



University of Wales Trinity Saint David

School of Engineering

**Combustion and Emission Study: Modelling Fuels
and NOx**

Powertrain and Sustainability

(M6X01206)

George Jones

P149914

(BEng) Motorsport Engineering

05.01.2020

Contents

List of Figures	3
List of Tables	4
1. Introduction	5
I. Aims.....	5
II. Objectives.....	5
III. Ideal Fuels	5
2. Molecular Study of an Iso-Octane & Methanol Blend	6
I. Molar Masses for Individual Fuels in Mixture.....	7
II. Combined Molar Masses	8
III. Mass Percentages for Blend.....	9
IV. Air Fuel Ratio by Mass.....	10
V. Enthalpy of Formation	12
VI. Mixture Heating Values.....	13
VII. Lower Heating Value (LHV)	13
VIII. Higher Heating Value (HHV).....	14
IX. Mass of CO ₂ Produced per Kilogram of Fuel Burned	15
.....	15
3. Iso-Octane NO _x Model for Lean Conditions	16
I. Iso-Octane Chemical Balancing for Lean Conditions	17
II. Enthalpy of Formation and Lower Heating Value due to Fuel Equivalence Ratios	18
III. Reaction Enthalpy & Flame Temperatures	19
IV. Temperature Rise of Burned Gas to Peak Pressure	22
V. Concentrations of Nitrogen & Oxygen.....	23
a) Assumptions.....	23
b) Calculations.....	23
c) Oxygen Concentration	24
d) Nitrogen Concentration	24
VI. Zeldovich Model.....	25
4. Investigation into the effects of Exhaust Gas Recirculation	26
I. Start of Combustion & Burn Zone Temperatures	26
II. NO _x Particles Per Million Produced With Exhaust Gas Recirculation.....	28
5. Conclusion.....	29
I. Limitations to the Model	29
II. Further Improvements for the Model	30
References	31

List of Figures

Figure 1 - MATLAB Script Molar Masses	7
Figure 2 - MATLAB Script Methanol Molar Mass.....	7
Figure 3 - MATLAB Script Iso-Octane Molar Mass	8
Figure 4 - MATLAB Script Total Molar Mass	8
Figure 5 - MATLAB Script Mass Percentage Methanol	9
Figure 6 - MATLAB Script Air Molar Mass	11
Figure 7 - MATLAB Script AFR by Mass	11
Figure 8 - MATLAB Script Enthalpy in (Products)	13
Figure 9 - MATLAB Script Enthalpy out (Reactants LHV)	13
Figure 10 - MATLAB Script LHV	14
Figure 11 - MATLAB Script Enthalpy out (Reactants HHV)	14
Figure 12 - MATLAB Script Net Enthalpy (HHV)	15
Figure 13 - MATLAB Script HHV	15
Figure 14 - MATLAB Script CO2 Mass per kg Fuel Burned	15
Figure 15 - MATLAB Script XLS Read	16
Figure 16 - MATLAB Script Fuel Equivalence Ratio	16
Figure 17 - MATLAB Script Enthalpies.....	18
Figure 18 - MATLAB Script Net Enthalpy.....	18
Figure 19 - Enthalpy against Temperature with Sub Ambient Values	19
Figure 20 - MATLAB Script Curve Fitting Enthalpies	20
Figure 21 - Curve Fitted Enthalpies against Temperature	20
Figure 22 - MATLAB Script Flame Temperature Enthalpy	21
Figure 23 - MATLAB Script Starting Flame Temperatures	21
Figure 24 - MATLAB Script Temp Rise for Pressure Rise	22
Figure 25 - MATLAB Script Charge Quantity per Cycle	23
Figure 26 - MATLAB Script Alpha	24
Figure 27 - MATLAB Script n3 Values.....	24
Figure 28 - MATLAB Script O2 Concentration.....	24
Figure 29 - MATLAB Script N2 Concentration	24
Figure 30 - MATLAB Script NOx Model	25
Figure 31 - MATLAB Script Total Exhaust kmols	25
Figure 32 - MATLAB Script NOx PPM	25

Figure 33 - MATLAB Script EGR Flame Temperatures	26
Figure 34 - MATLAB Script EGR Temperature Rise	26
Figure 35 - Temperature Rise per FER	27
Figure 36 - NOx PPM against Fuel Equivalence Ratio	28
Figure 37 - NOx Reduction Rate.....	28

List of Tables

Table 1 - Net Enthalpies per Fuel Equivalence Ratio	18
Table 2 - Temperature Increase due to Fuel Equivalence Ratio	21
Table 3 - Table of Assumptions.....	23

1. Introduction

I. Aims

- Investigate the molecular properties of a Methanol/Iso-Octane fuel blend
- Generate a simplified NO_x model for a typical road car through a range of lean conditions and identify the estimated NO_x particles per million.
- Include an Exhaust Gas Recirculation element to the model to evaluate its effects on the emission of NO_x.

II. Objectives

- Create a MATLAB script to analyse the molecular properties of a fuel blend including molar masses, enthalpies and stoichiometric air/fuel ratio.
- Produce a MATLAB combustion and emissions model for pure Iso-Octane in a theoretical engine
- Analyse the results to find limitations and areas of further improvement for the model.

III. Ideal Fuels

The properties of an ideal fuel are considered to include:

- No harmful reactants from the combustion process
- High energy density (calorific value)
- Ideal ignition temperature for the system
- Renewable/sustainable energy source
- Cheap to implement worldwide
- Safe to store, transport and use

2. Molecular Study of an Iso-Octane & Methanol Blend

The concept of blending different fuels is advantageous for the automotive industry as renewable fuels such as alcohols and biofuels can be implemented to reduce fossil fuel consumption. However, blending fuels will also adjust the combustion characteristics of the combined fuel.

A MATLAB script has been developed to extract the molecular properties of a pre-determined fuel mixture of Iso-Octane (50%) and Methanol (50%) and the resulting properties can be analysed to show the effects.

The addition of methanol to Iso-Octane increases the flame speed through combustion. The methanol molecule is significantly lighter than Iso-Octane due to the disparity of carbon atoms.

(Qianqian Li[†], 2016) expresses that a methanol content of over 40% will significantly increase flame speeds when the fuel equivalence ratio is greater than 1.0, whereas a lean mixture only produces small changes to flame speeds. Where methanol content is below 40%, a mild increase to flame temperatures can be observed throughout 0.7 to 1.6 equivalence ratios.

I. Molar Masses for Individual Fuels in Mixture

The atomic weights for each constituent molecule within the fuel blend has been obtained from the periodic table. These values have been introduced to the MATLAB script for processing and the resultant molecular formations for the fuel mixture are detailed in this section. The molecular masses can also be verified from the combustion tables included in the appendix (S McAllister, 2013).

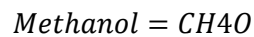
```
% Molar Masses

% C = 12.011;
% H = 1.008;
% O = 15.999;
% N = 14.007;

Mmass = [ 12.011 , 1.008 , 15.999 , 14.007]';
```

Figure 1 - MATLAB Script Molar Masses

Since,



Thus,

```
% Methanol Molar Mass

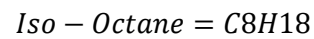
MethMass = ( (Mmass(1,1)) + (4*Mmass(2,1)) + (Mmass(3,1)) );
```

Figure 2 - MATLAB Script Methanol Molar Mass

$$\text{Methanol Molar Mass} = 12.011 + (4 \times 1.008) + 15.999$$

$$\text{Methanol Molar Mass} = \mathbf{32.042 \text{ kg/kmol}}$$

Since,



Thus,

```
% Iso-Octane Molar Mass  
IsoMass = ( (8*Mmass(1,1)) + (18*Mmass(2,1)) );
```

Figure 3 - MATLAB Script Iso-Octane Molar Mass

$$\text{Iso} - \text{Octane Molar Mass} = (8 \times 12.011) + (18 \times 1.008)$$

$$\text{Iso} - \text{Octane Molar Mass} = \mathbf{114.232 \text{ kg/kmol}}$$

II. Combined Molar Masses

As the molar composition of the fuel blend is 50/50, the equivalent mass distribution of this mixture can be determined by summing the individual molar masses for each fuel.

Since,

```
% Total Molar Mass  
TMass = MethMass + IsoMass;
```

Figure 4 - MATLAB Script Total Molar Mass

Thus,

$$\text{Total Molar Mass} = 32.042 + 114.232$$

$$\text{Total Molar Mass} = \mathbf{146.274 \text{ kg/kmol}}$$

III. Mass Percentages for Blend

To calculate the mass distribution as a percentage, the individual fuels can be divided by the total mass and multiplied by 100.

Since,

```
% Mass Percentage Methanol  
MethPer = (MethMass / TMass) * 100;  
  
% Mass Percentage Iso-Octane  
IsoPer = (IsoMass / TMass) * 100;
```

Figure 5 - MATLAB Script Mass Percentage Methanol

Thus,

$$\text{Methanol Mass Percentage} = \left(\frac{32.042}{146.274} \right) \times 100$$
$$\text{Methanol Mass Percentage} = \mathbf{21.9055\%}$$

And,

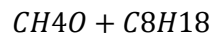
$$\text{Iso - Octane Mass Percentage} = \left(\frac{114.232}{146.274} \right) \times 100$$
$$\text{Iso - Octane Mass Percentage} = \mathbf{78.0945\%}$$

IV. Air Fuel Ratio by Mass

A stoichiometric reaction is an ideal ratio between the fuel and oxidant and is required to achieve complete combustion (Pulkrabek, 2015). In this instance, the Iso-Octane/Methanol blend is the fuel and standard air is considered the oxidant. A ratio of molar mass will be the method used for obtaining the stoichiometric value for this reaction.

Since,

$$\text{Fuel Blend} = \text{Methanol} + \text{Iso - Octane}$$

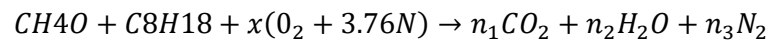


And

$$\text{Standard Air} = (\text{Oxygen} + \text{Nitrogen})$$

$$O_2 + 3.76N$$

Thus,



Where n_n and x = Balance Coefficients

Values of n_1 and n_2 must first be found from the products. From this, x and n_3 can be calculated.

$$n_1 = C + C_8 = 9$$

$$2n_2 = H_4 + H_{18} = 22$$

$$n_2 = 11$$

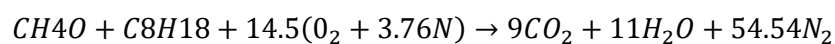
$$2x = 2n_1 + n_2$$

$$2x = (2 \times 9) + 11$$

$$x = 14.5$$

$$n_3 = 14.5 \times 3.76 = 54.52$$

Finally, the balanced stoichiometric equation can be satisfied for this fuel mixture.



With the quantity of Oxygen (x) established, the air molar mass can be calculated as follows.

Since,

```
% Air Molar Mass  
AirMass = 14.5 * ( (2*Mmass(3,1)) + 3.76 * (2*Mmass(4,1)) );
```

Figure 6 - MATLAB Script Air Molar Mass

Thus,

$$\text{Air Molar Mass} = 14.5 \times (31.998 + 763.662)$$

$$\text{Air Molar Mass} = \mathbf{1991.3 \text{ kg/kmol}}$$

The AFR by molar mass can be determined from,

```
% AFR By Mass  
AFR = AirMass / TMass;
```

Figure 7 - MATLAB Script AFR by Mass

Thus,

$$\text{AFR by molar mass} = \frac{1991.3}{146.274} = \mathbf{13.6135}$$

V. Enthalpy of Formation

There is usually a change in enthalpy when molecules are combined to create a compound. This is commonly referred to as the Enthalpy of Formation, with notation $\Delta \overline{h}_f^0$.

Δh Denotes a change in enthalpy.

The superscript ⁰ denotes a *standard datum state* of 298.15K (temperature) and 1 atmosphere (pressure) is being applied to the process, of which all other thermodynamic states are referred to (Heywood, 1988).

The subscript *f* denotes that the change in enthalpy is due to *formation*.

The Enthalpies of Formation for the most common compounds and species can be found in combustion tables. These usually display $\Delta \overline{h}_f^0$ as a function of temperature for convenience. Where tabulated data is not available, the Enthalpy of Formation can be found from the constituent molecules in the products and reactants using Hess's law. This law is an example of conservation of energy, illustrating that the route from the initial to final state in the reaction is irrelevant to the outcome.

VI. Mixture Heating Values

The Heating Value (Calorific Value) of the fuel blend is defined as being the value of heat energy from a reaction of complete combustion and can be determined from the enthalpies of the products and reactants.

Since,

```
% Enthalpy IN (Products)
EnthalpyP = FuelProp(14,10) + FuelProp(19,10);
```

Figure 8 - MATLAB Script Enthalpy in (Products)

Thus,

$$\begin{aligned} \text{Enthalpy of Mixture Products} &= 259.2 + 201.5 \\ \text{Enthalpy of Mixture Products} &= \mathbf{460.7 \text{ kJ/kmol}} \end{aligned}$$

VII. Lower Heating Value (LHV)

The LHV is referred to where the H_2O content of the reaction is in a vapour state. This is the value that is applicable to automotive internal combustion engines.

Since,

```
% Enthalpy OUT (Reactants for H2O gas)
EnthalpyRG = (9 * 393.5) + (11 * 241.8);
```

Figure 9 - MATLAB Script Enthalpy out (Reactants LHV)

Thus,

$$\text{Enthalpy of Mixture Reactants (H}_2\text{O as gas)} = \mathbf{6.2013 \text{ MJ/kmol}}$$

Since,

```
% Net Enthalpy (LHV)
EnthalpyNetG = EnthalpyRG - EnthalpyP;
```

Thus,

$$\text{Net Enthalpy of Mixture (H}_2\text{O as gas)} = \mathbf{5.7406 \text{ MJ/kmol}}$$

Since,

```
% LHV
LHV = EnthalpyNetG / TMass;
```

Figure 10 - MATLAB Script LHV

Thus,

$$\text{Mixture Lower Heating Value (LHV)} = \mathbf{39.2455 \text{ MJ/kmol}}$$

VIII. Higher Heating Value (HHV)

The HHV is referred to where the H_2O content of the reaction runs to a liquid state. The heating values can be physically determined using a Bomb Calorimeter (Yahya Al-Degs, 2012)

Since,

```
% Enthalpy OUT (Reactants for H2O liquid)
EnthalpyRL = (9 * 393.5) + (9 * 285.8);
```

Figure 11 - MATLAB Script Enthalpy out (Reactants HHV)

Thus,

$$\text{Enthalpy of Mixture Reactants (H}_2\text{O as liquid)} = \mathbf{6.1137 \text{ MJ/mol}}$$

Since,

```
% Net Enthalpy (HHV)

EnthalpyNetL = EnthalpyRL - EnthalpyP;
```

Figure 12 - MATLAB Script Net Enthalpy (HHV)

Thus,

$$\text{Net Enthalpy of Mixture (H}_2\text{O as liquid)} = \mathbf{5.653 \text{ MJ/mol}}$$

Since,

```
% HHV

HHV = EnthalpyNetL / TMass;
```

Figure 13 - MATLAB Script HHV

Thus,

$$\text{Mixture Higher Heating Value (HHV)} = \mathbf{38.6466 \text{ MJ/mol}}$$

IX. Mass of CO₂ Produced per Kilogram of Fuel Burned

```
% TMass (mol/g) = (kmol/kg)

CO2kg = 9 * (Mmass(1,1) + (2*Mmass(3,1))) / TMass;
```

Figure 14 - MATLAB Script CO₂ Mass per kg Fuel Burned

$$\text{Mass of CO}_2 = \mathbf{2.7078 \text{ kg}}$$

3. Iso-Octane NO_x Model for Lean Conditions

This section will investigate the emissions from Iso-Octane (C_8H_{18}) combustion through a range of lean fuel equivalence ratios (ϕ). The MATLAB study will be carried out as a theoretical model using sensible or ideal assumptions. The resulting emissions data will be analysed to determine the effects of lean burning on NO_x production.

The molar mass for Iso-Octane is established in section 2.

The combustion tables are imported to MATLAB as detailed below. These tables are referred to for the enthalpy values through a range of temperatures.

```
% Reads the Excel file for Properties of fuels, air and required
molecules
PropFuel = xlsread ('Fuels Database','Fuel Properties');
PropAir = xlsread ('Fuels Database','Air Properties');

PropCO2 = xlsread ('Fuels Database','CO2');
PropH2O = xlsread ('Fuels Database','H2O');
PropO2 = xlsread ('Fuels Database','O2');
PropN2 = xlsread ('Fuels Database','N2');
PropCO = xlsread ('Fuels Database','CO');
```

Figure 15 - MATLAB Script XLS Read

The fuel equivalence range for this investigation is,

```
% Phi (1/Lambda)

Phi = [0.6 :0.05: 0.9 0.95 :0.01: 1];
```

Figure 16 - MATLAB Script Fuel Equivalence Ratio

I. Iso-Octane Chemical Balancing for Lean Conditions

As the study will be considering lean conditions, the chemical balance equation must be satisfied to account for the addition of oxygen as a reactant. In the case of rich conditions, the oxygen content would be replaced with carbon monoxide.

Since,

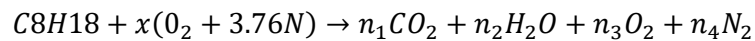
$$\text{Iso - Octane} = C_8H_{18}$$

And

$$\text{Standard Air} = (\text{Oxygen} + \text{Nitrogen})$$

$$O_2 + 3.76N$$

Thus,



Where n_n and x = Balance Coefficients

Values of n_1 and n_2 must first be found from the products. From this, x , n_3 and n_4 can be calculated.

$$n_1 = C_8 = 8$$

$$2n_2 = H_{18} = 18$$

$$n_2 = 9$$

$$2x = 2n_1 + n_2$$

$$2x = (2 \times 8) + 9$$

$$x = 12.5$$

$$n_3 = x(1 - \varphi)$$

$$n_4 = 12.5 \times 3.76 = 47$$

The fuel equivalence ratio (φ) will be used to manipulate the values of the balance coefficients through this study.

II. Enthalpy of Formation and Lower Heating Value due to Fuel Equivalence Ratios

As explained in section 2, Hess's Law can be used to find the enthalpy of formation in Iso-Octane, through the stated fuel equivalence range.

Since,

```
% Enthalpy For Products Due To Phi
hP = ((Phi)*PropFuel(14,10));

% % Enthalpy For Reactants Due To Phi
hR = ((Phi*8) * 393.5) + ((Phi*9) * 241.8);
```

Figure 17 - MATLAB Script Enthalpies

Thus,

```
% Net Enthalpy
hNet = hR - hP;

% Lower Heating Value
LHV = hNet / MassIso;
```

Figure 18 - MATLAB Script Net Enthalpy

The resultant enthalpies (as a function of FER) for the reaction can be viewed in the table below. These values will be later used to find the corresponding Start of combustion (SOC) temperatures.

Table 1 - Net Enthalpies per Fuel Equivalence Ratio

0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	0.96	0.97	0.98	0.99	1
3039	3292	3546	3799	4052	4305	4559	4812	4862	4913	4964	5014	5065

FER
Enthalpy

III. Reaction Enthalpy & Flame Temperatures

The enthalpy per temperature from the combustion tables are used in this section to obtain the start of combustion (SOC) temperatures for the fuel.

As illustrated in the graph below, the initial temperatures in the tables are below ambient and therefore can be disregarded. The Enthalpy values below 300k have an opposite trend to those above, thus have the ability to corrupt the fitted curve.

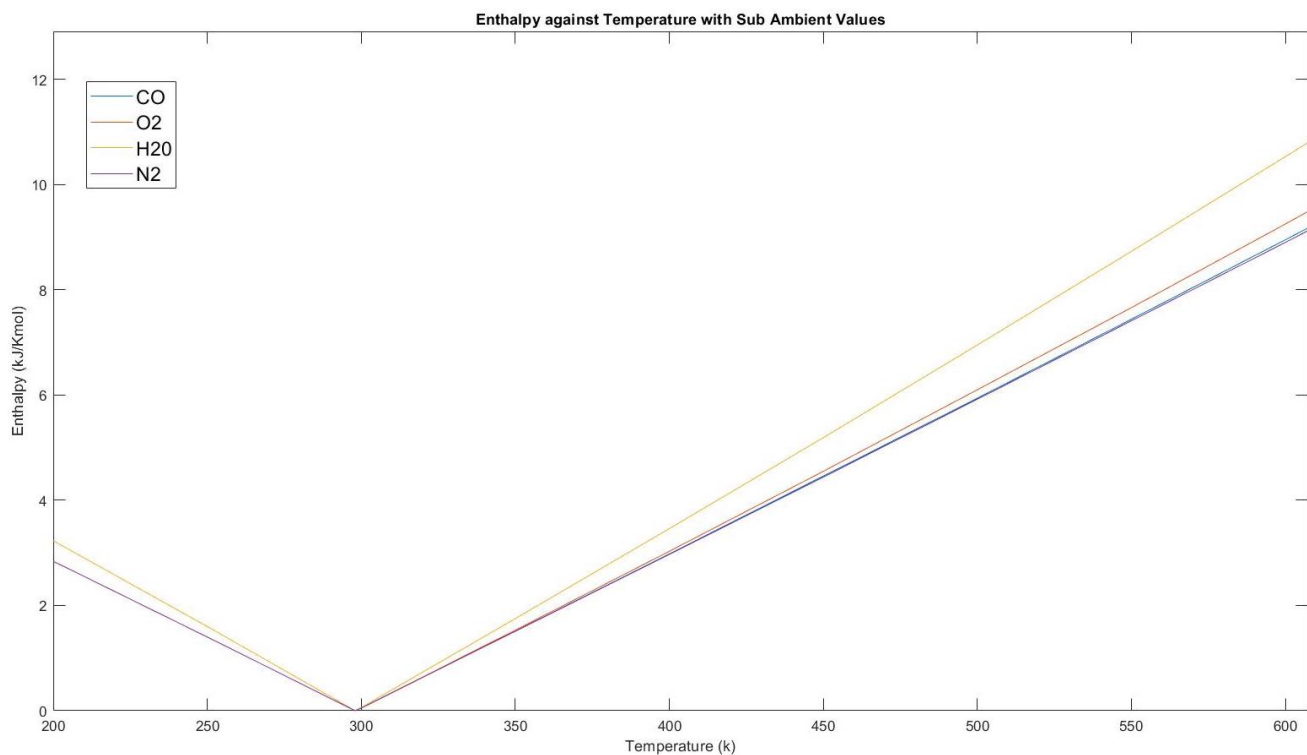


Figure 19 - Enthalpy against Temperature with Sub Ambient Values

The MATLAB curve fitting function is used to 9th order polynomial to generate an equation for the enthalpies. A temperature range from 300k to 3500k is included into the equation to give the corresponding enthalpy values for temperatures in 1k increases.

% Curve Fitting Temperatures & Enthalpies from Tables

```
FCO2 = fit( (PropCO2(4:68,1)) , (PropCO2(4:68,3)) , 'poly9');
FH2O = fit( (PropH2O(4:68,1)) , (PropH2O(4:68,3)) , 'poly9');
FO2 = fit( (PropO2(4:68,1)) , (PropO2(4:68,3)) , 'poly9');
FN2 = fit( (PropN2(4:68,1)) , (PropN2(4:68,3)) , 'poly9');
FCO = fit( (PropCO(4:68,1)) , (PropCO(4:68,3)) , 'poly9');

PCO2 = FCO2(Temp);
PH2O = FH2O(Temp);
PO2 = FO2(Temp);
PN2 = FN2(Temp);
PCO = FCO(Temp);
```

Figure 20 - MATLAB Script Curve Fitting Enthalpies

These curves can be seen below for each constituent molecule of the reactants.

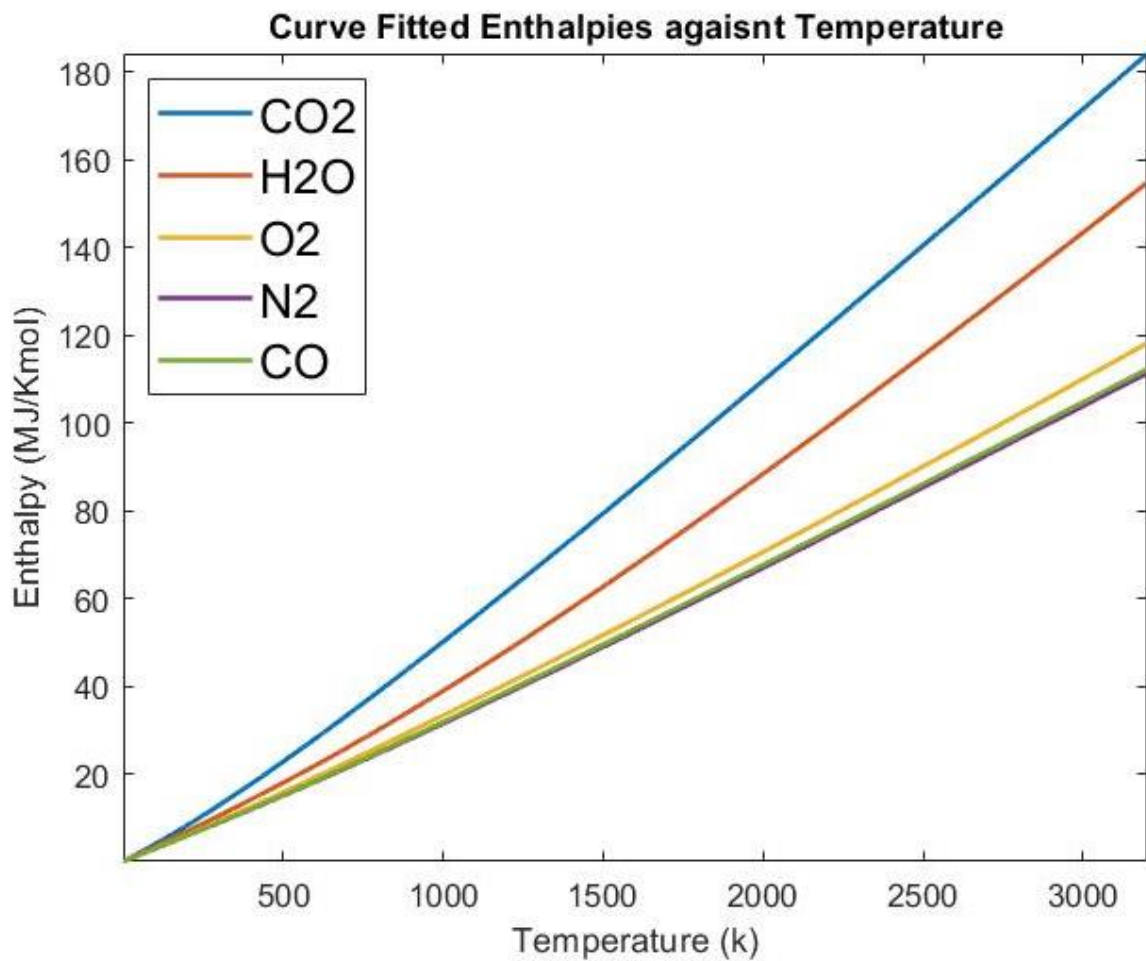


Figure 21 - Curve Fitted Enthalpies against Temperature

The fuel equivalence ratio is now multiplied by each of the reactants, except for oxygen, where φ is added using the method described in section 3.I. The resultant equation is as follows.

Enthalpies for Flame Temperature Calculations

$$(\varphi \times 8 \times CF \text{ CO}_2) + (\varphi \times 9 \times CF \text{ H}_2\text{O}) + (12.5 \times (1 - \varphi) \times \text{O}_2) + 47 \times CF \text{ N}_2$$

Where CF = 9th order Polynomial Curve Fit Results

```
% Flame Temperatures (Enthalpy)

FlameTemp = ( (Phi.*8).*PCO2) + ((Phi.*9).*PH2O) +
(12.5.*(1-Phi).*PO2) + 47.*PN2);
```

Figure 22 - MATLAB Script Flame Temperature Enthalpy

The resultant matrix is split into each fuel equivalence ratio and a 9th order polynomial curve is fitted with respect to the temperature range. This facilitates the ability to call up the required temperatures for each net enthalpy value as calculated earlier, otherwise known as the SOC flame temperatures.

```
% Starting Flame Temperatures
ft1 = feval(PhiF1, hNet(1,1));
ft2 = feval(PhiF2, hNet(1,2));
ft3 = feval(PhiF3, hNet(1,3));
ft4 = feval(PhiF4, hNet(1,4));
ft5 = feval(PhiF5, hNet(1,5));
ft6 = feval(PhiF6, hNet(1,6));
ft7 = feval(PhiF7, hNet(1,7));
ft8 = feval(PhiF8, hNet(1,8));
ft9 = feval(PhiF9, hNet(1,9));
ft10 = feval(PhiF10, hNet(1,10));
ft11 = feval(PhiF11, hNet(1,11));
ft12 = feval(PhiF12, hNet(1,12));
ft13 = feval(PhiF13, hNet(1,13));
```

Figure 23 - MATLAB Script Starting Flame Temperatures

Table 2 - Temperature Increase due to Fuel Equivalence Ratio

0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	0.96	0.97	0.98	0.99	1
1700	1794	1885	1975	2062	2147	2230	2311	2327	2343	2359	2375	2391

FEV
SOC Flame Temp

IV. Temperature Rise of Burned Gas to Peak Pressure

For this theoretical study, the pressure increase occurs over 16° of crank angle and is assumed to rise at a linear rate of 2 bar per degree, from 10 bar to its peak at 40 bar. The peak pressure is determined from assuming a part load scenario at 1800 RPM. The polytropic index is assumed to be constant at 1.17.

The temperatures in the burn zone are found using an iterative procedure, driven by a polytropic process (an adaption of Boyles Law). When combined with the Ideal Gas Law, the following equation can be used to find the rise in temperature.

$$T_2 = \sqrt[n]{\frac{P_2^{(n-1)}}{P_1^{(n-1)}}} \times T_1^n$$

Where T = Temperature, P = Pressure, n = Polytropic Index (1.17)

A MATLAB “for loop” function was used to find the rise in temperature through the pressure range.

```
% Temp Rise Due To Pressure Rise

TempRise = ones(16,13);
TempRise(1,:) = StartFlame;
for i= 1:1:15
    TempRise(i+1,:) = nthroot (((((Pres(i+1,:)).^(n-1))) ./
    (((Pres(i,:)).^(n-1)))) .* ((TempRise(i,:)) .^(n))), 1.17);
end
```

Figure 24 - MATLAB Script Temp Rise for Pressure Rise

V. Concentrations of Nitrogen & Oxygen

a) Assumptions

It is assumed that O_2 and N_2 concentrations are constant through combustion for all fuel equivalence ratios.

Table 3 - Table of Assumptions

Constant	Value
Cylinder Displacement	0.0004 m ³
Volumetric Efficiency	40 %
Cylinder Pressure @ Inlet Valve Close (IVC)	100,000 N/m ²
Charge Temperature	293 k
Combustion Chamber Volume	0.0004 m ³
Universal Gas Constant	8,314 kmol ⁻¹ k ⁻¹
Engine Speed	10,800 °/s

b) Calculations

The quantity of charge drawn into the cylinder per cycle is calculated from the following method.

Ideal Gas Law Derived Charge Quantity

$$\frac{\text{Cylinder Pressure IVC} \times (\text{Cylinder Displacement} \times \text{Volumetric Efficiency})}{\text{Universal Gas Constant} \times \text{Charge Temperature}}$$

% Charge Quantity in per cycle

$$\text{MIX} = (((\text{IVCpres}) * (\text{CylDisp} * \text{VolEff})) / ((\text{UGC}) * (\text{ChargeT})));$$

Figure 25 - MATLAB Script Charge Quantity per Cycle

From this, the actual number of kmols in the mixture can be determined for each fuel equivalence ratio.

Actual Number of kmols in Mixture per Cycle (α)

$$\frac{\text{Ideal Gas Law Derived Charge Quantity}}{\varphi + \text{Air}}$$

```
% Alpha (actual number of kmols in the mixture)

Alpha = ( (MIX) ./ ((Phi) + (12.5.*(1+3.76))) );
```

Figure 26 - MATLAB Script Alpha

c) Oxygen Concentration

The balance coefficient for oxygen (n_3) must be calculated for each value of FER to find the oxygen concentrations from the reaction.

```
% n3 As a Vector (Due To Phi Changing)

n3 = ( ((25) - (2.*(Phi.*8)) - (Phi.*9)) / 2);
```

Figure 27 - MATLAB Script n3 Values

```
% O2 Concentration

O2Con = ( (n3 .* Alpha) / (CCV) );
```

Figure 28 - MATLAB Script O2 Concentration

d) Nitrogen Concentration

```
% N2 Concentration

N2Con = ( (47 .* Alpha) / (CCV) );
```

Figure 29 - MATLAB Script N2 Concentration

Both Oxygen and Nitrogen concentrations are assumed to be constant through combustion. These concentrations are used in The Merker Zeldavich model to calculate Nitrous Oxide (NO_x) content in exhaust gases.

VI. Zeldovich Model

The Merker version of the Zeldovich model is used to calculate NO_x in this section.

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

```
% NOx [Gunter P Merker Model] (kmols/deg)

NOx = (((4.7e+13) .* N2Con .* (O2Con .^0.5)) .*exp(-
        67837./TempRise)) ./ degsec ) *CCV;
```

Figure 30 - MATLAB Script NOx Model

Total exhaust kmols is determined,

```
% Total Exhaust kmols

TotEx = Alpha .* ((Phi .* 8) + (Phi .* 9) + n3 + 47);
```

Figure 31 - MATLAB Script Total Exhaust kmols

NO_x PPM is sum of NO_x values from Zeldovich matrix per FER.

```
% NOx Parts Per Million (PPM)

NOxPPM = ((NOxSUM* 1e+06) ./ TotEx);
```

Figure 32 - MATLAB Script NOx PPM

The particles per million produced can be compared with the effects of adding EGR to the system in figure 36.

4. Investigation into the effects of Exhaust Gas Recirculation

The process of recirculating a proportion of exhaust gas back into the cylinder has become a common method in reducing the harmful gases emitted from the engine. This investigation will determine its effects on the engine during lean and stoichiometric conditions **TALK MORE HERE OR LATER?**

I. Start of Combustion & Burn Zone Temperatures

The same method (as previously demonstrated) is used to find the SOC flame temperatures. However, the additional mass percentage due to EGR must be included to the reactant enthalpies.

```
% Flame Temperatures (EGR Enthalpy)

EGRFlameTemp = (((Phi .* EGRvalue) .* 8) .* PCO2) + (((Phi .*
    EGRvalue) .* 9) .* PH2O) + ((47 .* PN2) .* EGRvalue);
```

Figure 33 - MATLAB Script EGR Flame Temperatures

The updated enthalpies are processed through the curve fitting methods to find the temperature rise due to EGR per FER.

```
% Temp Rise Due To Pressure Rise

EGRTempRise = ones(16,13);
EGRTempRise(1,:) = EGRStartFlame;
    for i= 1:1:15
EGRTempRise(i+1,:) = nthroot (((((Pres(i+1,:)).^(n-1))) ./
    (((Pres(i,:)).^(n-1)))) .* ((EGRTempRise(i,:)).^(n)),
    1.17);
    end
```

Figure 34 - MATLAB Script EGR Temperature Rise

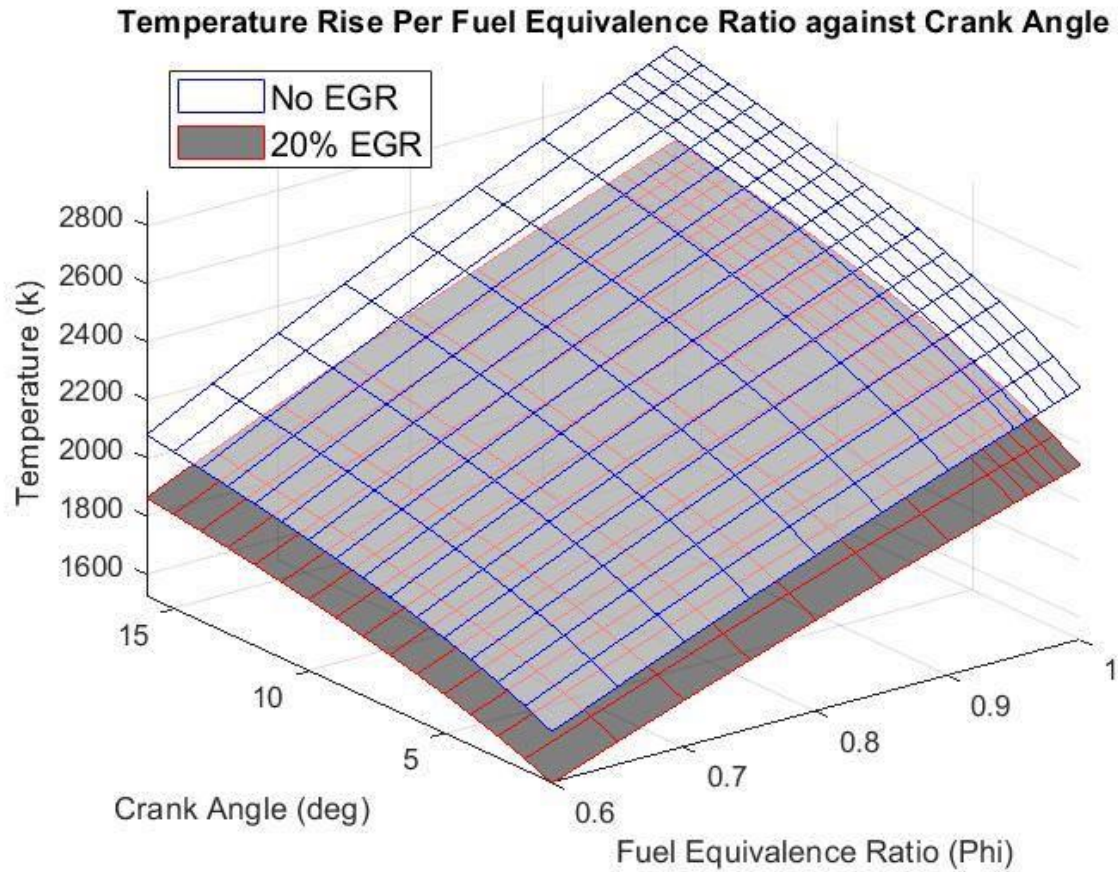


Figure 35 - Temperature Rise per FER

Addition of 20% EGR reduces peak combustion temperatures @ Stoichiometric FER by 200k.

The thermal efficiency of an engine also usually benefits from a slight increase with EGR at low engine loads. (J Hussain, 2012)

II. NO_x Particles Per Million Produced With Exhaust Gas Recirculation

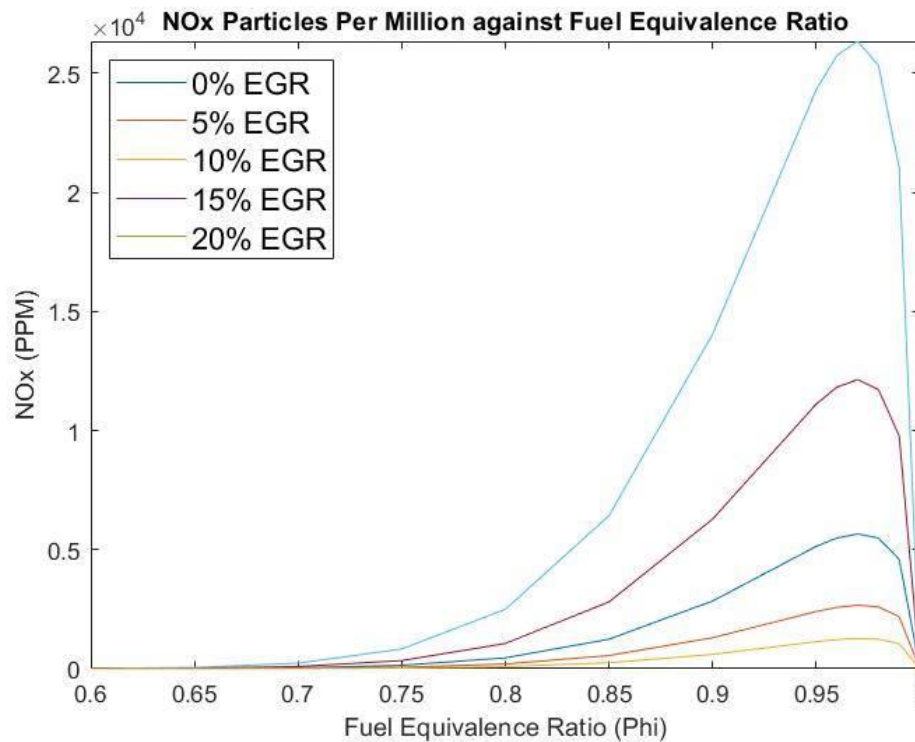


Figure 36 - NOx PPM against Fuel Equivalence Ratio

The model predicts the peak NO_x output to be an estimated 26,000 PPM at 0.97ϕ with no EGR added. The introduction of 5% EGR can be seen to reduce the overall NO_x content by approximately 60%. This linear trend is illustrated in the graph below.

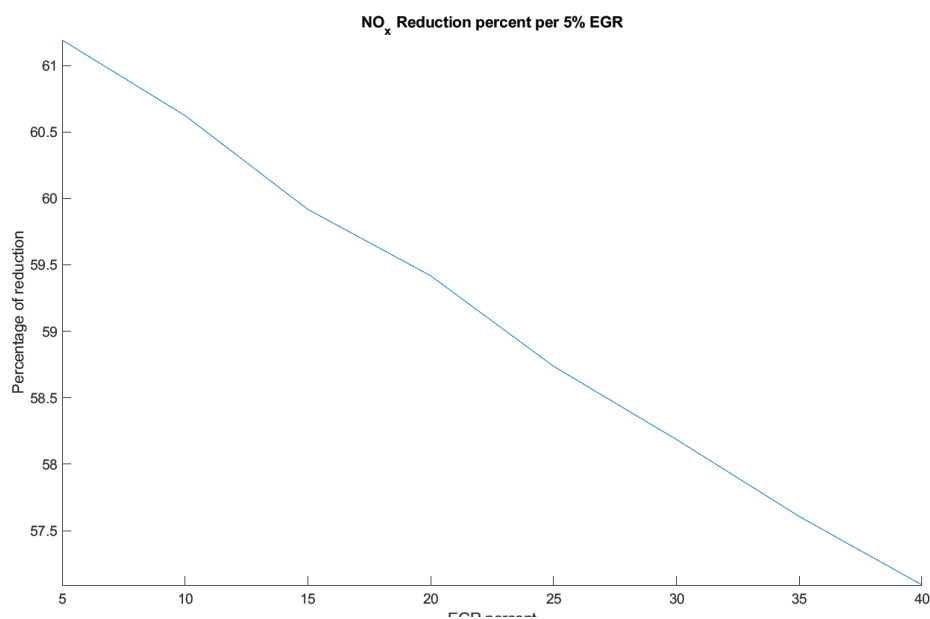


Figure 37 - NOx Reduction Rate

5. Conclusion

I. Limitations to the Model

The combustion and emissions model does provide reasonable trends for the theoretical conditions that have been applied. However, the limitations from idealised methodology and assumptions mean that significant improvements can be made to improve accuracy.

- The Zeldovich model is an empirical formula that has been created to predict the NO_x PPM for given oxygen and nitrogen concentrations. As there are many versions of this model available, it is unrealistic to assume the values are correct based on the individual driving factors Merker has used (in this study). To achieve high accuracy, an extended version of the Zeldovich model should be calibrated with real exhaust data for the type of engine and conditions that are being tested. The vast range in engine size, fuel mixtures and other variables makes it too difficult to have a direct mathematical solution (Zeldovich, 1951).
- The fuel balance equations are solved based on the assumption of pure fuel strains and only oxygen and nitrogen to comprise air. In reality, small quantities of other molecules such as sulphur would be present and thus have an influence on the reaction and emissions, to some extent.
- Although the volume of the combustion chamber is taken into consideration for the calculation of temperature rise in the burn zone, an isochoric process is implied through the volume remaining constant per degree of crank angle.
- Heat loss through cylinder walls, piston and cylinder head is not accounted for as an adiabatic process is assumed.
- The volumetric efficiency is assumed to be constant at 40% through all aspects of the model. The addition of varying levels of Exhaust gases would change this value if all other engine parameters remained stable.

- The polytropic index is assumed to be constant. This is not a realistic assumption due to the relationship between pressure and volume around the combustion event.
- The universal gas constant changes for cylinder gases over the duration of a cycle as a function of pressure, temperature and volume (P.P Walsh, 1998)
- The oxygen and nitrogen concentrations vary through combustion in reality.
- All variables in the model will undergo cyclic variation in a real internal combustion engine. This variation can be measured on an engine dynamometer over a duration of time to provide enhanced average values for each assumption, with greater precision.

II. Further Improvements for the Model

The accuracy of the model can be further developed by refining the assumptions that have been highlighted, through real world data correlation.

In addition, the MATLAB script could be redesigned to offer a fully automated fuel balancing, combustion and emissions program. This would greatly enhance the ability to compare different blends of fuels and reactions.

References

- Heywood, J. B., 1988. *Internal Combustion Engine Fundamentals*. 1 ed. s.l.:McGraw-Hill, Inc.
- J Hussain, k. P. N. A. R. M., 2012. Effect of Exhaust Gas Recirculation (EGR) on Performance and Emission of a Compression Ignition Engine with Staged Combustion (Insertion of Unburned Hydrocarbon). *International Journal of Energy Engineering*, pp. 285-292.
- P.P Walsh, P. F., 1998. *Gas Turbine Performance*. 2nd Edition ed. Oxford: Blackwell Publishing.
- Pulkrabek, W. W., 2015. *Engineering Fundamentals of the Internal Combustion Engine*. New Jersey: Prentice Hall.
- Qianqian Li†, W. Z. W. J. Y. X. Z. H., 2016. Laminar flame characteristics and kinetic modeling study of methanol-isooctane blends at elevated temperatures. *Fuel* 184, pp. 836-845.
- S McAllister, J.-Y. C. A. C. F.-P., 2013. *Fundamentals of Combustion Processes*. 1st ed. New York: Springer.
- Yahya Al-Degs, M. A.-G. G. W., 2012. Determination of Higher Heating Value of Petro-Diesels Using Mid-Infrared Spectroscopy and Chemometry. *Journal of Thermal Analysis and Calorimetry*, 107(2), pp. 853-862.
- Zeldovich, Y., 1951. *Theory of Flame Propagation*. Washington: NACA.