account for any geometric features only that of volume, the NOx formation may change; this is would be further work into Computational Fluid Dynamics for accurate results. (Andersson, Johansson, Hultqvist, & Noehre, 2006)

The chemistry behind NOx formation is still being researched and new formulas being used based on engine to engine; this seems to be the case where a model is fine-tuned towards a specified criteria. Seen with the Zeldovich mechanism this is well known method based on empirical formulas but the reverse reaction are deemed irrelevant as the values are small. With the regulations on the NEDC becoming stricter every 1% of accuracy is needed, so it will need to be included in greater detail for further precision.

The assumptions that are covered are well known to be relevant through extensive testing of difference sources, such as the in cylinder gases are assumed to be ideal, the compression/expansion strokes are assumed to be adiabatic, the mixture is 100% homogeneously mixed in-cylinder thus no locally lean patches, MFB assumes 100% burn and a rapid rise in temperature throughout the combustion chamber. These are assumptions have provided fairly accurate data for research uses; as the model can easily be changed to suit different variables or engine parameters. From the last NOx prediction the overall accuracy is within 78% at the anomaly RPM and within 33% when following the engine data trend.

Although some of the analysis can result in many variables within reasons without being able to freeze the engine as that specific degree to find out what is happening in cylinder at that time frame. As the NOx is such a difficult subject and is at the top of research and development for most engine manufacturers it is well documented although there is not one sole fix. The simple combustion model with some complex elements to provide an approximation of a real engine under observation, gives fairly accurate results.

8. Bibliography

- Andersson, M., Johansson, B., Hultqvist, A., & Noehre, C. (2006). *A Predictive Real Time NO_x Model for Conventional and Partially Premixed Diesel Combustion*. Toronto: SAE.
- Baulch et al. (1994). *Evaluated Kinetic Data For Combustion Modelling Supplement*. US: Journal of physical and chemical reference data.
- Beavon. (2016). *The oxidation of nitrogen monoxide*. Retrieved from www.rod.beavon.org.uk/nitrogenmonoxide.htm
- Bosch, R. (2011). *Automotive Handbook*. Germany: WILEY.
- Burton, K. (2017). *Combustion emissions and calculations*. Swansea.
- EPA. (1999). *Nitrogen Oxides, Why and How Are They Controlled*. Carolina: EPA.
- Ferguson, C. R., & Kirkpatrick, A. T. (2001). *Internal Combustion Engines - Applied thermosciences*. US: John Wiley & Sons.
- Ford, M. C. (2012). *Fox GTDI*. London: Ford.
- Glassman, I. (2008). *Combustion*. London: Elsevier.
- Goodger, E. (2000). *Transport Fuels Technology: from Well to Wheels, Wings, and Water*. Norwich: Landfall Press.
- Heywood, J. B. (1988). *Internal combustion engine fundamentals*. USA: McGraw-Hill.
- McDonald, M. (2017). Lecture Notes. *Chemistry*. Swansea.
- McGrath, P. J. (1996). *Assesment and improvement of current computantional spark ignition engine NO_x formation models for auto industry development and design use*. Massachusetts: MIT.
- Merket, G., Schwarz, C., stiesch, G., & Otto, F. (2006). *Simulating Combustion*. Berlin: Springer.
- Miller, R., Davis, G., Lavoie, G., Newman, C., & Gardner, T. (1998). *A Super-Extended Zel'dovich Mechanism for NO_x Modelling and Engine Calibration - 980781*. Detriot: SAE.
- P.G. Boulter, J. B.-K. (2012). *The Evolution and Control of NO_x Emissions*. Berlin: Springer-Verlag.
- Schwerdt, C. (2006). *Modelling NO_x-Formation in Combustion Processes*. Lund: Lund University.
- Supercomputing. (2017). *Coding Bilinear Interpolation*. Retrieved from Super Computing Blog: <http://supercomputingblog.com/graphics/coding-bilinear-interpolation/>
- Tazerout, M., Le corre, O., & Ramesh, A. (2000). *A New Method to Determine the Start and End of Combustion*. Nantes: Indian Institute of Technology Madras.

9. Appendix

9.1. Appendix A – Mass fraction burn dQ

During constant volume burning from P2n to P2.

1st law of thermodynamics

$$dQ = dU + P \cdot dV$$

But, $dV = 0$

$$\therefore dQ = dU = m \cdot C_v \cdot dT$$

From P2n $\rightarrow$ P2,

$$dQ = m \cdot C_v \cdot dT$$

Ideal gas law

$$PV = MRT$$

$$d(PV) = d(MRT) = m \cdot R \cdot dT$$

From P2n to P2, volume stays at V_2

$$\therefore d(PV) = V_2 \cdot dP = m \cdot R \cdot dT$$

Therefore heat released in 1 degree,

$$dQ = dU = m \cdot C_v \cdot dT = m \cdot R \cdot dT = V_2 \cdot dP$$

$$\therefore dQ = C_v \cdot V_2 \cdot dP \cdot R$$

Therefore, heat released in 1 degree is proportional to pressure rise;

$$\frac{\sum_{SOC \rightarrow \theta} dQ}{\sum_{SOC \rightarrow EOC} dQ} = \frac{\sum_{SOC \rightarrow \theta} \frac{C_v \cdot V_2 \cdot \Delta P}{R}}{\sum_{SOC \rightarrow EOC} \frac{C_v \cdot V_2 \cdot \Delta P}{R}}$$

Assuming C_v doesn't change, this produces MFB with greater precision;

$$\frac{\sum_{SOC \rightarrow \theta} V_2 \times \Delta P}{\sum_{SOC \rightarrow EOC} V_2 \times \Delta P}$$

$$C_p = C_v + R$$

$$\gamma = \frac{C_p}{C_v} = \frac{C_v}{C_v} + \frac{R}{C_v}$$

$$\therefore \gamma = 1 + \frac{R}{C_v}$$

$$\frac{R}{C_v} = \gamma - 1$$

$$\therefore dQR = \frac{V_2 \cdot dP}{\gamma - 1}$$

9.2. Appendix B – Real world Ford EGR usage

rr 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	3.2	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 31 Ford 1 Litre EcoBoost engines added EGR percentages (Ford, 2012)

Ford Motor Company's 1 litre Fox engine exhibits up to 33.3% EGR at 2% engine load with high EGR usage whilst being in the NEDC. Low levels of EGR are added whilst on full load. At the higher RPM EGR is used to cool down the combustion chamber due to the high heat produced from friction and lesser time for thermal runaway thus making the fuel is a more effective cooling agent. (Ford, 2012)

9.3. Appendix C – Specific heat ratio

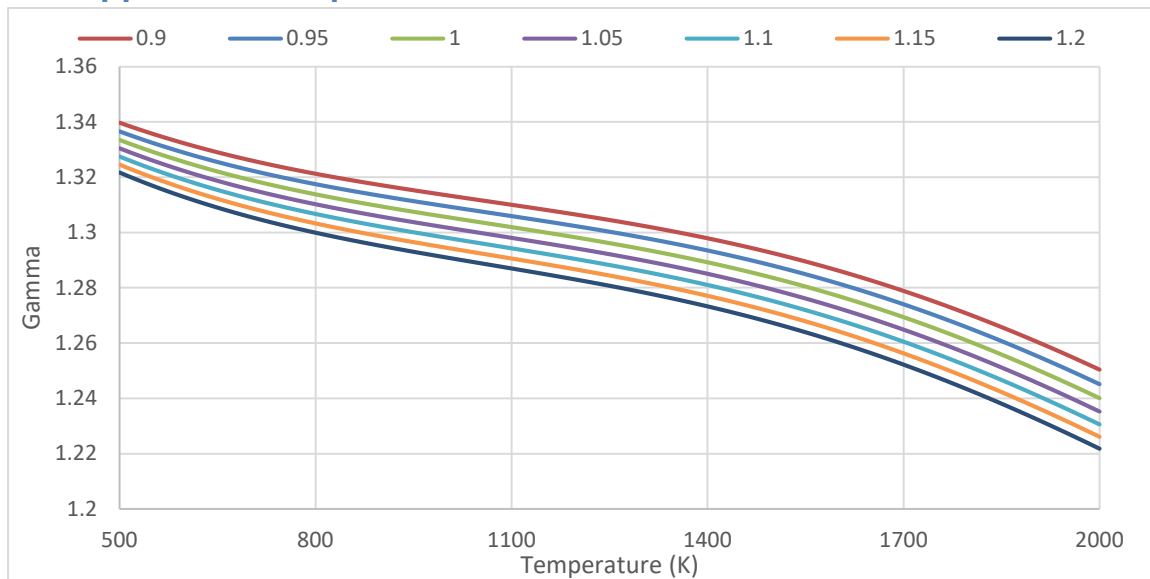


Figure 32 Gamma changing with temperature for Gasoline with varying FER

Showing the richer the mixture more lower the gamma, as more molecules thus more molecular weight so would require more energy to heat.

9.4. Appendix D – Reaction rate constants.

Continuing to get the constants for each degree Kelvin, the reaction rate table from used from Goodger, M. Fitting a polynomial to increase the accuracy of the model. Above 2800K the polynomial is slightly off, but as combustion temperatures hardly exceed 2800K it is ignored.

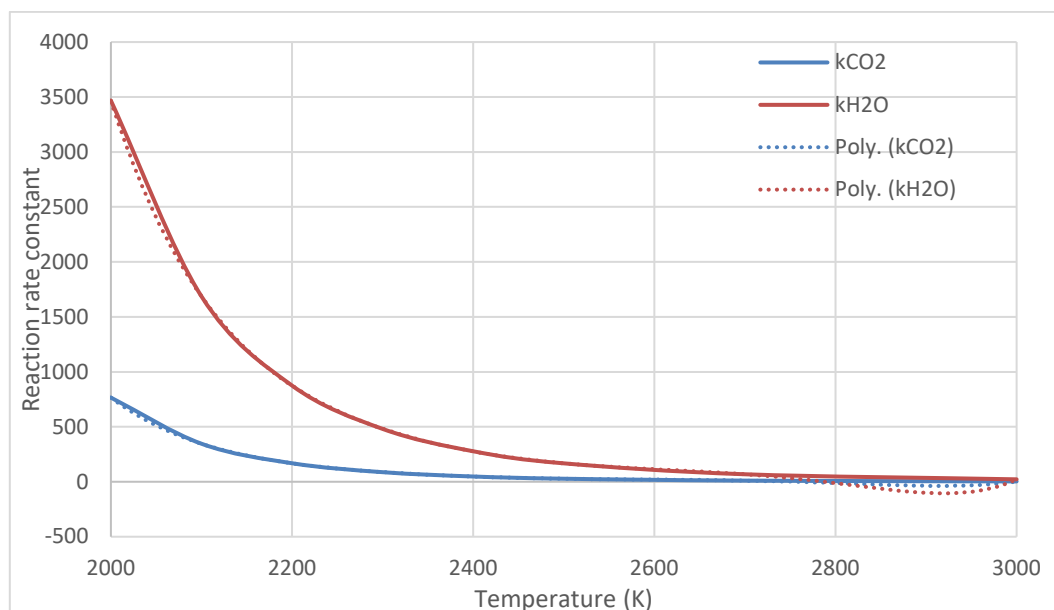


Figure 33 Reaction rate constant traces for CO₂ and H₂O. (Goodger, 2000)

Where polynomial with 'x' being the temperature needed, for CO₂;

$$y = 0.0000000000000782061135743534x^6 - 0.00000000118958594479025x^5 \\ + 0.00000753257874077333x^4 - 0.02542276484849073 \\ + 48.2507167698753x^2 - 48846.5459630743x + 20616109.6854172$$

Equation 59

Polynomial for H₂O;

$$y = 0.000000000000023036782841985300x^6 - 0.000000000349295715333898x^5 \\ + 0.00000220407421375471x^4 - 0.00741037925666485000000000000000x^3 \\ + 14.0049945950029x^2 - 14111.418168666x + 5924578.95644595$$

Equation 60

9.5. Appendix E – Oxygen (N₅) content after combustion

Fuel Equivalence ratio - 0.89																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	1.34717581	1.34358	1.34199	1.34146	1.34103	1.34068	1.34038	1.34013	1.3399	1.3397	1.33953	1.33937	1.33923	1.3391	1.33898	1.33887	1.33877	1.33867
2100	1.361577268	1.35383	1.35038	1.34924	1.34831	1.34755	1.3469	1.34634	1.34586	1.34543	1.34505	1.3447	1.34439	1.34411	1.34385	1.34361	1.34339	1.34318
2200	1.388429687	1.37306	1.36617	1.36388	1.36204	1.36051	1.35921	1.35809	1.35711	1.35625	1.35548	1.35479	1.35416	1.35359	1.35307	1.35259	1.35214	1.35173
2300	1.4348286	1.40665	1.39389	1.38964	1.3862	1.38334	1.38092	1.37883	1.377	1.37538	1.37394	1.37264	1.37148	1.37039	1.36941	1.36851	1.36767	1.36689
2400	1.508714137	1.46101	1.4391	1.43176	1.4258	1.42083	1.41661	1.41296	1.40977	1.40695	1.40442	1.40215	1.40008	1.3982	1.39648	1.39489	1.39342	1.39205
2500	1.617539673	1.54277	1.50782	1.49602	1.4864	1.47836	1.4715	1.46556	1.46036	1.45574	1.45161	1.44788	1.44449	1.4414	1.43856	1.43594	1.43352	1.43126
2700	1.960797597	1.81123	1.73835	1.71323	1.69256	1.67515	1.66019	1.64716	1.63566	1.62541	1.61619	1.60785	1.60024	1.59327	1.58684	1.58089	1.57537	1.57022
3000	2.768126394	2.48749	2.34179	2.28997	2.24665	2.20965	2.1775	2.14917	2.12395	2.10127	2.08071	2.06195	2.04474	2.02886	2.01414	2.00044	1.98764	1.97565
Fuel Equivalence ratio - 0.91																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	1.106064262	1.10201	1.10021	1.09962	1.09914	1.09874	1.0984	1.09811	1.09786	1.09764	1.09744	1.09726	1.0971	1.09695	1.09682	1.09669	1.09658	1.09647
2100	1.12225457	1.11355	1.10967	1.10838	1.10735	1.10648	1.10576	1.10513	1.10458	1.1041	1.10366	1.10328	1.10293	1.10261	1.10231	1.10204	1.10179	1.10156
2200	1.152263744	1.13512	1.1274	1.12484	1.12277	1.12105	1.11959	1.11834	1.11724	1.11627	1.11541	1.11463	1.11392	1.11328	1.1127	1.11215	1.11165	1.11119
2300	1.20363282	1.17251	1.15834	1.15361	1.14978	1.1466	1.14389	1.14156	1.13951	1.13771	1.13609	1.13464	1.13333	1.13213	1.13103	1.13002	1.12908	1.12821
2400	1.28438966	1.23237	1.20833	1.20025	1.19368	1.18819	1.18353	1.17949	1.17596	1.17283	1.17003	1.16751	1.16522	1.16313	1.16121	1.15945	1.15781	1.15629
2500	1.40156816	1.32125	1.28342	1.27059	1.26011	1.25134	1.24385	1.23736	1.23166	1.2266	1.22207	1.21798	1.21426	1.21086	1.20774	1.20485	1.20218	1.19969
2700	1.762956881	1.60661	1.52986	1.50331	1.48141	1.46292	1.44703	1.43315	1.42089	1.40995	1.40011	1.39118	1.38304	1.37556	1.36867	1.36229	1.35635	1.35081
3000	2.59312804	2.30613	2.15661	2.10332	2.05873	2.02059	1.98742	1.95817	1.9321	1.90864	1.88736	1.86793	1.85008	1.83361	1.81833	1.8041	1.7908	1.77833
Fuel Equivalence ratio - 0.99																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	0.160967586	0.15038	0.14547	0.14382	0.14247	0.14135	0.14039	0.13956	0.13883	0.13819	0.13761	0.13709	0.13662	0.13619	0.13579	0.13542	0.13509	0.13477
2100	0.198771462	0.1792	0.16993	0.16678	0.1642	0.16203	0.16018	0.15857	0.15715	0.15589	0.15476	0.15374	0.15282	0.15197	0.1512	0.15046	0.14979	0.14917
2200	0.258143294	0.22545	0.20972	0.20432	0.19980	0.19614	0.19293	0.19013	0.18767	0.18547	0.18349	0.18169	0.18006	0.17856	0.17718	0.1759	0.17471	0.1736
2300	0.344495246	0.29379	0.26912	0.26059	0.25356	0.24762	0.2425	0.23804	0.23409	0.23056	0.22738	0.2245	0.22186	0.21944	0.2172	0.21513	0.2132	0.2114
2400	0.462373644	0.3882	0.35178	0.33913	0.32868	0.31983	0.3122	0.30552	0.29961	0.29432	0.28954	0.2852	0.28123	0.27758	0.2742	0.27107	0.26815	0.26541
2500	0.615495535	0.51213	0.46097	0.44313	0.42835	0.41582	0.40499	0.39551	0.38709	0.37956	0.37275	0.36655	0.36088	0.35566	0.35082	0.34633	0.34215	0.33823
2700	1.038320365	0.86065	0.77098	0.73944	0.7132	0.69086	0.6715	0.65449	0.63936	0.62577	0.61347	0.60226	0.59198	0.58249	0.5737	0.56553	0.55789	0.55073
3000	1.934255045	1.62902	1.46865	1.41116	1.36291	1.32151	1.2854	1.25348	1.22495	1.19921	1.17581	1.1544	1.13469	1.11645	1.09951	1.08369	1.06889	1.05497
Fuel Equivalence ratio - 1.00																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	0.0634901	0.05047	0.04412	0.04192	0.0401	0.03856	0.03724	0.03608	0.03505	0.03413	0.0333	0.03255	0.03186	0.03122	0.03063	0.03009	0.02958	0.02911
2100	0.106405462	0.08466	0.07405	0.07037	0.06733	0.06476	0.06254	0.0606	0.05888	0.05734	0.05594	0.05468	0.05352	0.05246	0.05148	0.05056	0.04971	0.04891
2200	0.169591115	0.13515	0.1183	0.11245	0.10761	0.10352	0.09999	0.09689	0.09415	0.0917	0.08949	0.08747	0.08563	0.08393	0.08236	0.08091	0.07955	0.07828
2300	0.258653537	0.20658	0.18102	0.17214	0.16479	0.15856	0.15319	0.14848	0.14431	0.14057	0.13719	0.13412	0.13131	0.12872	0.12633	0.12411	0.12203	0.12009
2400	0.378465658	0.3032	0.26608	0.25316	0.24245	0.23338	0.22554	0.21867	0.21257	0.20711	0.20218	0.19769	0.19358	0.1898	0.18629	0.18304	0.18	0.17716
2500	0.533036294	0.42877	0.37702	0.35896	0.34398	0.33126	0.32027	0.31063	0.30207	0.2944	0.28746	0.28115	0.27536	0.27003	0.2651	0.26051	0.25623	0.25222
2700	0.958105825	0.77962	0.68948	0.65776	0.63136	0.60888	0.5894	0.57227	0.55703	0.54335	0.53096	0.51966	0.50929	0.49973	0.49087	0.48262	0.47492	0.4677
3000	1.857255325	1.55092	1.38997	1.33228	1.28385	1.2423	1.20606	1.17402	1.14538	1.11954	1.09605	1.07456	1.05477	1.03646	1.01945	1.00357	0.9887	0.97474
Fuel Equivalence ratio - 1.01																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	0.013939165	0.00768	0.00532	0.00461	0.00407	0.00364	0.0033	0.00301	0.00277	0.00257	0.00239	0.00224	0.0021	0.00198	0.00187	0.00178	0.00169	0.00161
2100	0.044064455	0.0274	0.02022	0.01792	0.01611	0.01464	0.01342	0.01239	0.01151	0.01075	0.01009	0.0095	0.00898	0.00851	0.00809	0.00771	0.00737	0.00705
2200	0.099925456	0.06857	0.05394	0.04902	0.04504	0.04172	0.03892	0.0365	0.0344	0.03254	0.03089	0.02942	0.02808	0.02688	0.02577	0.02476	0.02384	0.02298
2300	0.185080435	0.13483	0.1106	0.10228	0.09545	0.08971	0.08479	0.08051	0.07674	0.07338	0.07037	0.06765	0.06518	0.06291	0.06083	0.0589	0.05712	0.05546
2400	0.302818342	0.22862	0.1923	0.17972	0.16933	0.16055	0.15299	0.14638	0.14054	0.13532	0.13061	0.12634	0.12244	0.11886	0.11555	0.11248	0.10963	0.10696
2500	0.456329204	0.35264	0.30137	0.28351	0.26872	0.25619	0.24537	0.23589	0.22749	0.21996	0.21317	0.20699	0.20134	0.19613	0.19132	0.18685	0.18269	0.17879
2700	0.880906412	0.70239	0.61233	0.58066	0.55431	0.53188	0.51245	0.49537	0.48018	0.46655	0.45421	0.44296	0.43264	0.42312	0.41431	0.4061	0.39844	0.39126
3000	1.781608351	1.47452	1.31324	1.25544	1.20692	1.16531	1.12902	1.09693	1.06825	1.04239	1.01887	0.99735	0.97754	0.95922	0.94219	0.9263	0.91142	0.89744
Fuel Equivalence ratio - 1.02																		
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105
2000	0.00411996	0.0021	0.00141	0.00121	0.00106	0.00094	0.00085	0.00077	0.00071	0.00065	0.00061	0.00057	0.00053	0.0005	0.00047	0.00045	0.00043	0.0004
2100	0.017592947	0.0094	0.00643	0.00555	0.00488	0.00436	0.00394	0.00359	0.0033	0.00305	0.00284	0.00265	0.00249	0.00235	0.00222	0.0021	0.002	0.00191
2200	0.05492737	0.0324	0.0232	0.02034	0.01811	0.01633	0.01487	0.01366	0.01262	0.01174	0.01097	0.0103	0.0097	0.00917	0.00869	0.00827	0.00788	0.00752
2300	0.126996304	0.08308	0.06324	0.05673	0.05151	0.04722	0.04363	0.04057	0.03793	0.03562	0.03359	0.03178	0.03017	0.02871	0.0274	0.0262	0.0251	0.0241
2400	0.237045733	0.16688	0.1335	0.12216	0.1129	0.10517	0.09858	0.09288	0.08789	0.08347	0.07953	0.07599	0.07278	0.06986				

		Fuel Equivalence ratio - 1.05																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000641993	0.00032	0.00021	0.00018	0.00016	0.00014	0.00013	0.00012	0.00011	9.9E-05	9.2E-05	8.6E-05	8E-05	7.6E-05	7.1E-05	6.8E-05	6.4E-05	6.1E-05	0.00029		
2100	0.003028955	0.00152	0.00102	0.00087	0.00076	0.00068	0.00061	0.00056	0.00051	0.00047	0.00044	0.00041	0.00038	0.00036	0.00034	0.00032	0.00031	0.00029	0.00029		
2200	0.012097879	0.00618	0.00415	0.00356	0.00312	0.00278	0.0025	0.00228	0.00209	0.00193	0.00179	0.00168	0.00157	0.00148	0.0014	0.00132	0.00126	0.0012	0.0012		
2300	0.040060647	0.02138	0.0146	0.01261	0.01109	0.0099	0.00894	0.00815	0.00749	0.00693	0.00645	0.00603	0.00566	0.00533	0.00504	0.00478	0.00454	0.00433	0.00433		
2400	0.105434665	0.06097	0.04319	0.03772	0.0335	0.03013	0.02738	0.02509	0.02316	0.0215	0.02007	0.01881	0.01771	0.01673	0.01585	0.01505	0.01434	0.01369	0.01369		
2500	0.221056352	0.14007	0.10438	0.09285	0.0837	0.07625	0.07005	0.0648	0.06031	0.05641	0.05299	0.04997	0.04728	0.04487	0.0427	0.04073	0.03893	0.03729	0.03729		
2700	0.60866735	0.43847	0.35611	0.32775	0.30445	0.28485	0.26807	0.25349	0.24067	0.22927	0.21907	0.20986	0.20149	0.19385	0.18684	0.18038	0.1744	0.16885	0.16885		
3000	1.493582751	1.1875	1.0278	0.9708	0.92308	0.88224	0.8467	0.81534	0.78738	0.7622	0.73936	0.7185	0.69933	0.68163	0.66521	0.64992	0.63562	0.62221	0.62221		
		Fuel Equivalence ratio - 1.06																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000437523	0.00022	0.00015	0.00013	0.00011	9.7E-05	8.8E-05	8E-05	7.3E-05	6.7E-05	6.3E-05	5.8E-05	5.5E-05	5.2E-05	4.9E-05	4.6E-05	4.4E-05	4.2E-05	0.0002		
2100	0.002069962	0.00104	0.00069	0.00059	0.00052	0.00046	0.00042	0.00038	0.00035	0.00032	0.0003	0.00028	0.00026	0.00024	0.00023	0.00022	0.00021	0.0002	0.0002		
2200	0.006077211	0.00424	0.00264	0.00244	0.00213	0.0019	0.00171	0.00155	0.00143	0.00132	0.00122	0.00114	0.00107	0.00101	0.00095	0.0009	0.00086	0.0008	0.0008		
2300	0.028736015	0.01498	0.01014	0.00873	0.00766	0.00683	0.00616	0.00561	0.00515	0.00476	0.00442	0.00413	0.00388	0.00365	0.00345	0.00327	0.00311	0.00296	0.00296		
2400	0.08064866	0.04475	0.03108	0.02697	0.02382	0.02134	0.01932	0.01765	0.01625	0.01506	0.01403	0.01313	0.01234	0.01164	0.01101	0.01045	0.00994	0.00948	0.00948		
2500	0.181515486	0.1099	0.07975	0.07025	0.0628	0.05681	0.05187	0.04774	0.04422	0.04119	0.03855	0.03623	0.03417	0.03234	0.03069	0.02921	0.02786	0.02663	0.02663		
2700	0.548059882	0.38511	0.30669	0.27997	0.25816	0.23994	0.22441	0.211	0.19926	0.18889	0.17964	0.17134	0.16383	0.157	0.15076	0.14503	0.13975	0.13486	0.13486		
3000	1.425477237	1.12079	0.96231	0.90587	0.85867	0.81832	0.78325	0.75234	0.72481	0.70004	0.6776	0.65712	0.63832	0.62097	0.6049	0.58994	0.57597	0.56288	0.56288		
		Fuel Equivalence ratio - 1.07																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000315296	0.00016	0.00011	9E-05	7.9E-05	7E-05	6.3E-05	5.7E-05	5.3E-05	4.9E-05	4.5E-05	4.2E-05	3.9E-05	3.7E-05	3.5E-05	3.3E-05	3.2E-05	3E-05	3E-05		
2100	0.001493161	0.00075	0.0005	0.00043	0.00037	0.00033	0.0003	0.00027	0.00025	0.00023	0.00021	0.0002	0.00019	0.00018	0.00017	0.00016	0.00015	0.00014	0.00014		
2200	0.006077283	0.00306	0.00205	0.00176	0.00154	0.00137	0.00123	0.00112	0.00103	0.00095	0.00088	0.00082	0.00077	0.00073	0.00069	0.00065	0.00062	0.00059	0.00059		
2300	0.021290391	0.01094	0.00737	0.00633	0.00555	0.00494	0.00446	0.00405	0.00372	0.00344	0.00319	0.00298	0.0028	0.00263	0.00249	0.00236	0.00224	0.00213	0.00213		
2400	0.062423829	0.03364	0.02307	0.01994	0.01756	0.01568	0.01417	0.01293	0.01188	0.011	0.01023	0.00957	0.00898	0.00847	0.00801	0.00759	0.00722	0.00688	0.00688		
2500	0.148976144	0.08676	0.06166	0.05392	0.04792	0.04314	0.03922	0.03596	0.03321	0.03085	0.0288	0.02701	0.02543	0.02402	0.02276	0.02163	0.0206	0.01967	0.01967		
2700	0.493424336	0.33704	0.26323	0.2384	0.21828	0.20158	0.18745	0.17531	0.16475	0.15547	0.14724	0.13988	0.13326	0.12726	0.12181	0.11682	0.11224	0.10802	0.10802		
3000	1.359034795	1.05624	0.89935	0.84362	0.79708	0.75736	0.72288	0.69254	0.66554	0.64129	0.61934	0.59934	0.58099	0.56409	0.54845	0.5339	0.52033	0.50763	0.50763		
		Fuel Equivalence ratio - 1.08																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000236722	0.00012	7.9E-05	6.8E-05	5.9E-05	5.3E-05	4.7E-05	4.3E-05	3.9E-05	3.6E-05	3.4E-05	3.2E-05	3E-05	2.8E-05	2.6E-05	2.5E-05	2.4E-05	2.3E-05	2.3E-05		
2100	0.001121231	0.00056	0.00037	0.00032	0.00028	0.00025	0.00022	0.0002	0.00019	0.00017	0.00016	0.00015	0.00014	0.00013	0.00012	0.00012	0.00011	0.00011	0.00011		
2200	0.004578437	0.0023	0.00154	0.00132	0.00115	0.00103	0.00092	0.00084	0.00077	0.00071	0.00066	0.00062	0.00058	0.00054	0.00051	0.00049	0.00046	0.00044	0.00044		
2300	0.016234192	0.00827	0.00555	0.00477	0.00418	0.00372	0.00335	0.00305	0.00279	0.00258	0.0024	0.00224	0.0021	0.00198	0.00187	0.00177	0.00168	0.0016	0.0016		
2400	0.049020722	0.02589	0.0176	0.01518	0.01334	0.0119	0.01074	0.00978	0.00899	0.00831	0.00773	0.00722	0.00678	0.00638	0.00603	0.00572	0.00544	0.00518	0.00518		
2500	0.122556092	0.06914	0.04838	0.04208	0.03725	0.03341	0.03029	0.02771	0.02553	0.02367	0.02207	0.02067	0.01943	0.01834	0.01736	0.01648	0.01569	0.01496	0.01496		
2700	0.443017439	0.29418	0.22548	0.20269	0.18437	0.16927	0.15659	0.14575	0.13638	0.12819	0.12096	0.11453	0.10877	0.10358	0.09887	0.09458	0.09076	0.08705	0.08705		
3000	1.294304851	0.99393	0.83901	0.78415	0.73842	0.69946	0.66569	0.63603	0.60967	0.58604	0.56468	0.54524	0.52744	0.51106	0.49592	0.48187	0.46877	0.45653	0.45653		
		Fuel Equivalence ratio - 1.09																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000183392	9.2E-05	6.1E-05	5.2E-05	4.6E-05	4.1E-05	3.7E-05	3.3E-05	3.1E-05	2.8E-05	2.6E-05	2.4E-05	2.3E-05	2.2E-05	2E-05	1.9E-05	1.8E-05	1.7E-05	1.7E-05		
2100	0.000868397	0.00043	0.00029	0.00025	0.00022	0.00019	0.00017	0.00016	0.00014	0.00013	0.00012	0.00012	0.00011	0.00011	0.0001	9.7E-05	9.2E-05	8.7E-05	8.3E-05		
2200	0.003551993	0.00178	0.00119	0.00102	0.00089	0.00079	0.00071	0.00065	0.0006	0.00055	0.00051	0.00048	0.00045	0.00042	0.0004	0.00038	0.00036	0.00034	0.00034		
2300	0.012687397	0.00643	0.00431	0.0037	0.00324	0.00288	0.00259	0.00236	0.00216	0.002	0.00186	0.00173	0.00162	0.00153	0.00144	0.00137	0.0013	0.00124	0.00124		
2400	0.039080302	0.02035	0.01376	0.01185	0.0104	0.00927	0.00836	0.00761	0.00698	0.00645	0.006	0.0056	0.00526	0.00495	0.00468	0.00444	0.00422	0.00402	0.00402		
2500	0.101279118	0.05571	0.03853	0.0334	0.02947	0.02637	0.02387	0.0218	0.02006	0.01857	0.01729	0.01618	0.0152	0.01433	0.01356	0.01287	0.01224	0.01167	0.01167		
2700	0.396833716	0.25634	0.19303	0.17235	0.15585	0.14234	0.13107	0.12151	0.11328	0.10612	0.09983	0.09426	0.08929	0.08483	0.08079	0.07713	0.07378	0.07074	0.07074		
3000	1.231334911	0.93392	0.78135	0.72752	0.68274	0.64467	0.61174	0.58287	0.55726	0.53434	0.51366	0.49487	0.4777	0.46192	0.44736	0.43387	0.42131	0.40959	0.40959		
		Fuel Equivalence ratio - 1.1																			
		10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100	105		
2000	0.000145638	7.3E-05	4.9E-05	4.2E-05	3.6E-05	3.2E-05	2.9E-05	2.6E-05	2.4E-05	2.2E-05	2.1E-05	1.9E-05	1.8E-05	1.7E-05	1.6E-05	1.5E-05	1.4E-05	1.3E-05	1.3E-05		
2100	0.000689273	0.00034	0.00023	0.0002	0.00017	0.00015	0.00014	0.00013													

Fuel Equivalence ratio - 1.13																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	8.119E-05	4.1E-05	2.7E-05	2.3E-05	2E-05	1.8E-05	1.6E-05	1.5E-05	1.4E-05	1.2E-05	1.2E-05	1.1E-05	1E-05	9.6E-06	9E-06	8.1E-06
2100	0.0003834	0.00019	0.00013	0.00011	9.6E-05	8.5E-05	7.7E-05	7E-05	6.4E-05	5.9E-05	5.5E-05	5.1E-05	4.8E-05	4.5E-05	4.3E-05	3.7E-05
2200	0.001569276	0.00079	0.00052	0.00045	0.00039	0.00035	0.00031	0.00029	0.00026	0.00024	0.00022	0.00021	0.0002	0.00019	0.00017	0.00016
2300	0.005662997	0.00284	0.0019	0.00163	0.00143	0.00127	0.00114	0.00104	0.00095	0.00088	0.00082	0.00076	0.00071	0.00067	0.00063	0.00057
2400	0.018051452	0.00916	0.00614	0.00527	0.00461	0.0041	0.0037	0.00336	0.00308	0.00285	0.00265	0.00247	0.00232	0.00218	0.00206	0.00195
2500	0.050467447	0.02625	0.01775	0.01527	0.01341	0.01195	0.01077	0.00981	0.009	0.00832	0.00773	0.00722	0.00678	0.00638	0.00603	0.00572
2700	0.252028324	0.14795	0.1055	0.09235	0.08215	0.07399	0.06731	0.06175	0.05704	0.053	0.0495	0.04643	0.04372	0.04131	0.03916	0.03721
3000	0.997905375	0.71778	0.57836	0.53014	0.4905	0.45717	0.42865	0.40389	0.38215	0.36286	0.34562	0.33009	0.31601	0.30319	0.29144	0.27066
Fuel Equivalence ratio - 1.14																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	3.98759E-05	3.5E-05	2.3E-05	2E-05	1.7E-05	1.6E-05	1.4E-05	1.3E-05	1.2E-05	1.1E-05	1E-05	9.3E-06	8.7E-06	8.2E-06	7.3E-06	6.6E-06
2100	0.000329146	0.00016	0.00011	9.4E-05	8.2E-05	7.3E-05	6.6E-05	6E-05	5.5E-05	5.1E-05	4.7E-05	4.4E-05	4.1E-05	3.9E-05	3.7E-05	3.1E-05
2200	0.001346272	0.00067	0.00045	0.00039	0.00034	0.0003	0.00027	0.00025	0.00022	0.00021	0.00019	0.00018	0.00017	0.00016	0.00015	0.00013
2300	0.004862241	0.00244	0.00163	0.0014	0.00122	0.00109	0.00098	0.00089	0.00082	0.00075	0.0007	0.00065	0.00061	0.00058	0.00054	0.00049
2400	0.015546069	0.00787	0.00527	0.00452	0.00396	0.00352	0.00317	0.00288	0.00264	0.00244	0.00227	0.00212	0.00199	0.00187	0.00177	0.00167
2500	0.043826034	0.02265	0.01528	0.01314	0.01152	0.01026	0.00925	0.00842	0.00773	0.00714	0.00664	0.0062	0.00581	0.00548	0.00517	0.0049
2700	0.227363164	0.13119	0.09274	0.08095	0.07184	0.06458	0.05866	0.05373	0.04958	0.04602	0.04294	0.04024	0.03787	0.03576	0.03387	0.03218
3000	0.949607728	0.67456	0.53885	0.49217	0.45393	0.42187	0.39451	0.37083	0.35009	0.33173	0.31536	0.30064	0.28734	0.27523	0.26417	0.25401
Fuel Equivalence ratio - 1.18																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	3.98759E-05	3.5E-05	2.3E-05	2E-05	1.7E-05	1.6E-05	1.4E-05	1.3E-05	1.2E-05	1.1E-05	1E-05	9.3E-06	8.7E-06	8.2E-06	7.3E-06	6.6E-06
2100	0.00018258	9.1E-05	6.1E-05	5.2E-05	4.6E-05	4.1E-05	3.7E-05	3.3E-05	3E-05	2.8E-05	2.6E-05	2.4E-05	2.3E-05	2.1E-05	1.9E-05	1.7E-05
2200	0.000745077	0.00037	0.00025	0.00021	0.00019	0.00017	0.00015	0.00014	0.00012	0.00011	0.00011	9.9E-05	9.3E-05	8.8E-05	8.3E-05	7.5E-05
2300	0.002689406	0.00135	0.0009	0.00077	0.00067	0.0006	0.00054	0.00049	0.00045	0.00041	0.00039	0.00036	0.00034	0.00032	0.0003	0.00028
2400	0.008951789	0.00435	0.00291	0.00249	0.00218	0.00194	0.00175	0.00159	0.00146	0.00134	0.00125	0.00117	0.00109	0.00103	0.00097	0.00092
2500	0.024890127	0.01265	0.00848	0.00728	0.00638	0.00567	0.00511	0.00465	0.00426	0.00394	0.00366	0.00341	0.0032	0.00301	0.00285	0.0027
2700	0.145045149	0.07902	0.05442	0.04709	0.04151	0.03712	0.03356	0.03063	0.02817	0.02608	0.02427	0.0227	0.02132	0.0201	0.01901	0.01803
3000	0.754399438	0.50647	0.3896	0.35055	0.31906	0.29304	0.27114	0.25242	0.23622	0.22204	0.20952	0.19837	0.18838	0.17938	0.17121	0.16377
Fuel Equivalence ratio - 1.19																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	3.41483E-05	1.7E-05	1.1E-05	9.8E-06	8.5E-06	7.6E-06	6.8E-06	6.2E-06	5.7E-06	5.3E-06	4.9E-06	4.6E-06	4.3E-06	4E-06	3.8E-06	3.4E-06
2100	0.000160379	8E-05	5.3E-05	4.6E-05	4E-05	3.6E-05	3.2E-05	2.9E-05	2.7E-05	2.5E-05	2.3E-05	2.1E-05	2E-05	1.9E-05	1.8E-05	1.5E-05
2200	0.000653977	0.00033	0.00022	0.00019	0.00016	0.00015	0.00013	0.00012	0.00011	0.0001	9.3E-05	8.7E-05	8.2E-05	7.7E-05	7.3E-05	6.5E-05
2300	0.002359545	0.00118	0.00079	0.00068	0.00059	0.00053	0.00047	0.00043	0.00039	0.00036	0.00034	0.00032	0.0003	0.00028	0.00026	0.00023
2400	0.007594321	0.00382	0.00255	0.00218	0.00191	0.0017	0.00153	0.00139	0.00128	0.00118	0.00109	0.00102	0.00096	0.0009	0.00085	0.00081
2500	0.021903706	0.0111	0.00744	0.00638	0.00559	0.00497	0.00448	0.00407	0.00374	0.00345	0.0032	0.00299	0.00281	0.00264	0.00249	0.00236
2700	0.130078596	0.07015	0.0481	0.04157	0.03661	0.0327	0.02955	0.02696	0.02478	0.02293	0.02133	0.01995	0.01873	0.01765	0.01669	0.01583
3000	0.71059636	0.47041	0.35864	0.32158	0.29181	0.26732	0.24677	0.22926	0.21415	0.20095	0.18933	0.17901	0.16978	0.16147	0.15395	0.14711
Fuel Equivalence ratio - 1.23																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	2.14772E-05	1.1E-05	7.2E-06	6.1E-06	5.4E-06	4.8E-06	4.3E-06	3.9E-06	3.6E-06	3.3E-06	3.1E-06	2.9E-06	2.7E-06	2.5E-06	2.4E-06	2.1E-06
2100	0.000100467	5E-05	3.3E-05	2.9E-05	2.5E-05	2.2E-05	2E-05	1.8E-05	1.7E-05	1.5E-05	1.4E-05	1.3E-05	1.3E-05	1.2E-05	1.1E-05	9.6E-06
2200	0.000408324	0.0002	0.00014	0.00012	0.0001	9.1E-05	8.2E-05	7.4E-05	6.8E-05	6.3E-05	5.8E-05	5.4E-05	5.1E-05	4.8E-05	4.5E-05	3.9E-05
2300	0.001489682	0.00074	0.00049	0.00042	0.00037	0.00033	0.00029	0.00027	0.00025	0.00023	0.00021	0.0002	0.00018	0.00017	0.00016	0.00015
2400	0.004730505	0.00237	0.00158	0.00136	0.00119	0.00106	0.00095	0.00086	0.00079	0.00073	0.00068	0.00063	0.00059	0.00056	0.00053	0.00048
2500	0.013717877	0.00691	0.00462	0.00396	0.00347	0.00309	0.00278	0.00253	0.00232	0.00214	0.00199	0.00185	0.00174	0.00164	0.00155	0.00146
2700	0.08569698	0.04489	0.03042	0.0262	0.02301	0.02051	0.0185	0.01685	0.01547	0.0143	0.0133	0.01242	0.01166	0.01098	0.01038	0.00984
3000	0.555079606	0.34814	0.25693	0.2276	0.20442	0.18561	0.17003	0.15689	0.14567	0.13596	0.12748	0.12	0.11336	0.10742	0.10207	0.09724
Fuel Equivalence ratio - 1.24																
	10	20	30	35	40	45	50	55	60	65	70	75	80	85	90	105
2000	1.93286E-05	9.7E-06	6.4E-06	5.5E-06	4.8E-06	4.3E-06	3.9E-06	3.5E-06	3.2E-06	3E-06	2.8E-06	2.6E-06	2.4E-06	2.3E-06	2.2E-06	1.9E-06
2100	9.03244E-05	4.5E-05	3E-05	2.6E-05	2.3E-05	2E-05	1.8E-05	1.6E-05	1.5E-05	1.4E-05	1.3E-05	1.2E-05	1.1E-05	1E-05	9.5E-06	8.6E-06
2200	0.000366786	0.00018	0.00012	0.0001	9.2E-05	8.2E-05	7.3E-05	6.7E-05	6.1E-05	5.6E-05	5.2E-05	4.9E-05	4.6E-05	4.3E-05	4.1E-05	3.7E-05
2300	0.001319237	0.00066	0.00044	0.00038	0.00033	0.00029	0.00026	0.00024	0.00022	0.0002	0.00019	0.00018	0.00017	0.00016	0.00015	0.00013
2400	0.004245056	0.00213	0.00142	0.00122	0.00106	0.00095	0.00085	0.00077	0.00071	0.00066	0.00061	0.00057	0.00053	0.0005	0.00047	0.00043
2500	0.012317359	0.0062	0.00414	0.00356	0.00311	0.00277	0.00249	0.00226	0.00208	0.00192	0.00178	0.00166	0.00156	0.00147	0.00139	0.00131
2700	0.077579535	0.04043	0.02735	0.02354	0.02066	0.01842	0.01661	0.01512	0.01388	0.01283	0.01192	0.01114	0.01045	0.00984	0.0093	0.00882
3000	0.520983987	0.32263	0.2364	0.20887	0.1872	0.16967	0.15518	0.143	0.13261	0.12364	0.11582	0.10893	0.10283	0.09737	0.09247	0.08804

Figure 34 O₂/N₅ content at varying FER, Pressures and temperatures for gasoline C8.26H15.5

9.6. Appendix F – Bilinear interpolation coding

Used on Excel with the above tables in Appendix E to find the correct values for O₂. By using the many functions of Excel, it results in accurate values.

9.6.1. Q12 - Bottom left

=LOOKUP(IF(R358<\$AD\$18,\$AD\$18,IF(R358<\$AD\$19,\$AD\$19,IF(R358<\$AD\$20,\$AD\$20,IF(R358<\$AD\$21,\$AD\$21,IF(R358<\$AD\$22,\$AD\$22,IF(R358<\$AD\$23,\$AD\$23,IF(R358<\$AD\$24,\$AD\$24,IF(R358<\$AD\$25,\$AD\$25))))))))), \$AD\$18:\$AD\$25,IF(C358<\$AF\$17,\$AE\$18:\$AE\$25,IF(C358<\$AG\$17,\$AF\$18:\$AF\$25,IF(C358<\$AH\$17,\$AG\$18:\$AG\$25,IF(C358<\$AI\$17,\$AH\$18:\$AH\$25,IF(C358<\$AJ\$17,\$AI\$18:\$AI\$25,IF(C358<\$AK\$17,\$AJ\$18:\$AJ\$25,IF(C358<\$AL\$17,\$AK\$18:\$AK

9.6.2. Q11 – Top left

9.6.3. Q21 – Top right

9.6.4. Q22 – Bottom right

9.6.5. P - Final value

Kyle Burton - P131698

```

(FLOOR(C358,5))*((IF(R358<$AD$18,$AD$18,IF(R358<$AD$19,$AD$19,IF(R358<$AD$20,
,$AD$20,IF(R358<$AD$21,$AD$21,IF(R358<$AD$22,$AD$22,IF(R358<$AD$23,$AD$23,IF
(R358<$AD$24,$AD$24,IF(R358<$AD$25,$AD$25)))))))-
((LOOKUP(R358,AD$18:AD$25)))))))*W358))))+((((C358-
(FLOOR(C358,5))*(((IF(R358<$AD$18,$AD$18,IF(R358<$AD$19,$AD$19,IF(R358<$AD$2
0,$AD$20,IF(R358<$AD$21,$AD$21,IF(R358<$AD$22,$AD$22,IF(R358<$AD$23,$AD$23,I
F(R358<$AD$24,$AD$24,IF(R358<$AD$25,$AD$25)))))))-R358))/((CEILING(C358,5))-
(FLOOR(C358,5))*((IF(R358<$AD$18,$AD$18,IF(R358<$AD$19,$AD$19,IF(R358<$AD$2
0,$AD$20,IF(R358<$AD$21,$AD$21,IF(R358<$AD$22,$AD$22,IF(R358<$AD$23,$AD$23,I
F(R358<$AD$24,$AD$24,IF(R358<$AD$25,$AD$25)))))))-
(((LOOKUP(R358,AD$18:AD$25)))))*X358)+(((C358-(FLOOR(C358,5))))*(R358-
(LOOKUP(R358,AD$18:AD$25)))/((CEILING(C358,5))-
(FLOOR(C358,5))*((IF(R358<$AD$18,$AD$18,IF(R358<$AD$19,$AD$19,IF(R358<$AD$2
0,$AD$20,IF(R358<$AD$21,$AD$21,IF(R358<$AD$22,$AD$22,IF(R358<$AD$23,$AD$23,I
F(R358<$AD$24,$AD$24,IF(R358<$AD$25,$AD$25)))))))-
((LOOKUP(R358,AD$18:AD$25)))))*Y358)
    
```

9.7. Appendix G – Arrhenius function cont.

Originally derived from the function; where, k = rate constant, A = constant/pre-exponential factor, E_a = activation energy, R = gas constant, T = temperature

$$k = A \cdot e^{\left(\frac{-E_a}{R \cdot T}\right)}$$

(Beavon, 2016)

The function tells you the proportion with enough energy to start a reaction with the given molecules/atoms.

$$\frac{d[NO]}{dt} \propto [N_2] \cdot [O_2]^{0.5} \cdot e^{\left(\frac{-E_a}{R \cdot T}\right)}$$

$$\therefore \alpha = [N_2] \cdot [O_2]^{0.5} \cdot e^{\left(\frac{-E_a}{R \cdot T}\right)}$$

Where '4.7x10¹³' is an empirical constant found through research and engine development, to complete the Arrhenius function;

$$\therefore \alpha = 4.7 \times 10^{13} \cdot [N_2] \cdot [O_2]^{0.5} \cdot e^{\left(\frac{-67837}{T}\right)}$$

(Merket, Schwarz, stiesch, & Otto, 2006)

By finding the activation energy of N₂, the equation is simplified in the Zeldovich model equation above.

$$\frac{E_a}{Ru} = 67837 \therefore E_a = 563 \text{ MJ/Kmol}$$

This is the activation energy needed to start a reaction. The 'N₂' is hard to split up due to the bond so it has a high activation energy.

Temperature (K)	Probability (exp(-67837/T))
2000	1.85944E-15
2100	9.35062E-15
2200	4.06003E-14
2300	1.55156E-13
2400	5.30256E-13
2500	1.6425E-12
2600	4.66397E-12
2700	1.22583E-11
2800	3.00698E-11
2900	6.93352E-11
3000	1.51213E-10

The probability of a reaction to make NOx is approximately 10000 times more likely at 3000K than at 2000K. In reality below 1800K there is not enough probability that enough molecule/atoms have the necessary energy to equal the activation energy to start a reaction, hence NOx production isn't seen below this temperature.

9.8. Appendix H – NOx prediction Values

NOX. SOC->EOC											
	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000	6500
Calc	20.30016	1163.261	4186.341	810.658	2285.919	4882.689	3723.489	3338.85	3944.85	3137.554	3748.339
Ford	871	1553	1577	1787	1979	2467	2404	1695	1690	1335	1668
R1M	2518.188	17301.02	37626.48	8020.334	17521.05	31579.86	23286.94	17973.4	18991.16	14765.79	15557.91
Ford Cp	4.060031	232.6521	837.2681	162.1316	457.1838	976.5378	744.4919	667.77	789.154	627.5109	749.6678
Custom CP	10.98282	615.4565	1893.143	430.8848	1124.185	2533.26	1937.565	1927.699	2214.036	1724.223	1914.127

Figure 35 NOx predictions for SOC to EOC

NOX. SOC->T.Peak											
	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000	6500
Calc	8.901677	414.0038	1657.961	312.3124	852.6443	1612.398	1350.598	1102.207	1248.137	1016.542	1325.742
Ford	871	1553	1577	1787	1979	2467	2404	1695	1690	1335	1668
R1M	1267.426	5483.354	13075.73	2758.177	5862.742	9252.541	7477.815	5304.765	5204.529	4247.581	4946.881
Ford Cp	1.780335	82.80076	331.5923	62.46247	170.5289	322.4797	270.1195	220.4413	249.8114	203.3085	265.1484
Custom CP	4.493915	224.503	757.6646	174.6176	420.1651	841.675	694.8759	638.998	697.5416	558.5434	685.6859

Figure 36 NOx SOC to peak temperature

NOX. SOC.>T.Peak											
	1500	2000	2500	3000	3500	4000	4500	5000	5500	6000	6500
Calc	9.392156	388.7565	374.4219	286.2056	817.4408	1545.401	1360.692	775.8909	1167.845	961.5013	1277.982
Ford	871	1553	1577	1787	1979	2467	2404	1695	1690	1335	1668
Ford Cp	1.264069	77.75131	319.67	57.24113	163.4882	309.0802	235.7242	237.4743	233.569	192.3003	255.5964
Custom CP	3.197557	210.1303	982.0623	148.389	403.3225	804.7305	629.1092	709.1634	659.3573	533.0041	662.2064
1.7	15.96667	660.8861	636.5172	486.5496	1389.649	2627.182	2313.177	1319.015	1985.337	1634.552	2172.569

Figure 38 Polynomial burned temperature correction, for NOx prediction SOC to peak temperature

Figure 39 Excel worksheet for base data and fuel calculator

EDIT THESE CELLS					CALCULATION CELLS									
RPM	Lambda	AFR	AIRFLOW (KG/H)	(KG/M)	(KG/REV)	AirMass/Cyl	FuelMass/Cyl	Mtotal	φ=FuelEquivRatio	Mo/Wt.	R.un	Rb	Mo/Wt Pro	EGR
1500	1.1	16.05	121.6	2.026666667	3040	0.00900741	5.161209E-05	0.000956862	0.909090909	30.16932178	275.577955	287.8528637	28.882811	0.1
2000	0.99	14.45	165.5	2.75	5500	0.000916667	6.34371E-05	0.000980104	1.01010101	30.31444925	274.2586524	288.3750919	28.830507	0.8
2500	0.99	14.41	207.8	3.463333333	8658.333333	0.000923556	5.40913E-05	0.000987647	1.01010101	30.31444925	274.2586524	288.3750919	28.830507	0.1
3000	0.93	13.80	247.5	4.125	12376	0.000916667	5.161209E-05	0.000981668	1.075368817	30.40758461	273.4186259	292.0101315	28.471615	1.5
3250	0.94	13.71	261.1	4.351666667	14142.91667	0.000892055	5.10594E-05	0.000957759	1.063829787	30.39040588	273.6731807	291.3413276	28.536974	1.7
4000	0.97	14.07	304.9	5.081666667	20326.66667	0.000846944	6.01951E-05	0.00090714	1.039297835	30.34312822	273.9994354	289.4967994	28.718798	2.2
4500	0.95	13.89	312.5	5.208333333	23437.5	0.000771605	5.55511E-05	0.000827156	1.052637519	30.37465529	273.7150651	290.7273528	28.59724	2.7
5000	0.92	13.36	343.5	5.728333333	28641.66667	0.000753778	5.71659E-05	0.000829947	1.089565522	30.43232562	273.7771593	292.6222989	28.410252	3.1
5500	0.92	13.34	357.4	5.956666667	32761.66667	0.000723002	5.41245E-05	0.000776145	1.089565522	30.43232562	273.7771593	292.6222989	28.410252	3.1
6000	0.9	13.04	362.7	6.045	36270	0.000716667	5.15082E-05	0.000723175	1.111111111	30.45907877	272.5658399	294.0103872	28.277912	4.1
6500	0.89	13.13	331.9	5.916666667	35955.83333	0.00056735	4.32102E-05	0.000610561	1.123595506	30.46722955	272.8027757	294.675095	28.214125	4.1

Fuel	Formula	Mo,Wt		Element	Hydrogen	Carbon	Nitrogen	Oxygen
Isocetane	C8H18	114.2		Molecular Wt	1	12	14	16
Gasoline	C8.26H15.5	114.62						

Stoichiometric - DON'T EDIT KEEP AT 1 ALWAYS FOR FUEL CHEM CALCS										
Fuel Equiv Ratio (φ)	= 1	0.833333333	Lambda	= 1.2						
Chemical structure	C	H	+	x	(O2)	(+N2)	= 1.0	a.CO2	+b.H2O	+c.N2
Isocetane (C8H18)	8.26	15.5			2	3.76		8.26		
					O = 2x			7.75		
					12.135	=x*3.76		24.27		
						45.6276			45.6276	
Resultant	8.26	15.5	+	12.135	2	45.6276	+	8.26	7.75	45.6276

Stoichiometric - DON'T EDIT KEEP AT 1 ALWAYS FOR FUEL CHEM CALCS												
RICH	Fuel Equiv Ratio	1.1										
Structure	C	H	+	X	(O2)	(+N2)	=>	a.CO2	+b.CO	+c	+d	C=a+b (1)
Isocetane	9.086	17.05			12.135	2	3.76					2a+b=25-c (3)
C8H18							15.745	6.659		8.525		a=1.2
					O =	24.27			2.427		45.6276	b=C-a
Resultant	9.086	17.05	+	12.135	2	45.6276	=>	6.659	2.427	8.525	45.6276	

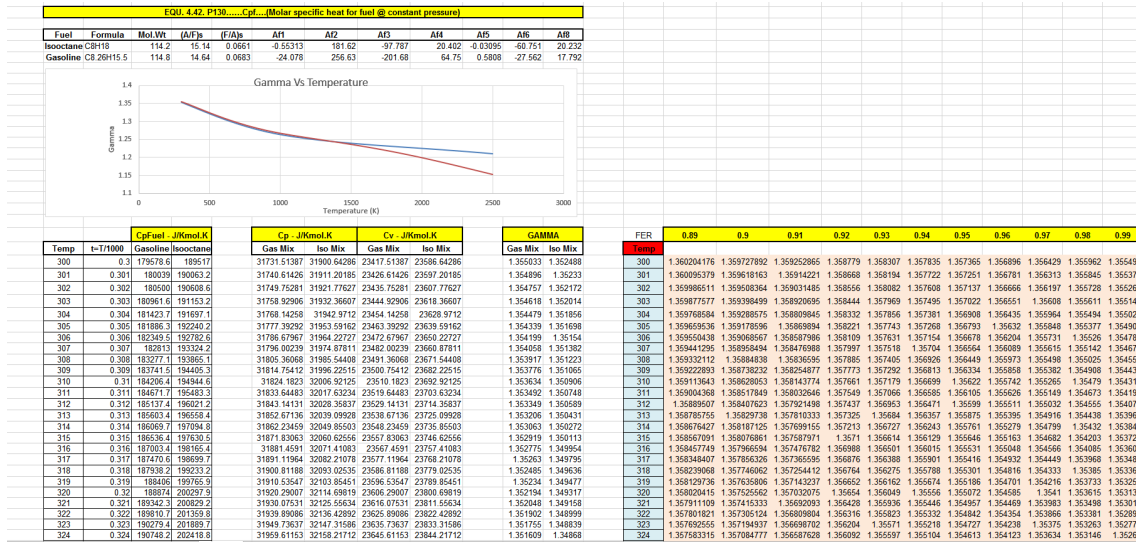
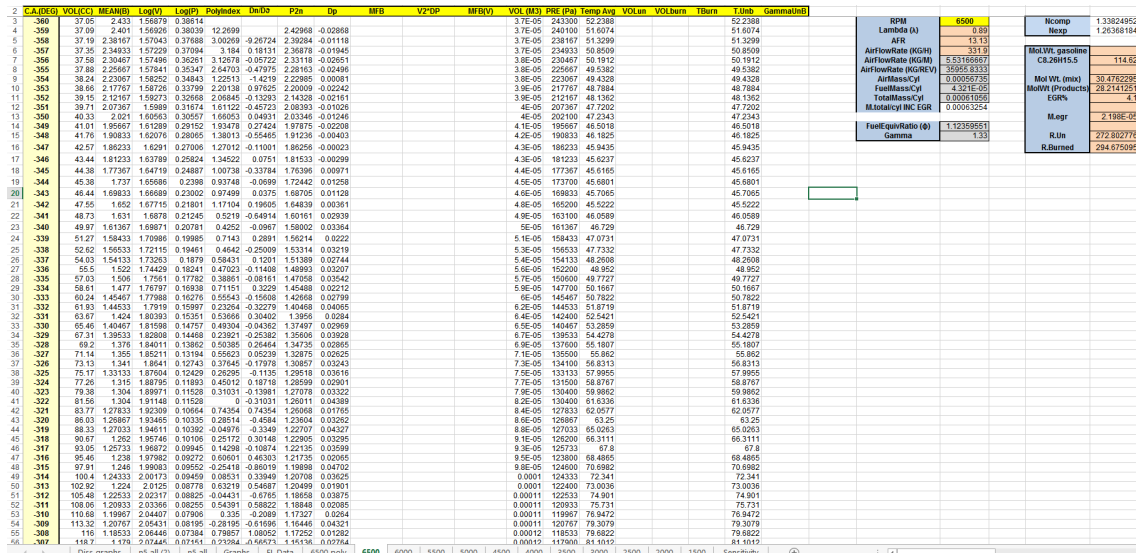


Figure 40 Variable Gamma calculations with polynomial



Combustion Modelling for NOx Production Analysis

[illegible]

Figure 42 Two zone calculation sheet

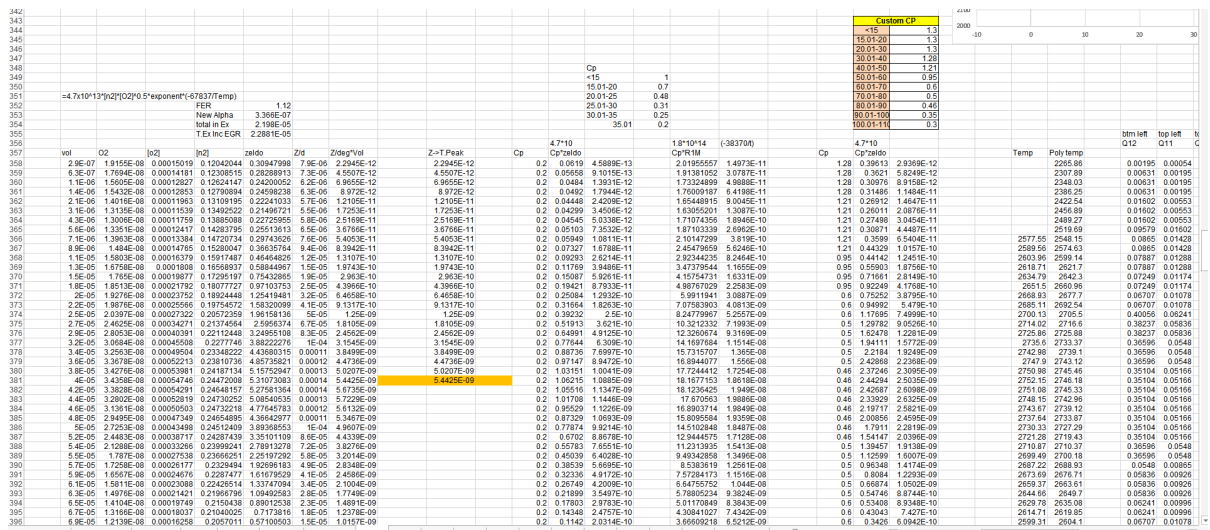


Figure 43 Bilinear interpolation calculations with different methods of NOx predictions and custom Cp table at top left. Far left is the polynomial temperature correction