

CFD and Emissions Modelling

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Abstract - This paper explores the feasibility of synthetic combustible fuels for internal combustion engines, particularly in the context of upcoming EU regulations that mandate 0g CO₂/km for L class vehicles from 2035. Utilizing Ansys Forte and Ricardo Wave, the research aims to model and simulate the combustion process within a Ford Sigma 1.6 petrol engine. The study focuses on building a Sector Mesh combustion model to validate the simulated data against actual recorded data, thereby assessing the effectiveness of CO₂ emissions-free fuel strategies.

Key steps include the adaptation of a petrol-based simulation for initial validation, followed by adjustments to model CO₂-free fuel strategies using data from Forte simulations to construct a Ricardo Wave model. This approach allows for detailed analysis of engine architectural characteristics, enhancing the simulation's accuracy.

The paper also delves into the specific setup for Ansys simulations at different RPMs, exploring variables such as spark timing, fuel equivalence ratio, and spark positioning. The simulation results are closely compared with measured data to evaluate the model's precision and identify areas requiring further refinement. The findings underscore the potential of synthetic fuels to meet stringent emissions standards but highlight the need for ongoing development in simulation accuracy and fuel strategy optimization to fully realize their benefits in practical applications.

1. INTRODUCTION

The following paper presents the use of Ansys Forte and Ricardo Wave in order to attempt to study the feasibility of synthetic combustible fuels for internal combustion engines should the regulations on the sale of L class vehicles not change in 2035.

From 2035 Onwards, the EU has proposed regulations for both cars and vans, allowing 0g CO₂/km in order to decrease greenhouse gasses and global warming [1].

Objectives:

Build a Sector Mesh combustion model in order to validate combustion simulation with recorded data. A Ford Sigma 1.6 petrol engine was used for this as data was readily available to the author.

Investigate CO₂ emissions free fuelling strategy. Use combustion data acquired from Forte simulations in order to build a Ricardo Wave Model.

Using the Ricardo wave model further consideration to architectural engine characteristics can be given.

2. ANSYS Modelling

An Ansys Forte combustion model has been built according to the Ford Sigma specifications in order to be able to compare simulated results to known data with an initial Petrol simulation in order to confirm validity of the simulation.

The diesel sector mesh tutorial from Ansys Forte has been used as a base for the construction of the following model.

In the sector Mesh Generator, the Sigma engine parameters are defined. (Figure 1).

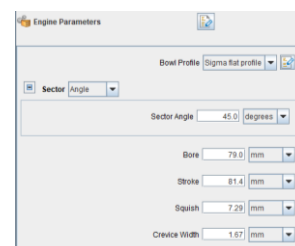


Figure 1: Sigma Engine Parameters Ansys (Iatrakis, 2024)

The Piston Crown of the Ford Sigma piston is a mostly flat crown with a shallow bowl (Figure 2). For ease of modelling, a completely flat crown is assumed. Figure 3 shows the configuration screen in Ansys for the piston profile.



Figure 2: Ford Sigma Pistons (RioSulense, 2024)

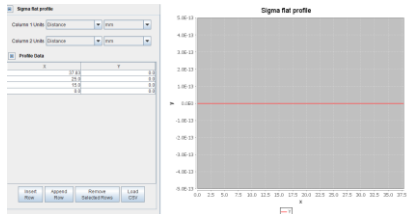


Figure 3: Piston Crown Configuration Ansys (Iatrakis, 2024)

The mesh settings used were the same as proposed by the Sigma tutorials. Figure 4 shows the used mesh settings and the generated mesh.

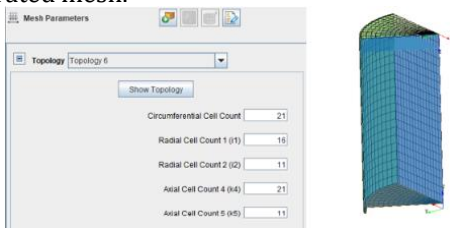


Figure 4: Mesh Settings & Generated mesh (Iatrakis, 2024)

3. Ansys Simulation Setup

Following part describes the model setup for the Sigma Forte simulations, Simulations at 1500RPM and 4500RPM have been conducted for comparison with the recorded data.

The used Ansys 'Gasoline 1 Comp 49SP' chemistry library is used. The Turbulent Flame Speed Ratio (b1) is set to 2. The remaining chemistry settings have been kept default.

As a Spark-Ignition engine configuration is used, a spark is introduced to the diesel model, and the soot model is disabled. Figure 5 shows the settings for the Flame Propagation model.

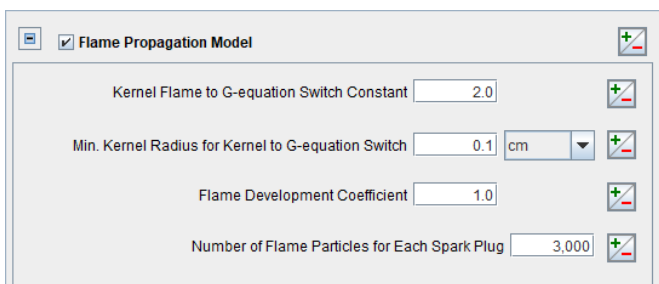


Figure 5: Flame Propagation Settings (Iatrakis, 2024)

Figure 6 shows the positioning of the spark.

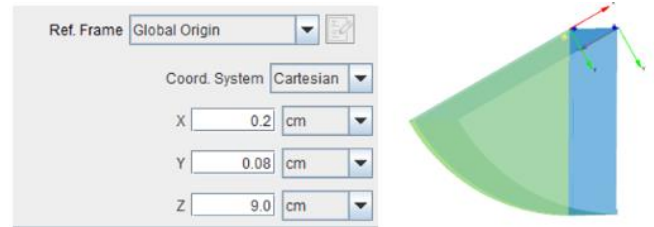


Figure 6: Spark Positioning Settings. (Iatrakis, 2024)

The spark timing and duration settings were changed throughout the different simulations and will be discussed later.

The boundary conditions were kept as default.

Since the model is ran as a simplified port injection model, the initial conditions are used to control fuelling. The sigma data shown has used a consistent 0.9 lambda value for the fueling during the measurements. Which relates to a 1.1 equivalence ratio. Using a stoichiometric fuel balance calculator, the fuel mixture composition was calculated, iso-octane was assumed as fuel. Figure 7 shows the used fuel balance for 'petrol'.

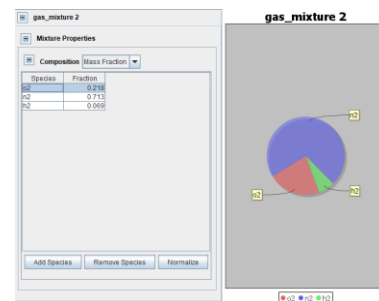


Figure 7: Petrol Mixture Configuration (Iatrakis, 2024)

All combustion simulations was ran between -165° Crank Angle and 125° Crank Angle, thus the same pressure as measured in the Sigma Data at -165° Crank Angle was defined as initial pressure. The exact pressure will be defined further on depending on simulation.

4. 1500 RPM Validation

The simulation settings were all set as shown in the previous part. A fuel equivalence ratio of 1.1 was used. Spark timing was set to -5.5° Crank angle to best match the sigma data. Changing spark duration showed no effect on the combustion. Initial pressure was set to 1.128 Bar, as measured at -165° C.A. in the sigma data.

Figure 8 shows both the simulated and measured in-cylinder pressures over the crank angle. An attempt to match spark

timing has been made through trial and error. As visible from the sigma data, combustion starts around -5° crank angle. Despite these efforts, a precise match with the measured data has not been achieved. Adjusting the spark timing to be more advanced with the same amount of fuel results in excessively high pressures, while aligning the spark timing more closely with the original leads to slower combustion and maintains a delayed pressure drop, even with a fuel equivalence ratio of 1.

The most accurate approximation of pressure was achieved at -5.5° crank angle using a 1.1 fuel equivalence ratio, mirroring the sigma data's settings. It is important to highlight that significant geometric differences, evident from the mismatch in pressures even before combustion starts, likely contribute to the discrepancies observed. This discrepancy underscores the need for further refinement of the model to bridge the gap between simulated and real-life conditions.

The author notes that no further accuracy was obtained, and for subsequent comparisons, the settings of -5.5° crank angle and a 1.1 fuel equivalence ratio will be maintained.

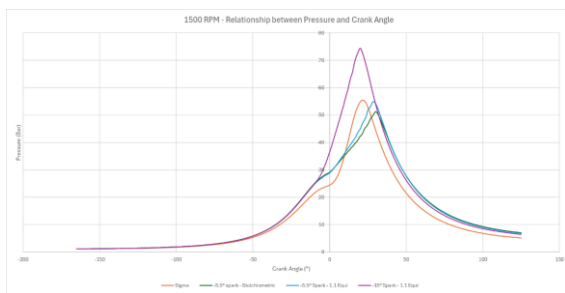


Figure 8: 1500 RPM Spark Timing Comparison (Iatrakis, 2024)

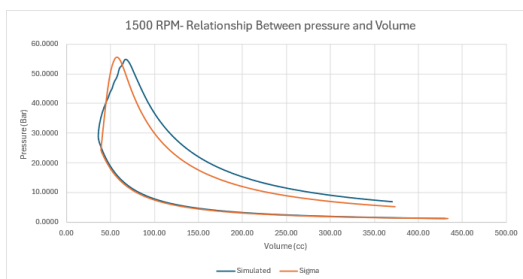


Figure 9: 1500RPM Pressure over Volume plot (Iatrakis, 2024)

The graph above shows the relationship between pressure and volume, showing similar indications to the combustion as Figure 9 showing a slower combustion process of the simulated data compared to measured, similar peak pressure between the two is shown, it also shows the pressure starts dropping down later, although the actual pressure drop seems to be at a similar rate as the measured data, indicating a similar heat release rate.

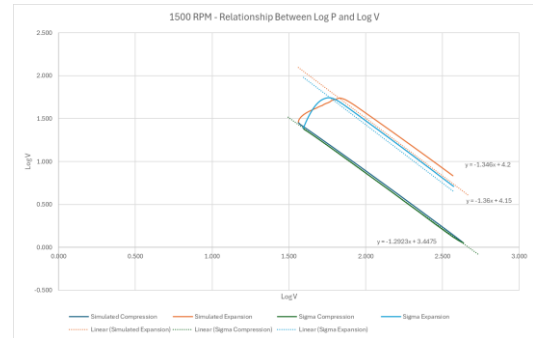


Figure 10: 1500RPM LogV over LogP (Iatrakis, 2024)

Figure 10 allows for the determination of the polytropic index (n-values) by fitting trendlines to the linear segments of the graph, where the gradient corresponds to the polytropic index. It's evident that the rates of compression and expansion are closely matched between the Sigma data and the simulated results. However, as noted previously, there is a delayed pressure decrease, indicating that combustion extends longer than anticipated. The trendlines show very similar gradients, or n-values, suggesting that either the simulated or measured results could be reliably used for wave simulation purposes.

Figure 11 displays the simulated Mass Fraction Burned (MFB) plotted against crank angle. It illustrates the cumulative percentage of fuel burned throughout the engine cycle. Typically, fitting this data with a Wiebe function is useful for simulations in software like Ricardo WAVE. However, in this instance, such curve fitting is not required because ANSYS already provides detailed information regarding the start and end of combustion, as well as the duration of the combustion process.

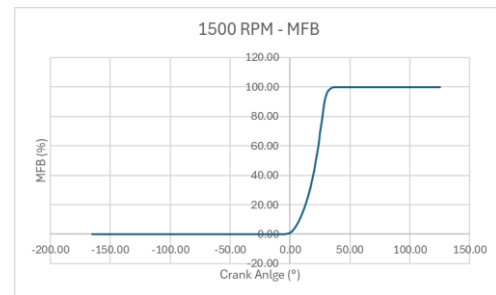


Figure 11: 1500RPM MFB (Iatrakis, 2024)

Table 1 shows a comparison of the MFB percentages between simulated and measured values, percentagewise the values aren't far off but the 10% to 90% burn duration confirms the elongated burn time as shown before. These differences are deemed acceptable and representative and can be used in the Wave simulation.

Table 1: MFB Comparison 1500RPM (Iatrakis, 2024)

MFB Comparison 1500 RPM				
MFB (%)	Simulated (C.A.)	Sigma (C.A.)	Offset (C.A.)	Diff %
2	2.03	3.80	-5.14	39.8%
10	9.00	7.76	-0.32	9.8%
50	22.01	22.62	-5.56	24.6%
90	30.02	30.90	-5.29	14.2%
10-90 Dur	21.02	23.14		2.5%

Table 2 offers a comparison of several key parameters such as compression ratio, clearance volume, displacement volume, maximum pressure, and temperature. While the maximum temperature recorded in the simulations is higher. The higher compression ratio also ties in with the difference in pre combustion pressure. Which is expected to be due to the difference in piston crown compared to the physical engine. The other parameters closely match each other. This consistency highlights the model's accuracy in replicating crucial engine characteristics effectively.

Table 2: 1500RPM Engine Parameters Comparison (Iatrakis, 2024)

1500 RPM Engine Parameters Comparison		
	Simulated	Sigma
Compression Ratio	11.95	11.16
Clearance Volume (mm ³)	35752.30	36428.96
Displacement Volume (mm ³)	398995.90	398995.90
Max Pressure (Bar)	54.83	55.47
Max Temperature (deg K)	2664.71	2454.15

5. 4500 RPM Validation

In the following part, some validation is shown at 4500RPM between the ford sigma measured data and the simulated data in Ansys, in order to learn and compare at higher rpm. Initial pressure was set to 1.224 Bar as with the sigma data at -165 Degrees C.A. Spark duration was found to have no influence on the combustion.

A fuel equivalence ratio of 1.1 was used as used during the ford sigma measurements. A spark timing of -29 degrees crank angle was found to match the combustion of the sigma measurements the best.

Figure 12 shows a comparison between Pressure and Crank Angle. Initially, it's clear that the angle at which the spark is ignited for the sigma occurs later than simulated, even though the simulation settings were set as close to reality, there are still discrepancies. The used spark angle was the only one with which a similar maximum pressure was reachable. As the Figure 13 shows, the rate of combustion and expansion is quite close, but occurs at different crank angles, pressure also stays higher for a while in the simulated result, decreasing pressure around 10° C.A. later than sigma. Figure 13 displays the relationship between pressure and volume, again shows the rate of pressure increase and decrease is quite similar, although burn duration seems to carry on longer as pressure drops later on.

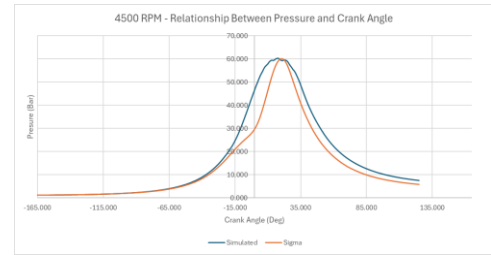


Figure 12: Pressure Comparison Simulated vs Sigma (Iatrakis, 2024)

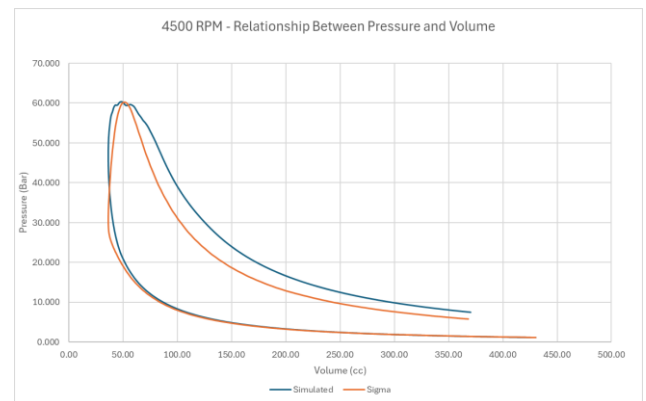


Figure 13: 4500RPM Pressure over Volume (Iatrakis, 2024)

Figure 14 shows the relationship between LogP and LogV, following the same trend as with the 1500RPM analysis, a similar rate of compression and expansion is seen between the simulated and measured data. The pressure decrease is delayed, indicating combustion carries on for longer, the trendlines show similar gradients/ n-values, indicating a match of the data sets for use in Wave.

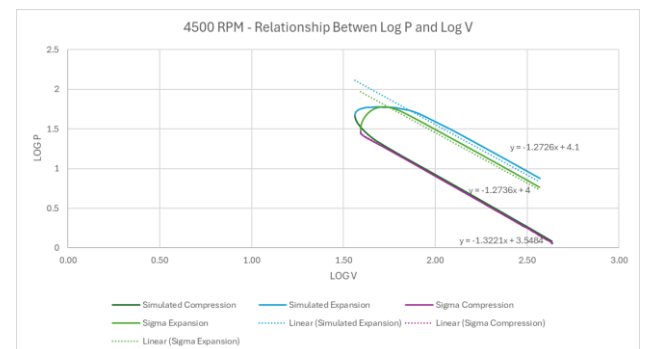


Figure 14: 4500RPM LogP over LogV (Iatrakis, 2024)

Figure 15 displays the simulated Mass Fraction Burned (MFB) plotted against crank angle.

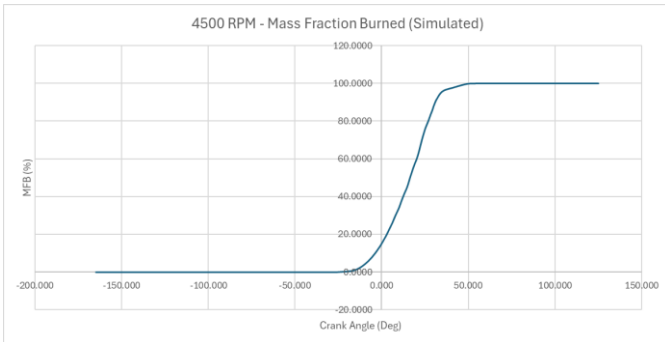


Figure 15: 4500RPM MFB (Iatrakis, 2024)

Table 3 presents a comparison of the Mass Fraction Burned (MFB) values alongside the corresponding crank angles from both simulated and measured datasets. While there are differences in the specific crank angles recorded between the two sets, the overall duration of the combustion process is similar. This consistency in duration suggests that, despite discrepancies in timing, the overall efficiency and pattern of fuel combustion are comparable across both simulations and real-world measurements.

Table 3: MFB Comparison 4500RPM (Iatrakis, 2024)

MFB Comparison 4500 RPM				
MFB (%)	Simulated (C.A.)	Sigma (C.A.)	Offset (C.A.)	Diff %
2	-12.914	-7.777	-5.137	40%
10	-2.924	-3.240	-0.316	10%
50	17.056	22.616	-5.560	25%
90	32.041	37.330	-5.289	14%
10-90 Dur	34.965	34.090		3%

Table 4 provides a comparison of key parameters showing the same accuracy as discussed before in the 1500RPM comparison, again showing a higher temperature, which may be contributed due to the longer burn duration.

Table 4: 4500RPM Engine Parameters Comparison (Iatrakis, 2024)

4500 RPM Engine Parameters Comparison		
	Simulated	Sigma
Compression Ratio	11.95	11.16
Clearance Volume (mm ³)	35752.30	36428.96
Displacement Volume (mm ³)	398995.90	398995.90
Max Pressure (Bar)	60.30	60.19
Max Temperature (deg K)	2537.92	2377.60

The simulations effectively display the correct trends, and the main values required for the Wave simulation are generally close to the observed data, suggesting that the model captures the essential dynamics of the engine. However, further refinement and more accurate modelling are necessary to achieve closer alignment with the measured values. Notably, the mixture composition and spark timing are the most significant discrepancies, seemingly getting less representative at higher engine speeds. Resulting in an inability to accurately match the pressure patterns observed in actual engine operations. Despite these issues, the accuracy of several key parameters indicates that the foundational

modelling is deemed correct enough for use in wave by the author.

6. ANSYS Hydrogen Simulation

As discussed previously hydrogen is the chosen fuel for the further investigation of this assignment, an initial simulation is ran at 1500 RPM using the same settings as the petrol, using a stoichiometric 1.0 equivalence hydrogen fuel mix. Figure 16 shows the used fuel mix.

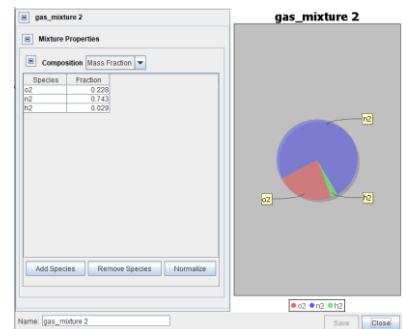


Figure 16: Stoichiometric Hydrogen Fuel Mix (Iatrakis, 2024)

Figure 17 shows a comparison of pressure over crank angle between the initial hydrogen simulation and petrol, the properties of hydrogen are clearly visibly with it's very high flame speed [2], as pressure increases almost instantly, it shows that using an advanced ignition timing doesn't pay in this instance as reverse work will be done during compression. A following run has been conducted using a +3° C.A. ignition timing. It shows a decrease in pressure and still a very high pressure, fast burn duration. Figure 20 shows a 17% increase in temperatures, which goes paired with the very high increase in NOx emissions Figure 18.

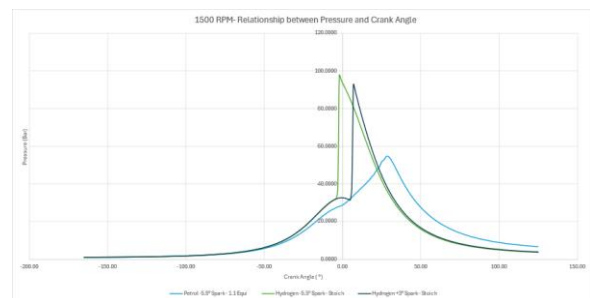


Figure 17: Hydrogen Pressure over C.A. (Iatrakis, 2024)

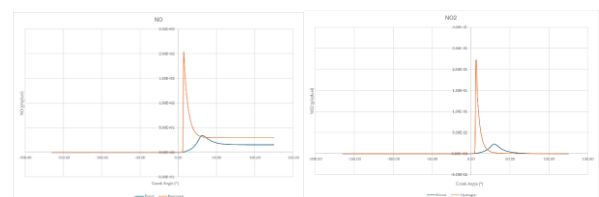


Figure 18: Hydrogen NOx Emissions (Iatrakis, 2024)

The high flame speed and high pressure related to hydrogen sparks interest whether if hydrogen could be introduced and ignited at different points throughout the cycle to improve the amount of work done and pressure in the cylinder for a higher MEP, such as used in the G-Cycle engine [3]. Water injection also sparks to mind in order to cool the reaction down and decrease pressures, decreasing losses and decreasing NOx emissions.

Where the G-cycle injects heated water for the first time during the compression of the combustion chamber in order to regulate the compression ratio, this is not something the author is looking for to increase the compression ratio. Early in the combustion/expansion phase, a second heated water injection (250-350°C or 523-623 K) cools the reaction, maintaining a peak temperature around 1,800 K. This cooling phase transforms water into superheated steam, expanding and increasing the chamber's mean effective pressure (MEP) for work. A third water injection (30°C) is injected late in the combustion/ expansion phase, cooling the exhaust gas, combustion chamber and aiding in vapor condensation for easier recovery of the used water.

An initial ANSYS simulation has been run with one water injection, the same injection settings as the ANSYS Diesel Mesh tutorial were used. The injection was configured to start at -5 degrees C.A. and injecting 0.005g of water for 4° C.A. Injecting water before the ignition has been chosen because the pressure and temperature rise occurs so quickly after combustion of the hydrogen. In a similar fashion as the G-Cycle's first water injection.

Figure 19 shows the pressure between no water injection and water injection has stayed fairly similar, meaning the work done will be comparable, the high pressure compared to petrol also means that hydrogen can be ran much leaner to reach the same pressures. A slight decrease in peak temperature is seen, a significant temperature drop past around 10° C.A. comes with a significant decrease in NOx emissions, proving the water injection technique effective. Temperature has now also dropped even more compared to petrol. A further run with 2 more water injections at 10° C.A. and 25° C.A., injecting 0.1g of water was deployed to reach a similar A.C.A. as the G-cycle to try to maintain pressure due to vaporisation and decrease temperature and emissions, the latter water injection is also meant to help with vapor condensation for water collection, which can't be confirmed in this case. The results show a clear decrease in temperature and NOx emissions with only some losses towards the end of the expansion cycle in pressure. With temperature coming close to starting temperature towards the end of the cycle, this shows improvement towards thermal efficiency.

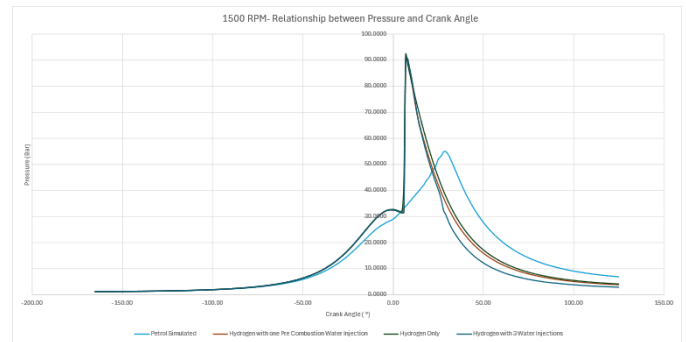


Figure 19: Pressure over C.A. hydrogen (Iatrakis, 2024)

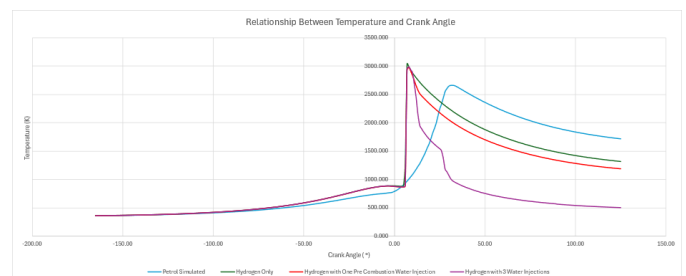


Figure 20: Temperature over C.A. Hydrogen Comparison (Iatrakis, 2024)

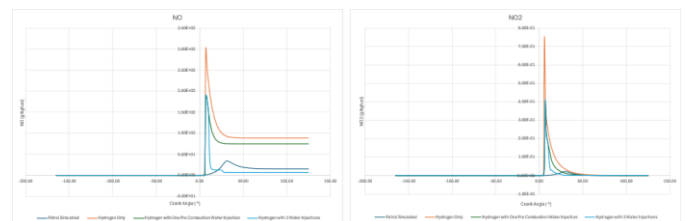


Figure 21: NOx Hydrogen Comparison (Iatrakis, 2024)

Another simulation was conducted using a lean hydrogen mixture with an equivalence ratio of 0.8, employing the same water injection settings as before. This resulted in pressures more aligned with those observed in petrol engines, a significant decrease in temperature, and reduced NO production. However, as anticipated, there was a notable increase in NO2 production, likely due to the higher oxygen content and possibly suboptimal combustion timing for this mixture. Despite these challenges, the results highlight the potential benefits of even leaner mixtures, warranting further

investigation.

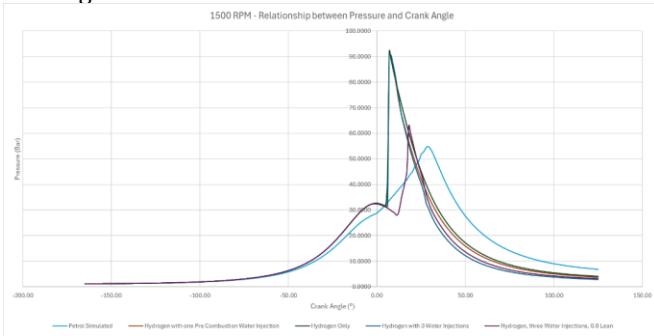


Figure 22: Pressure Hydrogen Lean + Water Comparison
(Iatrakis, 2024)

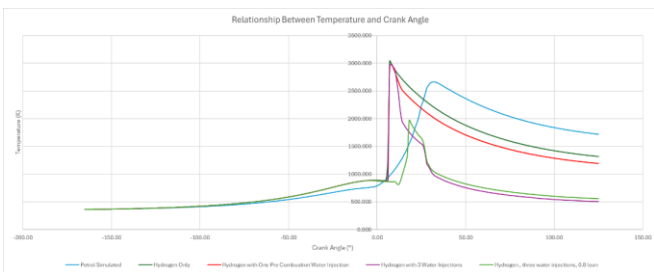


Figure 23: Temperature Hydrogen Lean + Water Comparison
(Iatrakis, 2024)

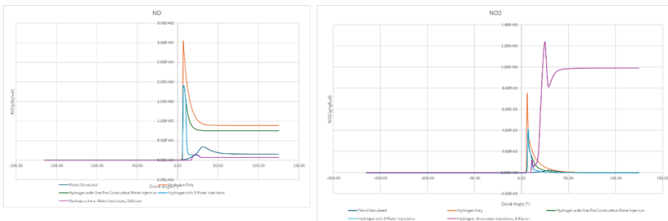


Figure 24: NOx Hydrogen Lean + Water Comparison
(Iatrakis, 2024)

The previous research has demonstrated the viability of using hydrogen and water injection as a combustible fuel combination to reduce emissions and potentially eliminate greenhouse gas emissions. Future work should focus on exploring direct hydrogen injection techniques to enhance control over injection points. Additionally, considering multiple point injection could allow for more effective utilization of hydrogen's combustion properties. These strategies aim to optimise the performance and environmental benefits of hydrogen as a fuel source.

7 Ricardo Wave Simulation

A simple simulation was conducted using Ricardo Wave to model the physical performance characteristics of an engine similar to the Sigma engine, but configured to run on hydrogen. A simplified single-

cylinder model was created, incorporating the Ford Sigma's engine parameters along with combustion parameters derived from hydrogen simulations in ANSYS Forte. The parameters utilized included those from three water injections and a 1.0 equivalence value for hydrogen combustion. Additionally, a boost map escalating from 1Bar to 2Bar at 2000RPM was applied, recognising that hydrogen combustion requires higher air pressures to generate comparable power [4]. The specific burn duration and Wiebe function parameters were extracted from the Ansys Forte simulations. The simulated results, when scaled to represent a 4-cylinder engine, indicate a peak power of 171 hp and a torque of 220 Nm, aligning with the performance of a modern 1.6L Ford Ecoboost engine [5]. However, the direct increase in torque from 1000rpm to 2000rpm suggested by the boost map is unrealistically abrupt, indicating that employing a supercharger or a more gradual boost map would likely yield more realistic outcomes.

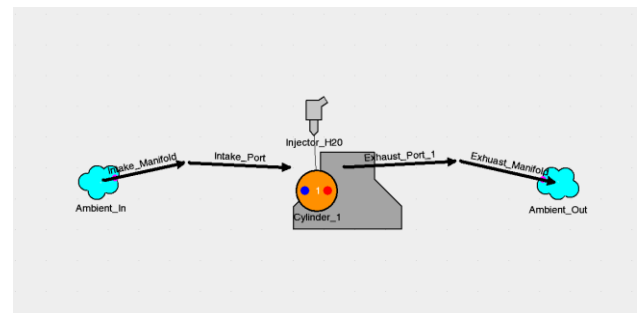


Figure 25: Simplified Single Cilinder Model Ricardo Wave
(Iatrakis, 2024)

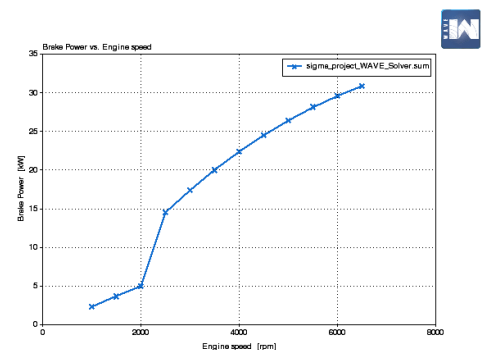


Figure 26: Power Graph 1 Cilinder Simulation Ricardo Wave
(Iatrakis, 2024)

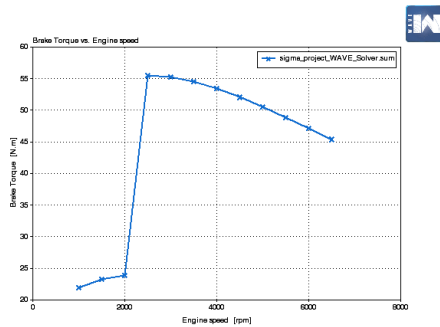


Figure 27: Torque Graph 1 Cilinder Simulation Ricardo Wave (Iatrakis, 2024)

6. CONCLUSIONS

The previous study presents a method for validating an Ansys Forte Combustion model against measured data, along with the development of a hydrogen combustion model using Ansys and Wave software. This research contributes positively toward utilizing hydrogen as a fuel in internal combustion engines to reduce emissions. It highlights hydrogen's characteristics as a combustible fuel, but emphasizes that further work is needed to enhance simulations with direct injection systems. Specifically, the study suggests exploring the effects of injecting hydrogen at various points throughout the engine cycle, adjusting timing, and other parameters. Additionally, water injection has been identified as a viable method to significantly reduce NO_x emissions from hydrogen combustion. With proper development, capturing water post-combustion could be optimized to maintain a high operational range.

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