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CFD & Emissions Modelling

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Alternative Fuels Combustion Modelling ACHA7002

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1 Introduction

The increase in long-term climate targets and strict environmental regulations has driven the transition to and development of sustainable powertrains and specifically low emission systems becoming an automotive industry critical focus. For the UK, the 2035 mandate would ban any new internal combustion engine (ICE) vehicle with emissions at the tailpipe, creating a substantial obstacle for conventional fuelling, but also increasing the uncertainty around the viable use of alternative fuels such as blends (e.g. E85), synthetics, and even Hydrogen. Ethanol blends like E85 can offer potential benefits as their emissions formation and combustion efficiency can be influenced by their increased oxygen compositions and renewability.

This paper aims to compare and investigate petrol and E85's combustion characteristics with the use of ANSYS Forte CFD (Computational Fluid Dynamics), followed up with MATLAB post-processing to attain Wiebe function metrics for implementation of simplified representations of combustion to be deployed in Realis Wave. Some major parameters such as cylinder pressure, heat release rate, temperature, and combustion phasing are investigated and analysed in an aim to evaluate trends of performance and emissions.

Petrol (100% Iso-Octane - C_8H_{18}), and E85 (15% Iso-Octane - C_8H_{18} and 85% Ethanol - C_2H_5OH) are modelled under their equivalent operating conditions. With the petrol study being used as a form of validation compared to the dynamometer data and thus baseline for further fuel type comparison, provides understanding of the performance, emission, and efficiency trade-offs between fuel types. The findings aim to supply insight into alternate fuelling's potential role within the tightening constraints of future regulations.

2 Literature Review

2.1 Regulations

The emissions regulations currently emplaced in the UK follow that of the European Union very closely, especially those descended from the Euro-6 regulations. The UK has however introduced a stricter policy set with the upcoming 2035 mandate of all new vehicles sold having zero emissions at the tailpipe (UK Government, 2020). If this mandate goes ahead in 2035, it has significant implications for any alternative fuels, due to all having some form of emissions with even hydrogen producing H₂O and Nox (White, Steeper and Lutz, 2006; Verhelst and Wallner, 2009), even with the elimination of Nox, depending on the exactness of the regulations to come, H₂O which is a harmless emission, would still render hydrogen combustion uncompliant despite its potential benefits. If the UK was to instead switch to following the EU with Euro-7 (UK Government, 2026), they would focus on tightening the limits of pollutants opposed to enforcing zero emissions across the board.

2.2 Fuel choice

A vast scope of alternate fuelling options has been investigated for their possible emissions reduction for ICEs, these include synthetics which aim to replicate performance of regular fuels (petrol and diesel) with renewable production methods; biofuels that aim to harness fuel from biomaterial such as food stock (corn, sugarcane, soy) (Goldemberg, Coelho and Guardabassi, 2008) or waste (animal fats, agricultural residues, used cooking oils) (Knothe, 2010); and hydrogen, a non-carbon based fuel which eliminates CO & CO₂ production.

Ethanol fuels including E85, due to their high-octane ratings, oxygen content, and renewability, have been extensively studied with reduction of specific emissions and increased efficiency of combustion being observed (Turner *et al.*, 2014; Costa and Sodré, 2010). Butanol fuelling has seen increased interest as a biofuel; this is in part due to its improved compatibility over ethanol with the existing fuel infrastructures as well as its increased energy density (Rakopoulos *et al.*, 2010; Siwale *et al.*, 2013). Hydrogen fuelling experiences setbacks due to the infrastructure updates required, storage challenges, and retention of Nox production, however, hydrogen does offer a carbon free fuel with high efficiency and rapid combustion times (White, Steeper and Lutz, 2006).

Additional alternatives like synthetic e-fuels and methanol are currently being studied and evaluated for their lifecycle emission reduction promise, however this study covers E85, selected due to its compatibility with current engine models, well documented behaviours, and its availability, while further studies would investigate butanol as a biofuel alternative; and hydrogen as a non-carbon-based alternative.

3 Methodology

3.1 Engine

Table 3-1: Ford Sigma 1.6L Engine Measurements

Measurement	Value
Bore	79mm
Stroke	81.4mm
Con-Rod Length	138mm
Compression Ratio	11.1:1

3.2 Ansys Forte Modelling

3.2.1 Assumptions & Simplifications

3.2.1.1 Sector Mesh

The sector mesh generated for the sigma cylinder used a flat piston head, decided upon due to the lack of available information or models of the piston bowl as well as differences between performance and commercial models.

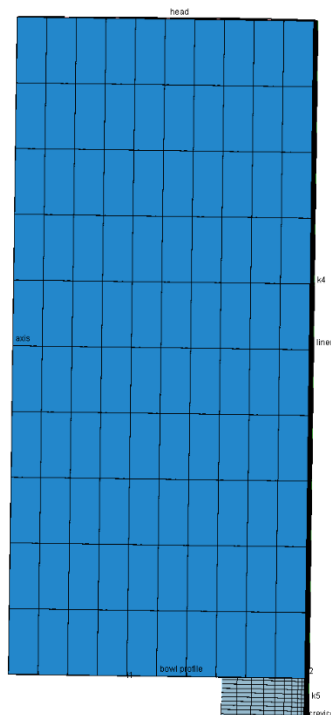


Figure 3-1: Forte Sector Mesh

3.2.1.2 RPM

For simplification and reduction of simulation count and time, a single RPM value of 6000 was used, this value was carried forward for every simulation with the exception of a multi-value run for the petrol.

3.2.1.3 Injection Modelling

The use of the injection modelling was not utilised

3.2.2 Setup

3.3 MATLAB Calculations

From the forte results files an Excel was created for both the petrol and E85 simulations, taking the columns for crank angle, cylinder mass, and unburnt hydrocarbon mass fraction, used to calculate the burnt mass fraction in addition to identifying the start of combustion (SOC) and end of combustion (EOC) estimated at 95% burn rate. MATLAB was then used to plot the burnt mass fraction against crank angle, then calculate and plot the points of 10, 50, and 90% burn rates. From this, the curve fitter tool was utilised with the bounds set to SOC and EOC, using the Wiebe function equation to determine the function exponent:

$$x_b(\theta) = 1 - \exp \left[-a \left(\frac{\theta - \theta_{soc}}{\Delta\theta_{dur}} \right)^{m+1} \right]$$

$x_b(\theta)$ = Mass fraction burned

θ = Crankshaft angle (°)

θ_{soc} = Crankshaft angle at start of combustion (°)

$\Delta\theta_{dur}$ = Crankshaft angle range during combustion (°)

a = Efficiency parameter

m = Shape parameter

Equation 3-1: Wiebe Function Formula

3.4 Realis Wave Modelling

3.4.1 Assumptions & Simplifications

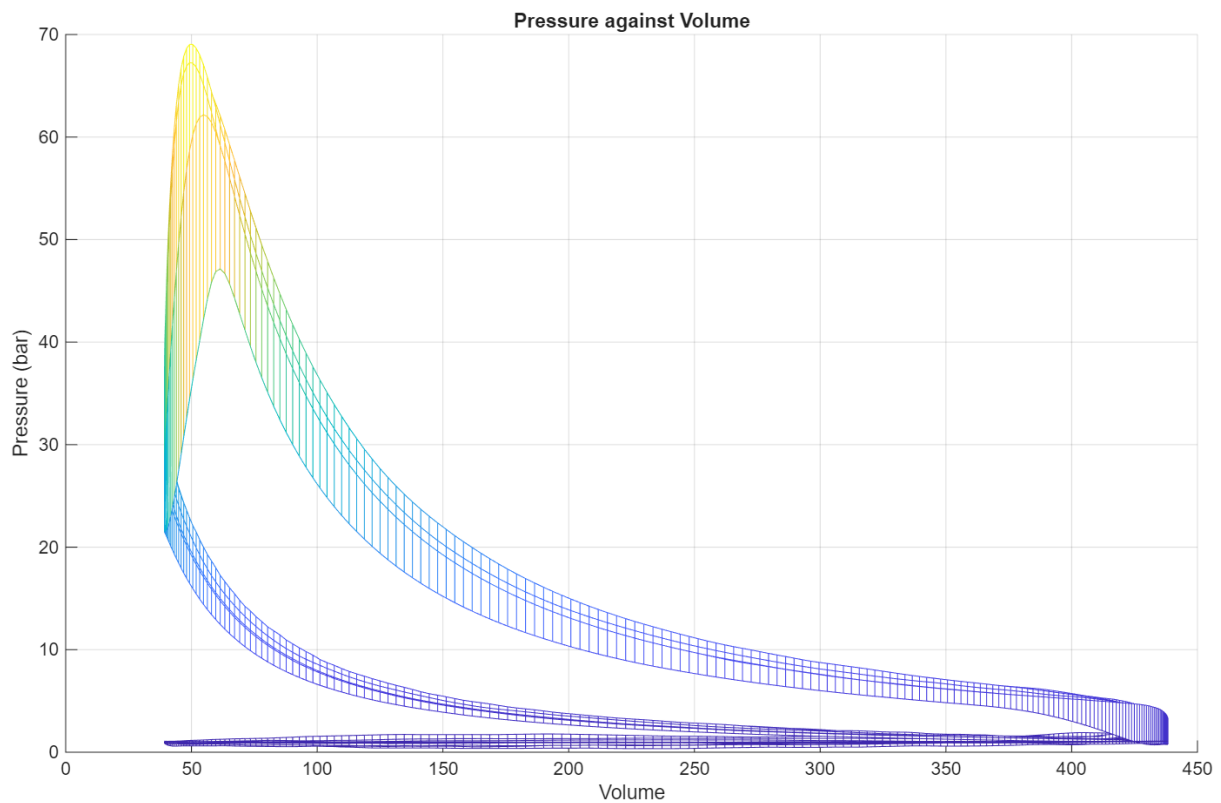
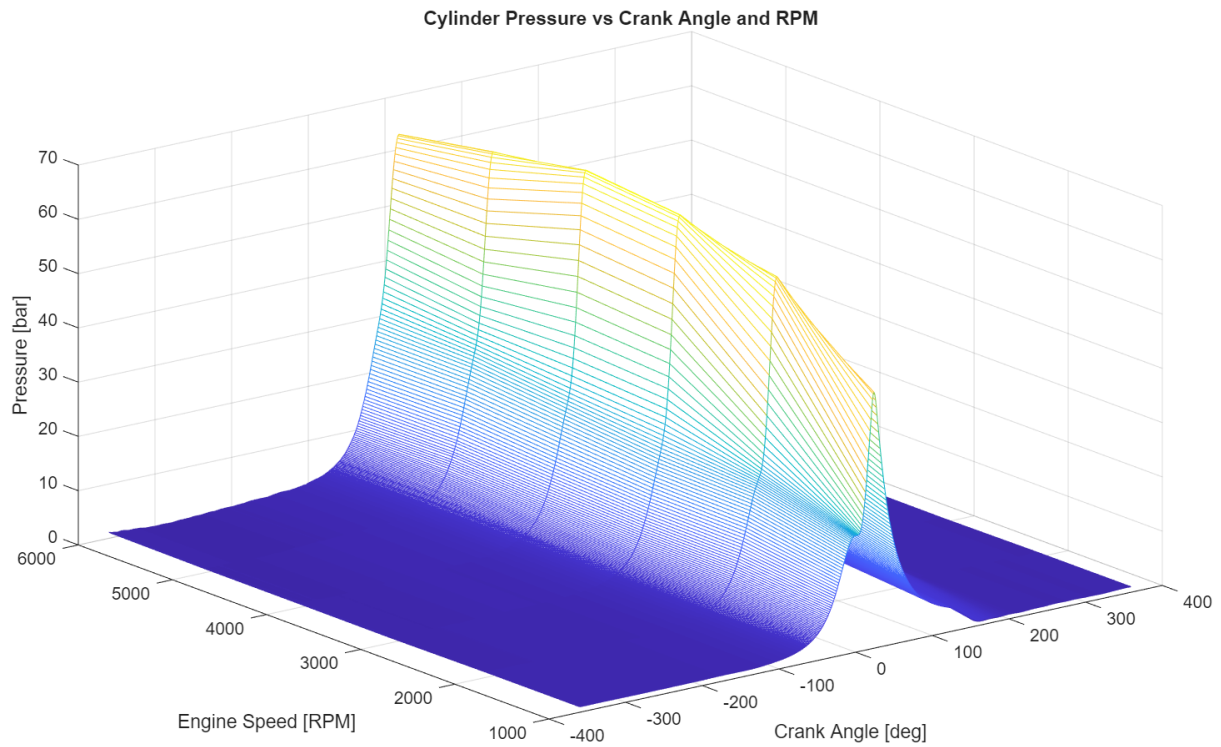
While the sigma 1.6L engine is an in-line 4, within wave only a single cylinder was modelled for simplicity and speed of simulations.

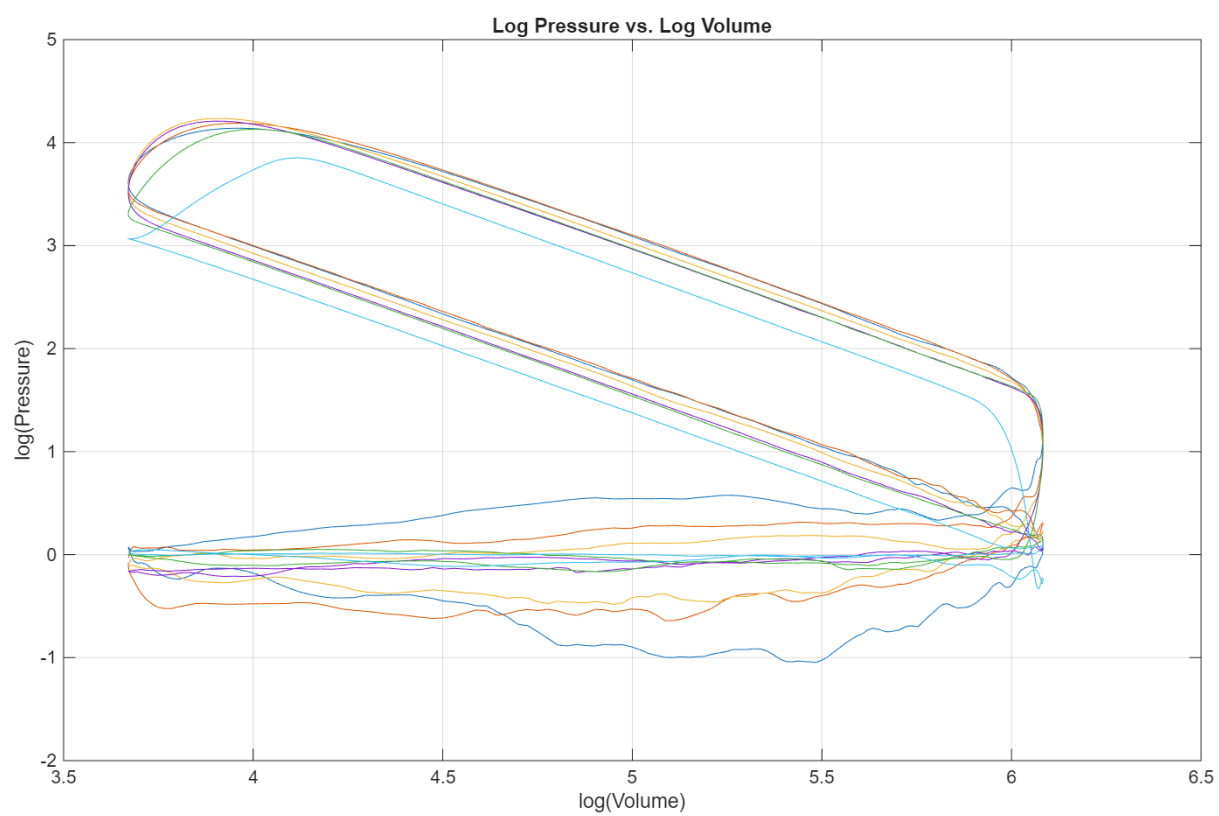
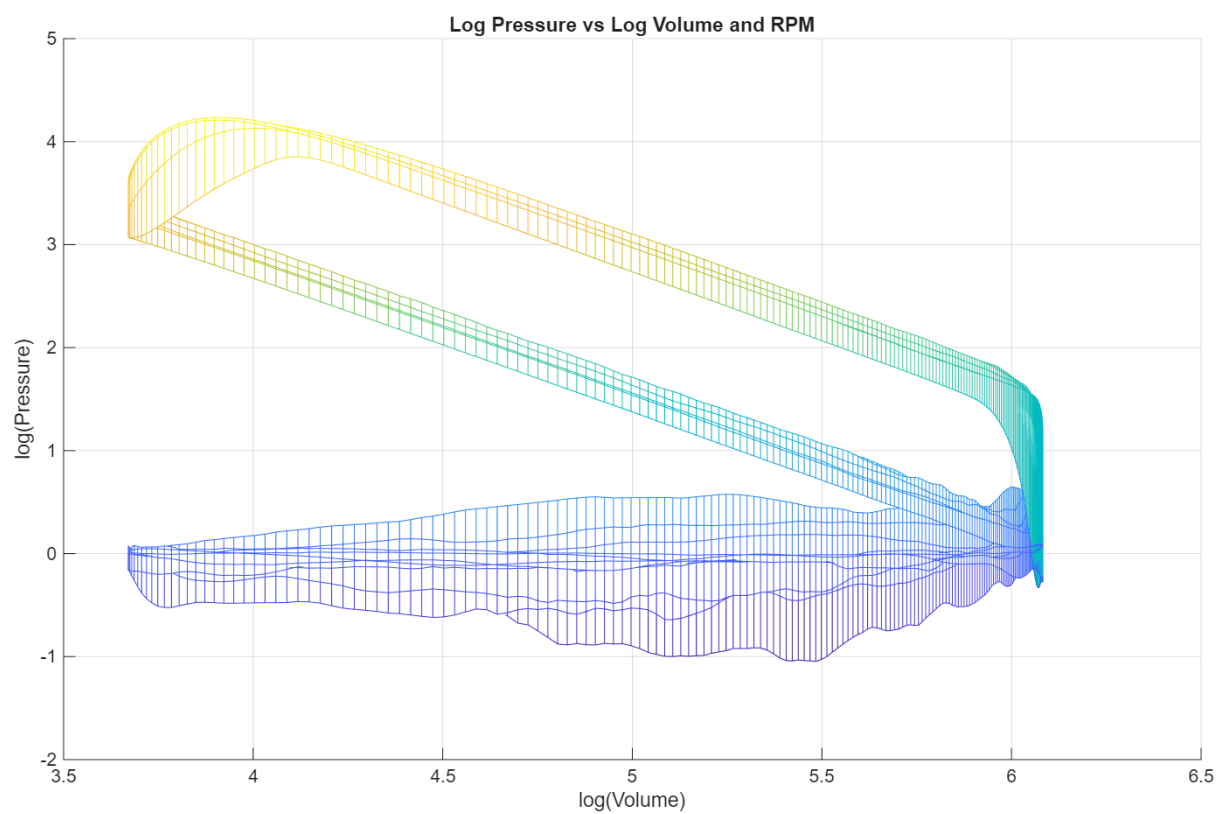
3.4.2 Set Up

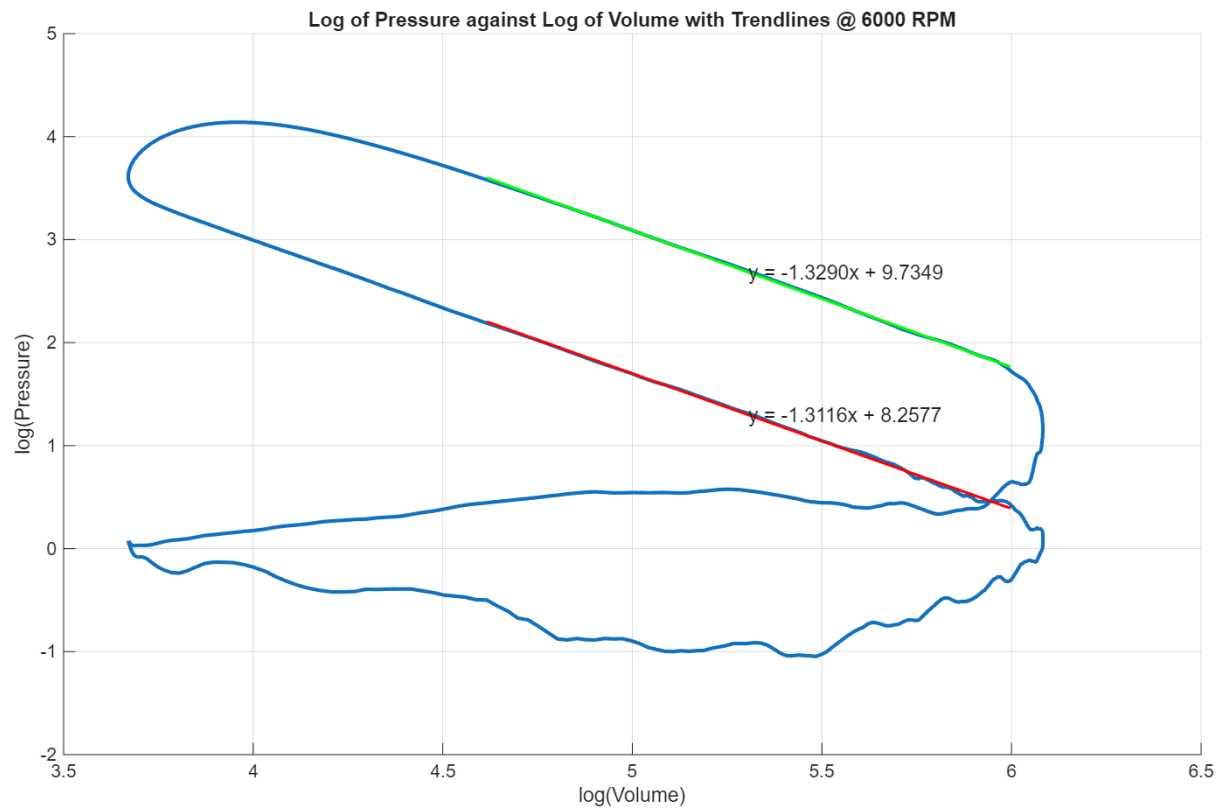
The values for the Wiebe function were pulled from the calculated values via MATLAB, these were 50% burn rate, combustion duration, and Wiebe exponent, the burn fraction at completion was left at 1. For the cases 6 were used with only the RPM differing with 1000-6000, AFR stayed constant at 14 for the petrol (based on the predefined petrol fuel in forte) and 9.8 for the E85 (chosen as the stoichiometric value). Injection timing was not altered from the original base.

4 Results

4.1 Dynamometer







RPM	N (Compression)	N (Expansion)
6000	1.3116	1.3290
5000	1.3254	1.3386
4000	1.3188	1.3241
2000	1.3083	1.3381
1000	1.3227	1.4174

Average N (Compression) = 1.3196

Average N (Expansion) = 1.3466

4.2 Ansys Forte

4.2.1 Base Petrol

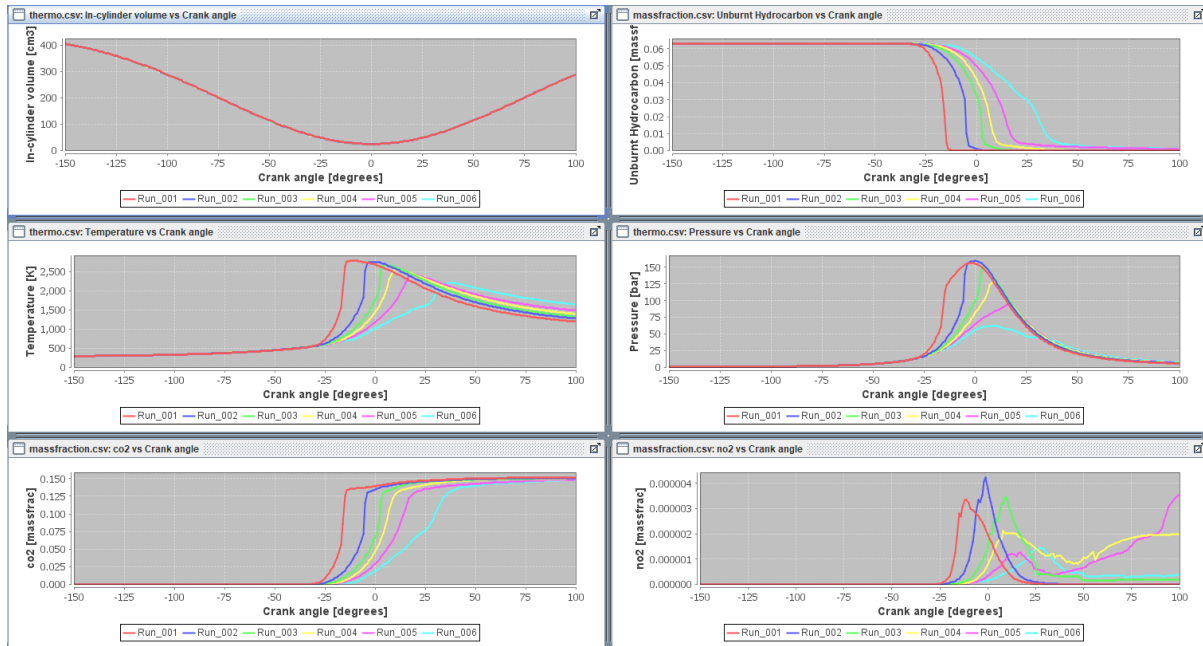


Figure 4-1: Petrol Multi-RPM sim at -35 Degree Spark

Initially for the petrol sims, a multi-rpm run was carried out, this was at -35 degrees of crank angle.

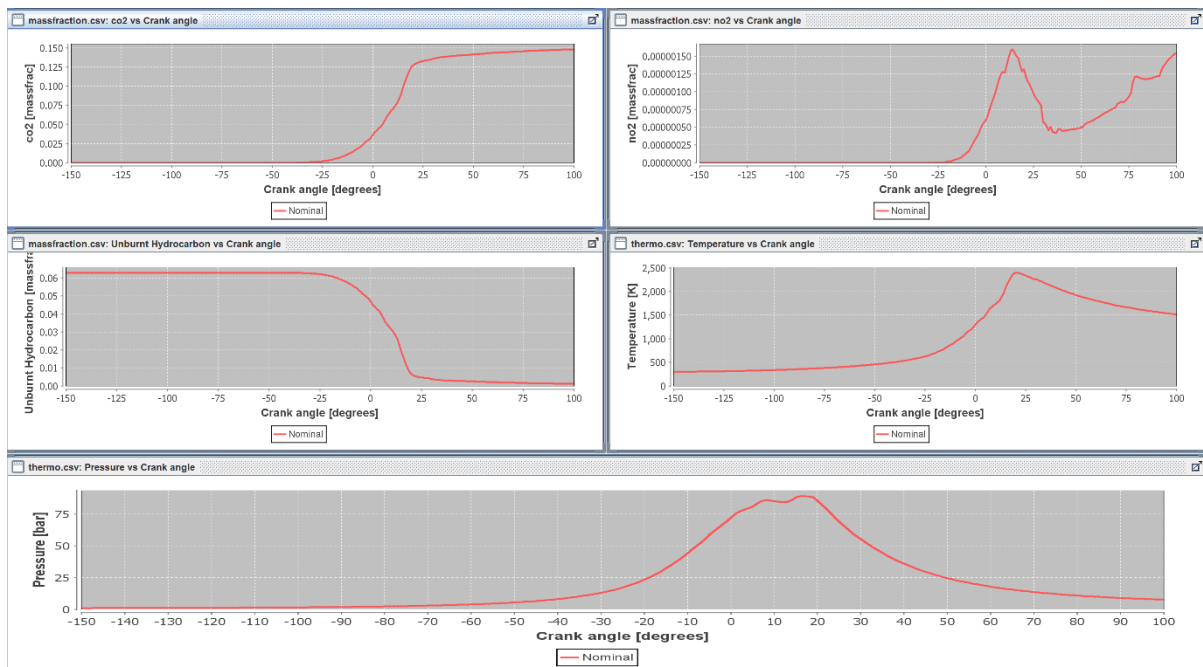


Figure 4-2: Petrol -45 Degree Spark

After the multi sim, 6000 RPM was selected and remained constant moving forward, with spark being advanced 10 degrees to achieve a quicker burn rate.

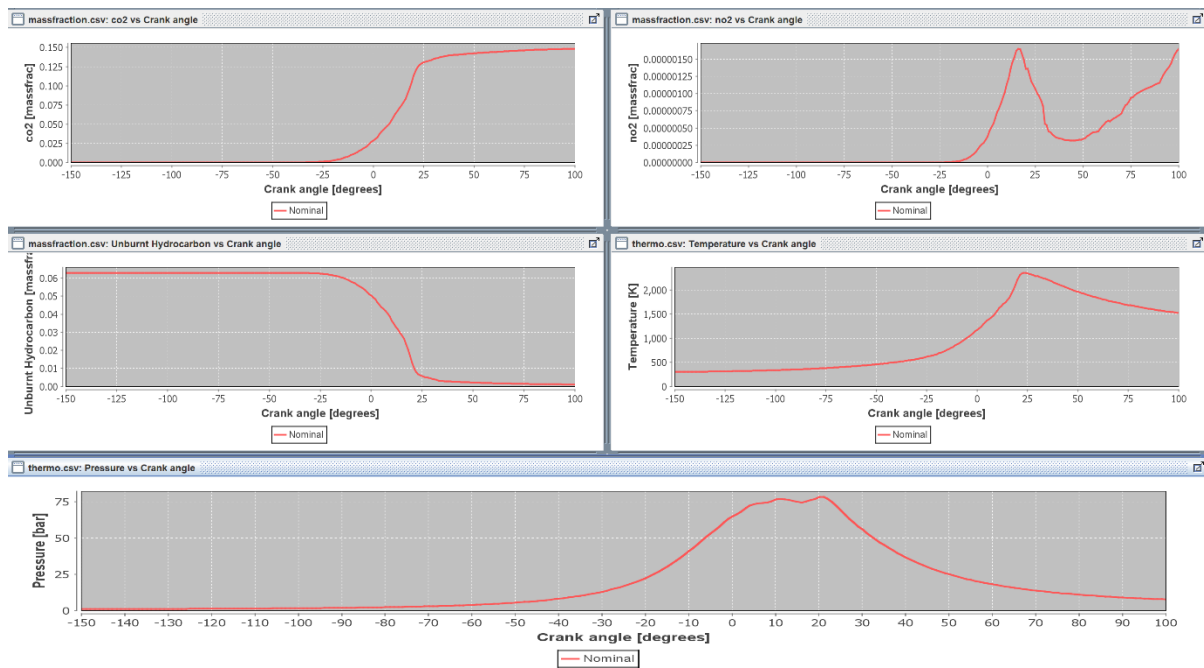


Figure 4-3: Petrol -40 Degree Spark

Spark timing was retarded 5 degrees; this was due to the high pressures found at -45

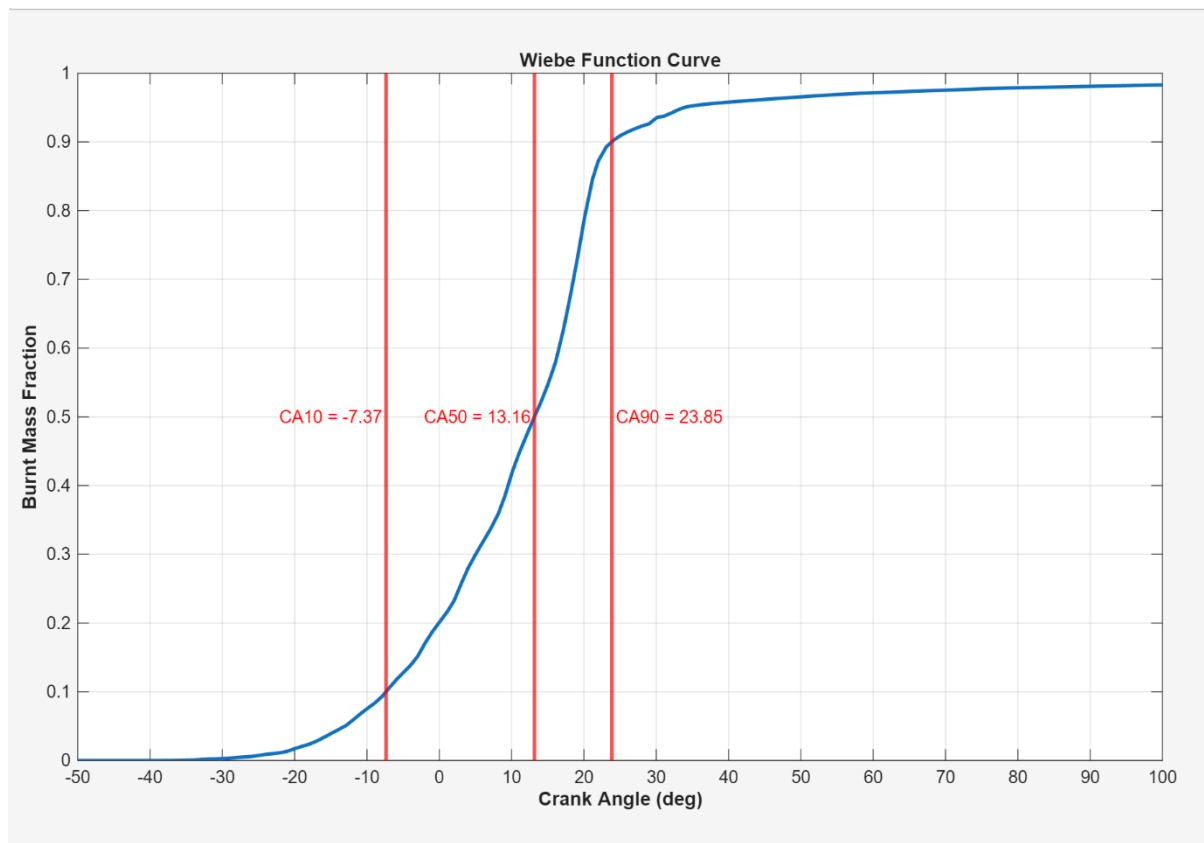


Figure 4-4: Petrol Wiebe Function With 10, 50 & 90 Percent Burn

The Wiebe function plotted in MATLAB from the Forte data calculated in Excel, this contains markers and values at 10, 50, and 90 percent burn.

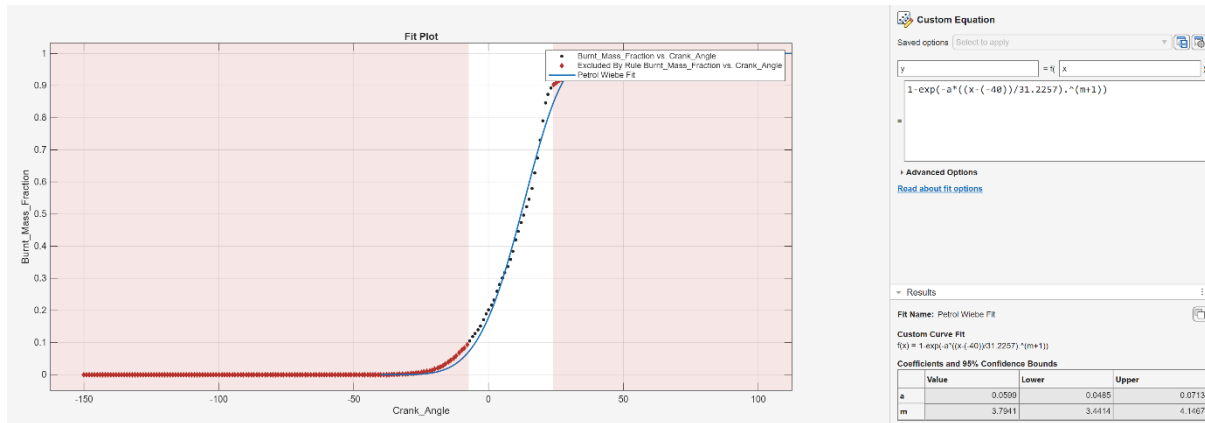


Figure 4-5: Petrol Curve Fitting

The fitted curve in MATLAB that gives the exponent values from the Wiebe formula.

4.2.2 E85

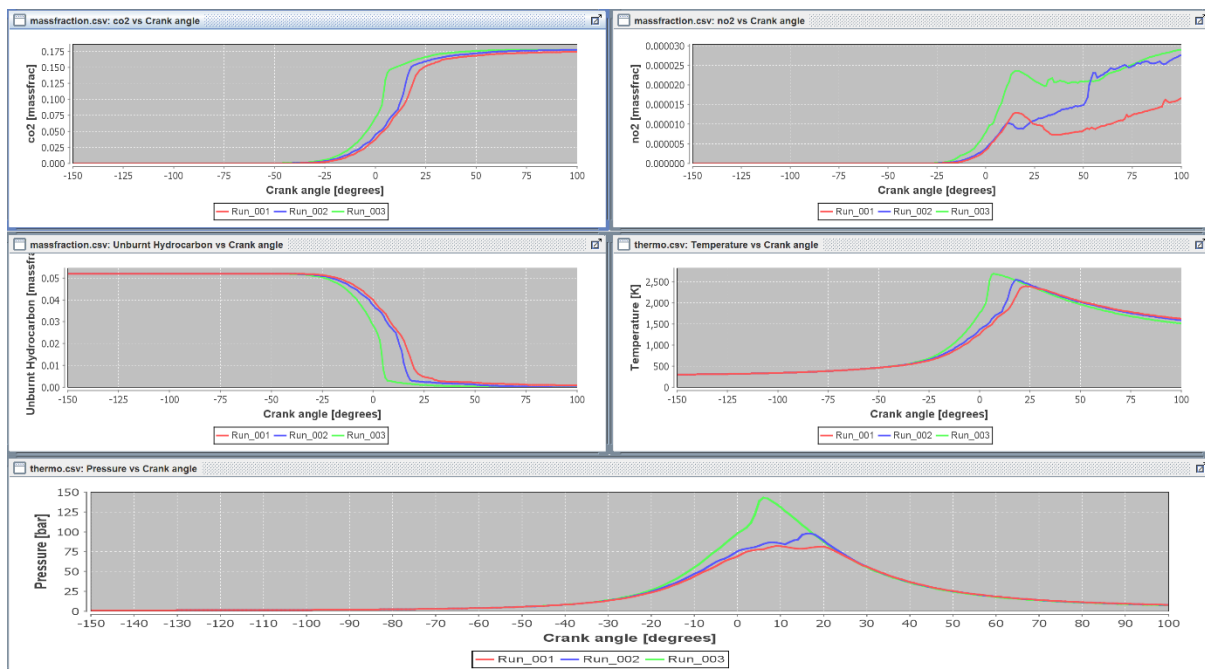


Figure 4-6:E85 Spark Testing

Spark timing was tested to look for a more realistic and balanced combustion

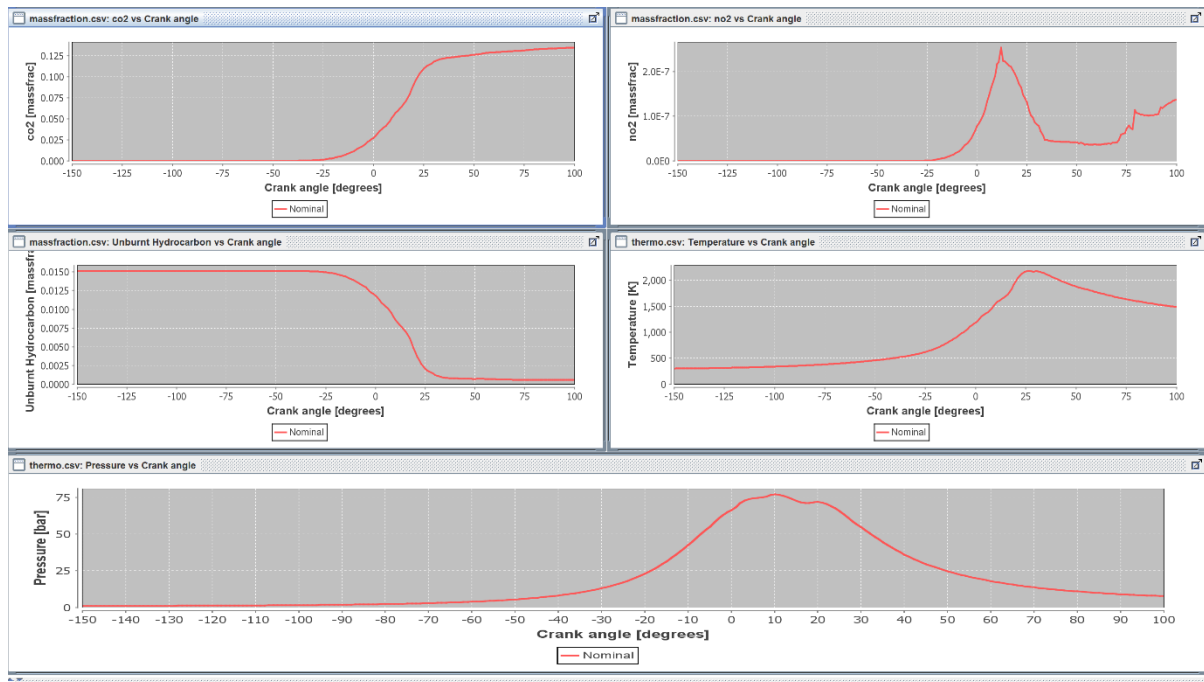


Figure 4-7: Petrol -45 Degree Spark

-45 degrees was selected for its balance between combustion time and pressure values, then the fuel mix was returned to stoichiometric and values taken.

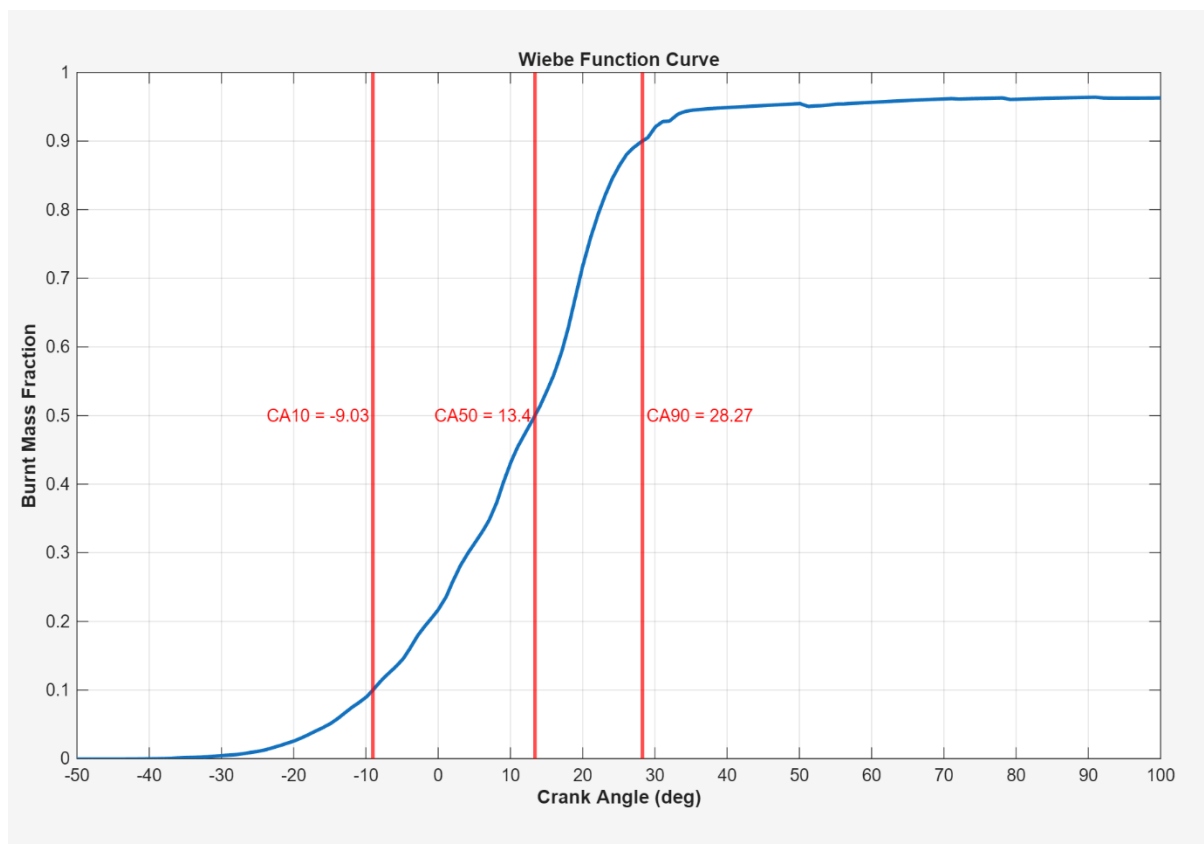


Figure 4-8: E85 Weibe Function With 10, 50 & 90 Burn

The Wiebe function plotted in MATLAB from the Forte data calculated in Excel, this contains markers and values at 10, 50, and 90 percent burn.

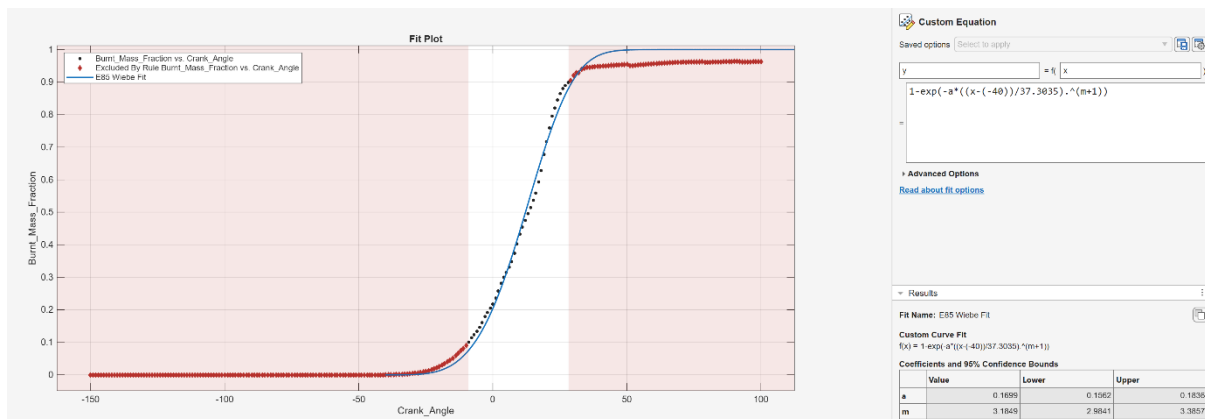


Figure 4-9: E85 Curve Fitting

The fitted curve in MATLAB that gives the exponent values from the Wiebe formula.

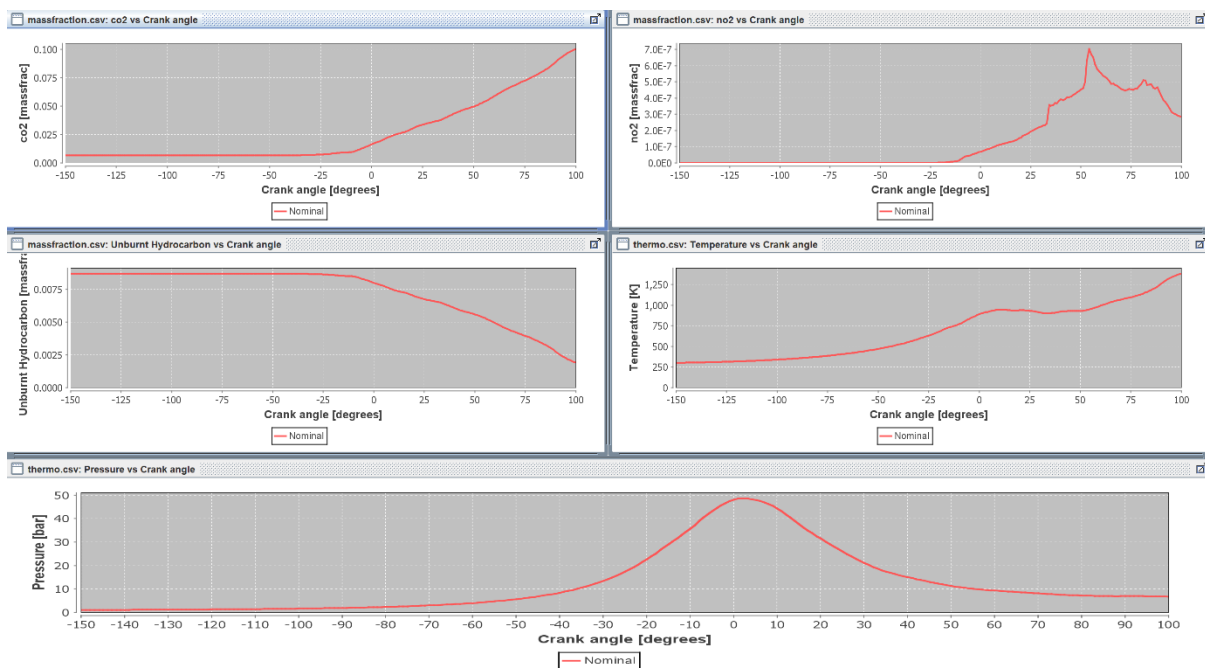


Figure 4-10: E85 5% EGR Test

A sim was run with E85 including a 5% exhaust gas recirculation added to the mix to investigate effect.

4.3 Realis Wave

4.3.1 Base Petrol

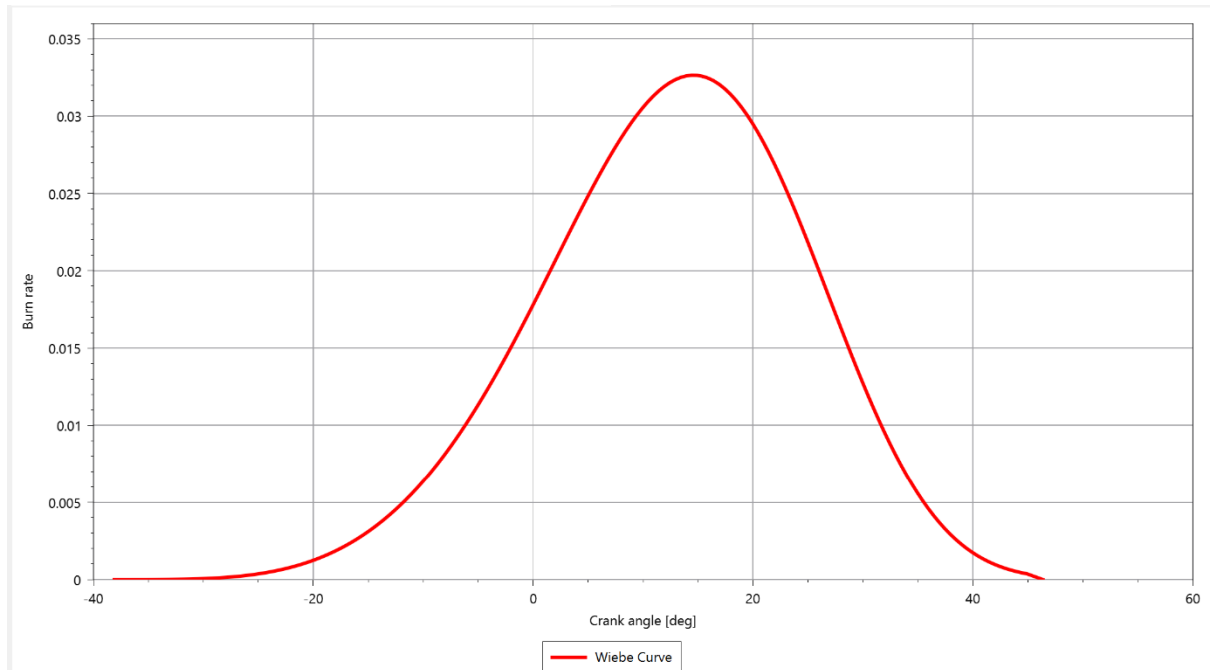


Figure 4-11: Petrol Wave Wiebe Plot

When all components were inserted to Wave's Wiebe plotter, this graph was plotted the burn characteristics.

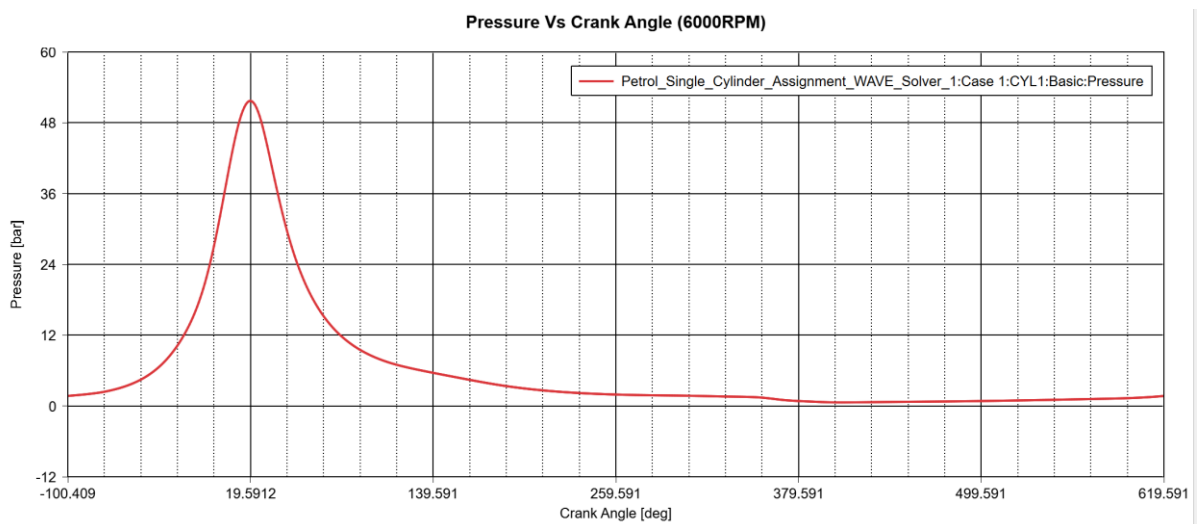


Figure 4-12: Petrol Pressures @6000 RPM

Pressure vs crank angle plot result from the Wave simulation at 6000 RPM

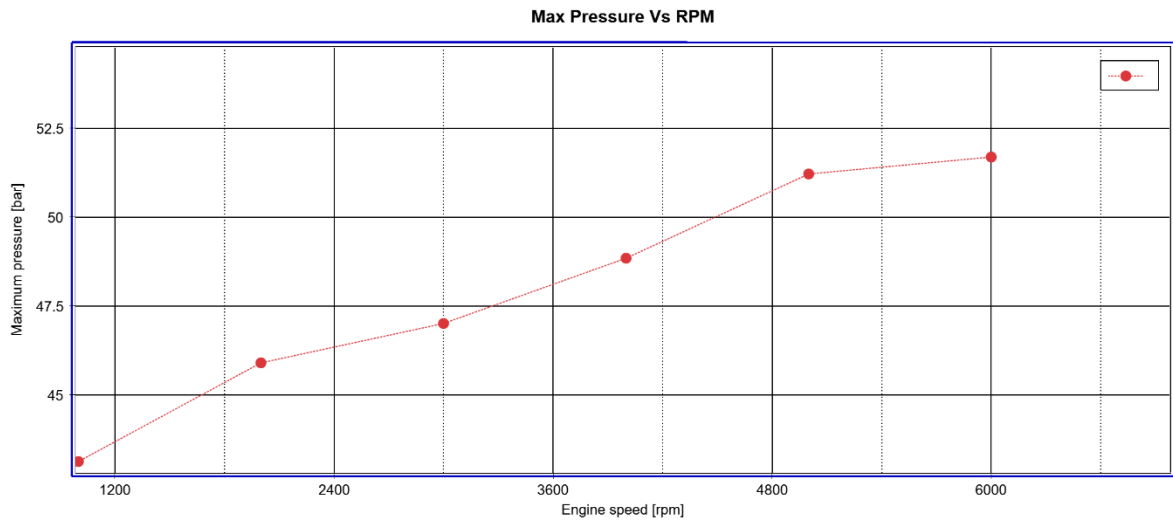


Figure 4-13: Petrol Max Pressure Vs RPM

Max pressure plots over the range of RPM values simulated.

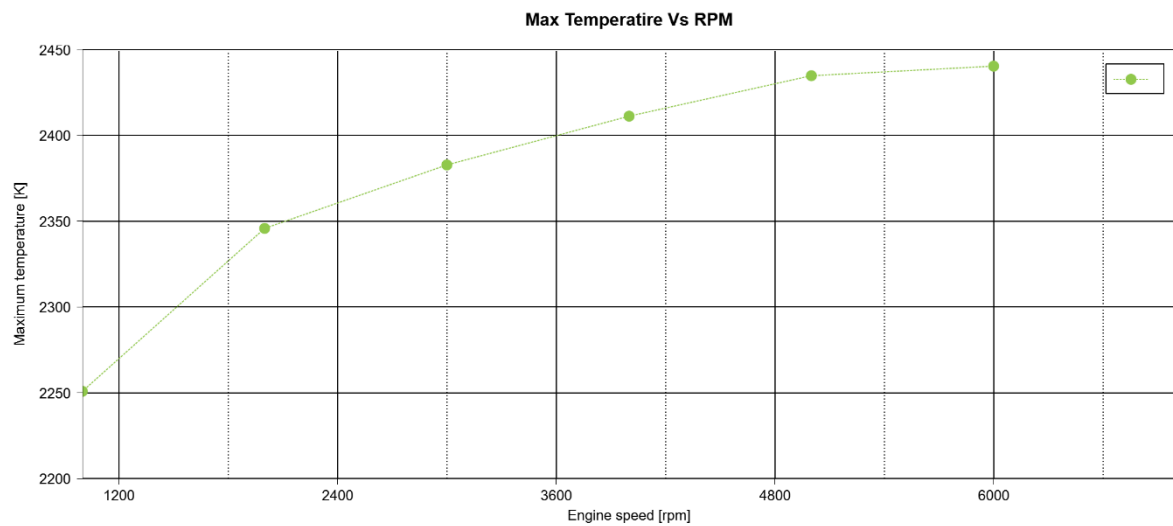


Figure 4-14: Petrol Max Temperature Vs RPM

Max Temperature plots over the range of RPM values simulated.

4.3.2 E85

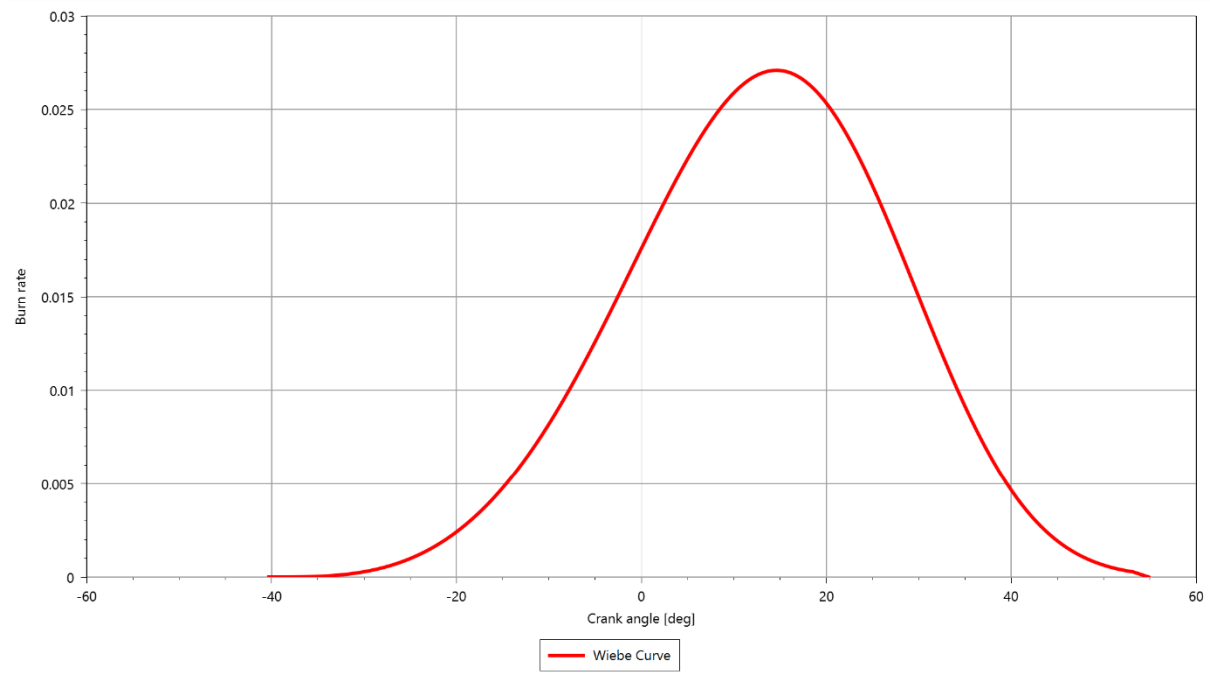


Figure 4-15: E85 Wave Wiebe Plot

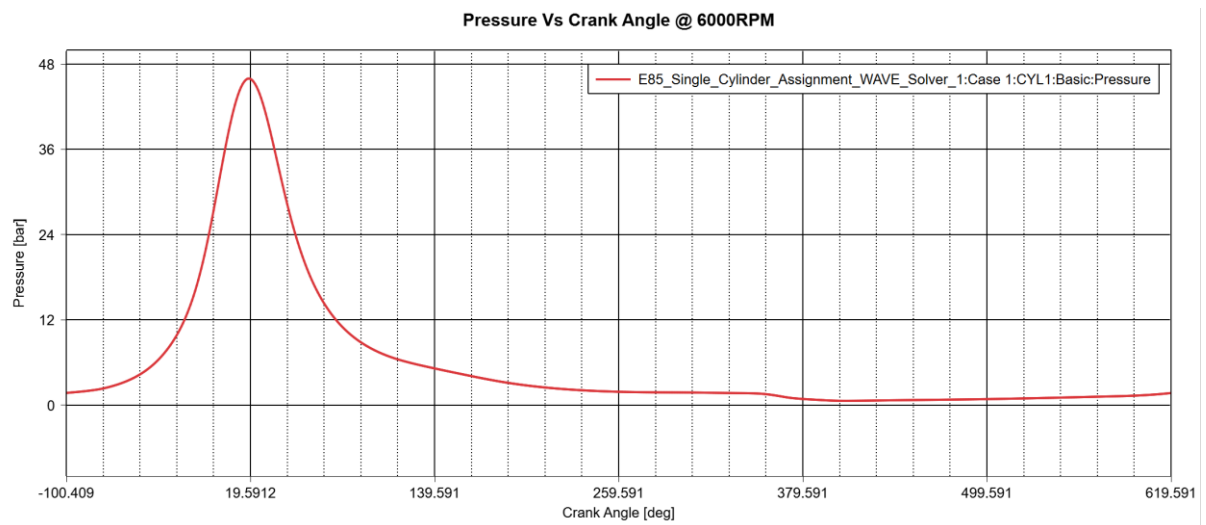


Figure 4-16: E85 Pressures @6000 RPM

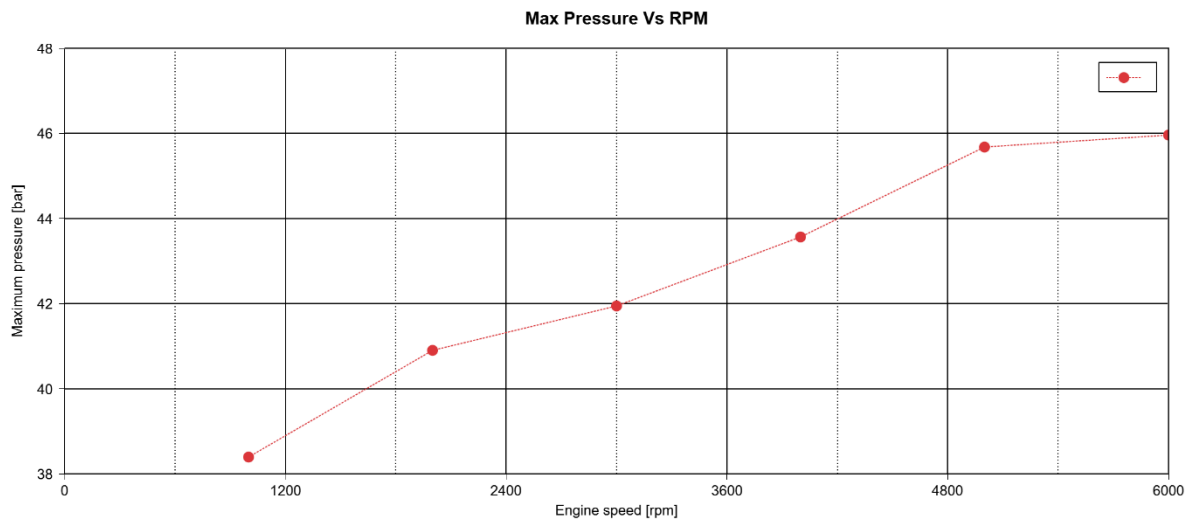


Figure 4-17: E85 Max Pressure Vs RPM

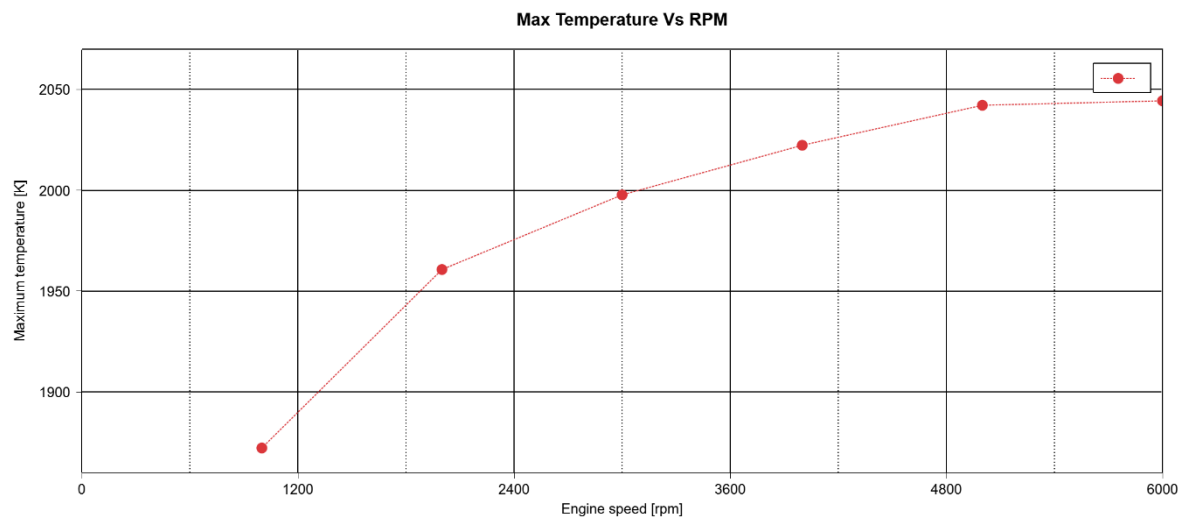


Figure 4-18: E85 Max Temperature Vs RPM

5 Evaluation

5.1 Ansys Forte

5.1.1 Petrol

After the spark timing was retarded from -55 to -45 degrees BTDC, the petrol validation runs supplied a fairly reasonable profile for the combustion, with peak pressure reduced to ~75-80 bar and acceptable phasing shown by the peak pressures appearing shortly after TDC and the majority of combustion taking place around TDC. The MATLAB extracted values for 10, 50, and 90 percent burn gave a burn duration ~31 degrees, which would be reasonable for spark combustion. An issue that arose was the compression ratio was calculated by Forte at ~16.5:1 vs the 11.1:1 of the actual engine, this likely due to assumptions and simplifications such as the use of a flat piston head over a defined bowl and as such would be the likely cause of the overprediction of pressures when compared with the real-world dynamometer results.

Further assumptions such as the omission of an injection model and the reliance on premixed gas mixes, simplification of heat transfer, and idealised combustion are large contributors to the higher peaks and sharper rises of pressure. Due to these limitations, the Forte petrol sims are acceptable for comparative analysis, however do not suit exact validation.

5.1.2 E85

Like the petrol simulations, once calibration of the spark timing had been carried out, the E85 simulation produces consistent combustion with -45 degrees BTDC being found as the best compromise between combustion speed and realistic pressures. Peak of pressure is observed in the 75-80 bar range, largely comparable to the petrol sims, with the temperature peaks showing a reduction to around 2200K. Burn duration was observed as approximately 37 degrees of crank angle, 6 degrees greater than that of the petrol, displaying similar phasing of the combustion but with an increased gradual burn time, which would be consistent with the difference in flame development and the higher latent heat of vaporisation typical of ethanol combustion behaviour. The same

limitations are present with peak pressures being caused by an increased compression ratio.

5.2 Realis Wave

Consistent combustion trends are largely shown by both petrol and E85 simulation results with variances in simulations aligning well with those to be expected in the different properties of each fuel. Petrol peaks at 52 bar in the 6000 RPM run with 2400K peak temperatures and displays a well-defined combustion, however the Forte based Wiebe metrics with advanced phasing of combustion is reflected by early peaks. Stable heat release is observed with symmetrical and smooth burn rate.

The same trends are observed for the E85 simulation but display peaks in temperature and pressure consistently lower at 2040K and 46 bar respectively. A reaction to be expected by the reduction of cylinder temperatures and cooled charge due to ethanol's higher latent heat of vaporisation. Combustion does however remain consistent with similar curve shapes and efficient but stable burn rates, suggesting the combustion characteristics from the Wiebe function are fairly adequate.

Key assumptions and limitations such as the compression ratio are carried forward into the wave results biasing the combustion phasing. Overall while the Wave simulations are able to produce a consistent model for comparison, with E85 displaying more gradual, cooler combustion, the results are simplified greatly but remain reasonable physically and acceptable for the identification of trends and comparison.

5.3 Further Work

Further work would include refinement to both Forte and Wave models with a reduction in assumptions such as the flat piston head. Also a detailed investigation of other alternative fuels in Butanol and Hydrogen to compare traditional fuels, ethanol mixtures, bio-fuels, and non-carbon fuels.

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