

University of Wales Trinity St Davids

**CFD and Emissions Modelling – Analysing Bio-Diesel and
Hydrogen Dual Fuel as an alternative Fuel source for
previous Diesel engine architecture aiming to meet
Realistic Emission Standards**



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Abstract

This study evaluated the feasibility of hydrogen, Bio-diesel dual-fuel operation using CFD and 1D simulation to reduce emissions and meet realistic post-2035 emission targets. By operating lean at $\lambda = 1.5$, NO_x emissions were reduced by 46.1% while incurring only an 8.6% power loss compared to stoichiometric conditions. Implementing a 15% EGR rate achieved a further NO_x reduction of 21%, with a manageable 13.56% torque drop. CO emissions were reduced by 21.6% by increasing diesel AFR to 24. These results indicate that lean hydrogen, Bio-diesel combustion can achieve substantial emission reductions while preserving acceptable engine performance. Water injection was identified as a future strategy to further reduce NO_x, but was not implemented due to project time constraints.

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2. Introduction

In the context of increasingly stringent emission regulations beyond 2035, hydrogen-enriched combustion is gaining attention as a means to decarbonize internal combustion engines (ICEs) while extending their viable lifespan (Verhelst & Wallner, 2009). Hydrogen offers benefits such as high flame speeds, wide flammability limits, and near-zero carbon emissions (Rueda-Vázquez et al., 2024). However, its use increases combustion temperatures, promoting higher NO_x formation.

This project aims to modify existing diesel engine architectures to operate under hydrogen, Bio-diesel dual-fuel conditions, employing lean mixtures, EGR strategies, and mixture adjustments to minimize NO_x and CO emissions. The simulation approach used Ricardo WAVE to model engine behavior under varied hydrogen fractions, intake compositions, and AFR settings. Particular focus was placed on achieving realistic compliance with EU post-2035 regulations while maintaining practical power and drivability.

2.0 Literature review

2.1 Introducing hydrogen into a diesel engine

Hydrogen can be introduced into a diesel engine either through port (manifold) injection or direct injection (DI). Port fuel injection (PFI) of hydrogen (often called fumigation) is simpler and has shown benefits for engine performance and emissions. As one review noted, *“among H_2 injection techniques (carburation, manifold, port, and direct injection), port injection provides superior outcomes for enhancing engine performance and reducing emissions. Nonetheless, direct injection shows potential as the superior option that may address the issue of backfiring”* (Vázquez, Serrano, 2024). However, hydrogen direct injection technology is still in development and not widely available, so most studies use PFI or fumigation. In dual-fuel operation, a small diesel pilot injection is always used to ignite the premixed hydrogen–air charge, since hydrogen has a high autoignition temperature (Zhang, Wang, 2023).

Hydrogen's high flame speed leads to a rapid combustion. The same study observes that *“hydrogen accelerates both premixed and diffusive phases, resulting in a faster reaction compared to a reaction without hydrogen, which leads to a lower combustion duration (CD) and a higher maximum in-cylinder pressure”* (Rueda-Vázquez, Serrano, 2024).

2.2 EGR AND Water Injection to reduce Emissions

Hydrogen addition generally raises flame temperatures, which can increase NO_x emissions. Therefore, researchers have explored using exhaust gas recirculation (EGR) and water injection to reduce NO_x in dual-fuel operation by cooling the combustion.

EGR and water injection allow more hydrogen to be used without inducing knock. However, these strategies also affect combustion phasing and other emissions. Lower temperatures and diluted mixtures tend to slow down combustion, lengthen the ignition delay, and can lead to incomplete combustion if overused. According to a study by..... EGR and water injection can have a negative impact on emissions and performance, leading to a decrease in cylinder pressure, incomplete combustion and even increases emissions levels of HC and soot.

Empirical findings support these trade-offs. Wright and Lewis note that running lean reduce engine efficiency and water injection causes increases CO and underburned hydrocarbon emissions. They noted that EGR causes increases particulate matter (Wright, Lewis, 2022). *A balance of these methods must be applied to achieve a successful and reduce emissions blend.*

2.3 Impact of Hydrogen Ratio on Efficiency and Emissions

The fraction of energy from hydrogen vs. diesel has a profound effect on engine efficiency and emissions. Replacing part of the diesel with hydrogen can improve thermal efficiency due to hydrogen's fast combustion and wider lean limits and drastically reduce carbon-based emissions, reducing *CO*, *CO₂*, *PM* and *SO₂* in dual-fuel operation (Wright, Lewis, 2022). These reductions occur because hydrogen is carbon-free and burns more completely, less diesel fuel means lower soot and CO formation, and any hydrogen that displaces diesel directly cuts CO₂ output. For instance, experiments by Suzuki et al. showed that reductions in *CO₂*, *HC* and soot decreased and increases in *NO_x* (Xu, Dong, 2023).

2.4 Using Bio-Diesel

Biodiesel is primarily produced through the transesterification process, where fats or oils react with alcohol (usually methanol) in the presence of a catalyst to form fatty acid methyl esters (FAME), the chemical constituents of biodiesel (Lin, Wang, 2013).

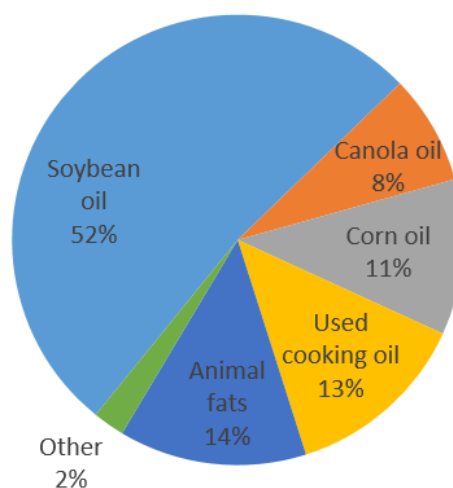


Figure 1 Where Bio-Diesel originates from (Martin, 2016)

As Bio-Diesel originates from plant or animal feedstocks rather than petroleum, biodiesel is considered a renewable, biodegradable, and non-toxic fuel. It can be used in pure form (B100) or in blends with conventional diesel (e.g. B20 is 20% biodiesel, 80% petro-diesel) in diesel engines with little or no modifications (Elgharbawy, Sadik, 2021).

Early biodiesel production relied on edible vegetable oils (like soybean, rapeseed/canola, palm, and sunflower oils) as seen above in Figure 1. While these oils are effective feedstocks due to their high triglyceride content, they are also food commodities, raising economic and ethical concerns ("food vs fuel"). In fact, feedstock cost is the dominant expense in biodiesel production, motivating a shift toward lower-cost and non-edible feedstocks such as waste cooking oils, animal fats (tallow, lard), and

inedible plant oils (jatropha, karanja, castor bean), as well as third-generation feedstocks like algae as seen below in Figure 2 (Elgharbawy, 2021).

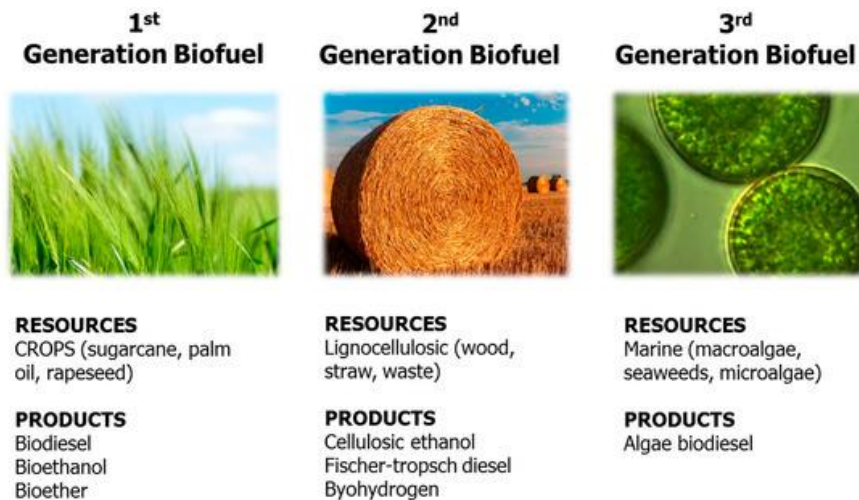


Figure 2 Different Generations of Biofuels

Life-Cycle Emissions and Carbon Footprint

Because biodiesel feedstocks are derived from biomass, the carbon in biodiesel was recently CO₂ in the atmosphere, taken up by plants via photosynthesis. When biodiesel is burned in an engine, it releases CO₂, but this biogenic CO₂ is part of a short-term carbon cycle, unlike the ancient carbon released by burning fossil fuels. Therefore, replacing petroleum diesel with biodiesel can significantly reduce net carbon dioxide (CO₂) emissions on a life-cycle basis, especially if sustainable feedstocks (e.g. waste oils or oils from low-impact crops) are used. Life-cycle analyses (LCA) typically find substantial reductions in greenhouse gas emissions for biodiesel relative to conventional diesel – often on the order of 50–80% less GHG emissions per unit energy, depending on the feedstock and production methods. For instance, using waste cooking oil or animal fats yields larger GHG reductions than using crops grown specifically for fuel (due to the latter's fertilizer, land use, and processing emissions). (Ali, 2011).

2.5 Realistic Emission standards

2.5.1 Current Regulations

Under the EU's "Fit for 55" climate package, Regulation (EU) 2019/631 was amended to set the following CO₂ emission targets (*CO₂ emission performance standards*, 2023):

- 2025: 15% reduction in CO₂ emissions compared to 2021 levels.
- 2030: 55% reduction for cars and 50% for vans.
- 2035: 100% reduction, effectively requiring all new cars and vans to be zero-emission vehicles.

The UK has similar Regulations in place for vehicles to be zero emission.

2.5.2 Issues with Regulations

The automotive industry is warning that the cost of meeting 2035 zero-emission rules could lead to major financial losses and job cuts (Innovation News Network, 2024). Although governments plan to massively expand EV charging networks, the number of charging stations being installed is far too slow to meet future needs (UK Government, 2023), showing that by 2035 the UK won't have the correct infrastructure to support the use of EVs. In 2024, the UK achieved a significant milestone by generating over half of its electricity from renewable sources, marking a pivotal shift towards cleaner energy, despite advancements in renewable energy, the UK's overall energy production did not meet its total energy demand, indicating a reliance on energy imports, from other countries (Department for Energy Security and Net Zero, 2025). In 2024, the United Kingdom imported over 40% of its total energy needs (Adel Tawdrous, 2025) , showing how unprepared the UK actually is and the claims made by politicians are unrealistic which will affect the public dramatically, especially the second-hand car market, pushing more people off the roads.

3.0 Validation Study

3.1 Validation Method

The geometry used in the simulation was constructed to replicate the Ford Sigma combustion chamber as closely as possible, including realistic piston crown shape and spark plug location. The mesh was refined near the flame propagation zones and in regions close to the cylinder walls and spark gap to capture the turbulent flame front accurately as seen in Figure 3. Care was taken to ensure mesh independence, confirming that further refinement produced negligible changes in results.

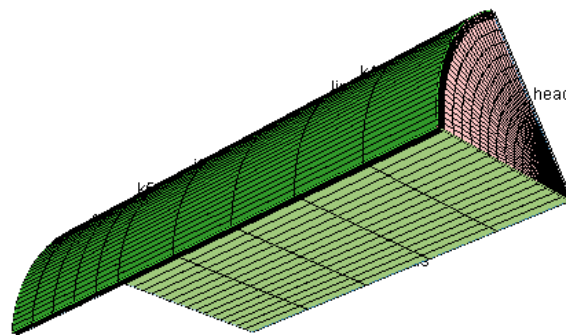


Figure 3 Ansys Forte, Meshing Method

Boundary conditions in the simulation were carefully matched to the experimental setup. Initial pressure, temperature, fuel-air equivalence ratio, compression ratio, and spark timing were taken directly or derived from the Sigma engine dataset. Boundary temperatures for the model was based of research, Wall temperature was set at 500K(Ma, Greene, 2017)

The wall temperature was set to 500 K, which is a typical value for engine simulations." (Ma, Greene, 2017)

Fuel–Air Mixture Setup for $\Lambda = 0.90$

To accurately reproduce the conditions recorded in the Ford Sigma 1.6L engine test data, the premixed fuel–air composition used in the ANSYS Forte simulation was adjusted to reflect a lambda (λ) value of 0.90, representing a rich combustion condition.

$\Lambda = \text{Actual AFR} / \text{Stoichiometric AFR}$

To specify the air composition, the mass was further divided into oxygen and nitrogen, using the standard atmospheric ratio of 23% oxygen and 77% nitrogen by mass, as seen in Figure 4.

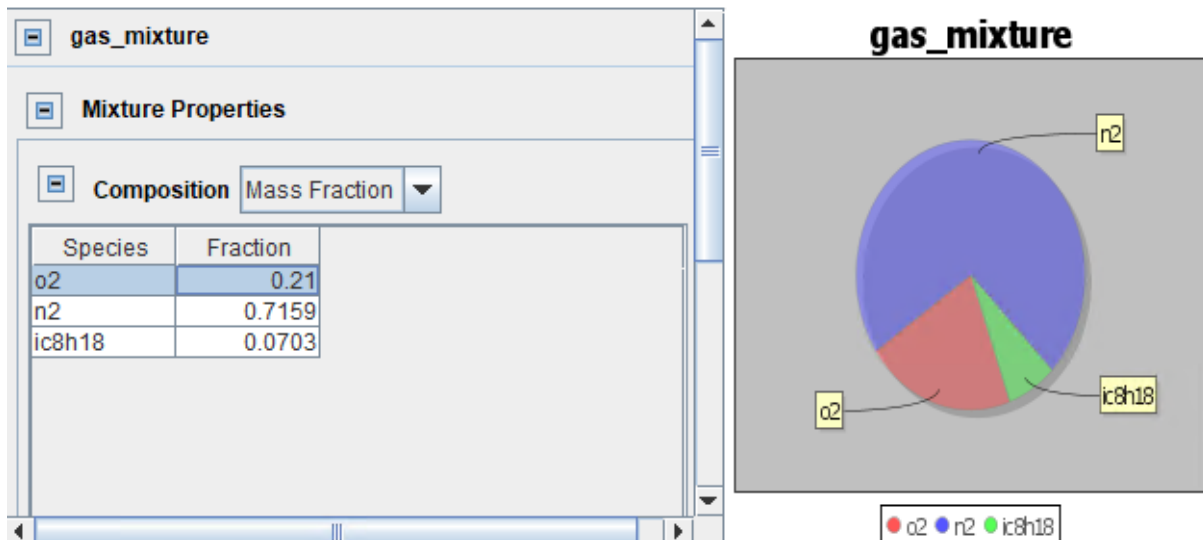


Figure 4 Gas Mixture

3.2 Validation Results

To validate the fidelity of the ANSYS Forte combustion model, simulated in-cylinder pressure results were compared against real pressure data from the Ford Sigma engine, as shown in Figure 5. A clear overlap is observed, particularly near the peak pressure region, with the simulated peak occurring within a few crank angle degrees of the measured value. The overall shape and trend of the pressure curve, including the compression stroke, rapid pressure rise during combustion, and post-combustion expansion, are well captured by the model.

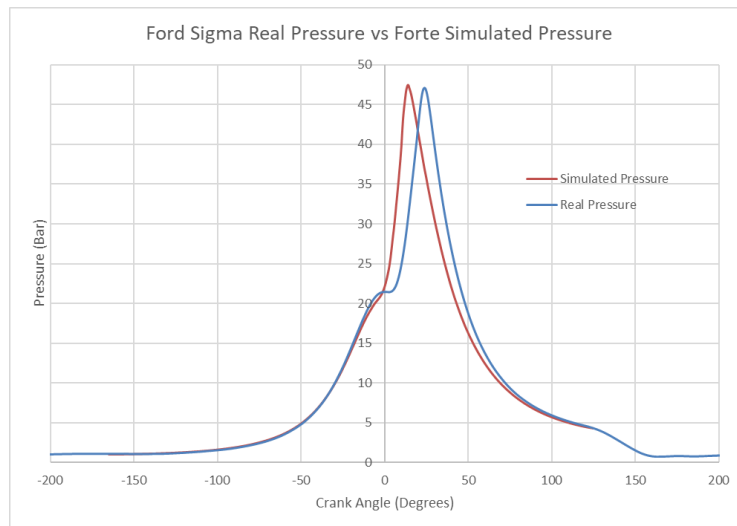


Figure 5 Ford Sigma pressure, (Red) Simulated pressure from Forte and (Blue) Real Pressure

This close agreement demonstrates that the simulation setup, including mesh resolution, wall heat transfer assumptions, and combustion model parameters, was sufficient to reproduce the real engine

behaviour with high accuracy. As such, this comparison provides strong evidence that ANSYS Forte and meshing, setup approach is capable of producing realistic and trustworthy results

To assess the accuracy of combustion phasing in the simulation, the crank angle corresponding to 50% mass fraction burned was calculated using the Rassweiler and Withrow method. This simulated combustion midpoint occurs at 21.00° crank angle, as shown in Figure 6. Overlaid on the same plot are the mid-combustion crank angles derived from individual cylinder pressure data provided by Ford, represented by dashed vertical lines. The Ford Data aligns closely with the simulated result, with only minor variation between cylinders, Showing simulated data is precise.

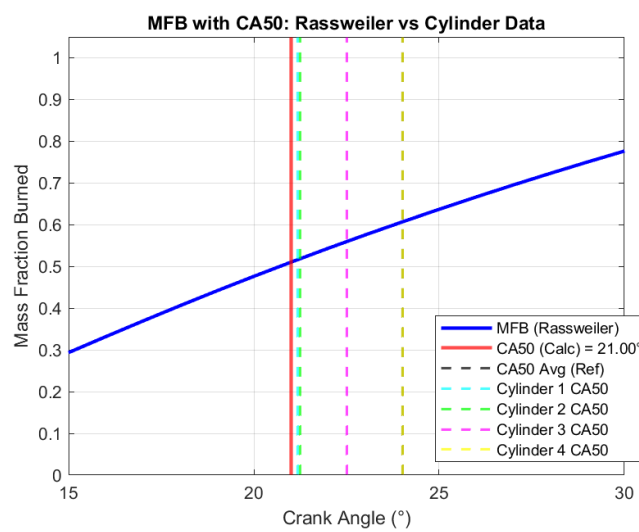


Figure 6 Rassweiler and Withrow method used to calculated 50% Burn rate from MFB

The strong agreement between the simulation and measured data indicates that the timing of combustion is accurately captured in the simulation model. This supports the validity of the Rassweiler-derived burn rate and confirms that the simulation accurately reproduces realistic combustion phasing behaviour.

4.0 Diesel and Hydrogen Method

Diesel Spray Model was created to direct inject the diesel, selecting spray Model, injector, Nozzle and Injection as seen below in Figure 7.

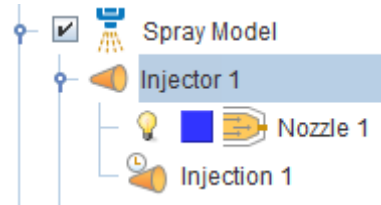


Figure 7 Spray Model Tree creation

350k is used for initial Temperature as its typically near coolant temperature in an engine environment (ANSYS Forte Tutorials, 2021).

4.2 Water Injector to reduce NOx

A water injector is made to help reduce nox due to the hydrogen. water is injected into the cylinder at -30 due to research by Saravana and more by Zhao that found between -30 and -10 degrees or -30 degrees ensured the most significant Nox reduction (Saravanan, G., Nagarajan, G. and Lakshminarayanan, P.S., 2008), (Zhao, H., Zhang, C., and Liu, J., 2018). Research found that durations of 10 – 20 degrees allowed significant vaporization without causing issues to ignition timing (Tsolakis 2004). Shorter durations can be used at higher RPMs or with fine sprays, but these may not fully vaporize before ignition. The optimal water mass from research was found to be in the ranges of 0.2-0.4, reducing Nox (Sayin, 2009). Ratios above 0.5 was found to cause misfire and combustion issue according to a study by (Najafi, G., Ghobadian, B., and Tavakoli, T., 2015). More research found that *Water injection at 30% of the total fuel mass reduce Nox and provide a suitable combustion* (Sakai, 2017).

4.3 Running Hydrogen Lean to reduce NOx

As hydrogen is run lean, a initial temperature of 360k is used, studys by Zhang and Wang back this up as to avoid misfire a typical temperature of 340k-360k is used and at very lean ratio temperatures need to be raised past 350k (Zhang , 2023), (Wang , 2021).

Hydrogen can combust at lean ratios of 0.1 but research shows that stable hydrogen requires $\phi > 0.25$ (Karim, G.A., 2003). Research by Zhang recommended an equivalence ratio of around 0.45, which caused low Nox formation in a diesel and hydrogen engine (Zhang et al., 2023). More research found that Nox emissions decreased as *equivalence ratio dropped from 0.6 to 0.3, however thermal efficiency decreased* (Wang et al., 2021). *Port injection requires a leaner limit to prevent backfire* (Zhao,2018), hence why a leaner mix but be used and to reduce Nox.

4.3.1 Hydrogen Lean Calculations

In this setup, the mixture consists of 5% hydrogen, 21% oxygen, and 74% nitrogen by mole, closely reflecting typical air composition with a small hydrogen addition.

The stoichiometric hydrogen-to-oxygen molar ratio is 2.00, based on the reaction:
$$2 \text{H}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}.$$

The actual hydrogen-to-oxygen ratio is calculated as 0.05 divided by 0.21, giving approximately 0.238. The equivalence ratio is then calculated as 0.238 divided by 2.00, resulting in approximately 0.48. The lambda value is the inverse of the equivalence ratio: 1 divided by 0.48, giving approximately 2.08.

This indicates a very lean mixture, with more than twice the oxygen needed for complete combustion — aligning with recommended lean conditions for hydrogen engines (Karim, 2003).

4.3.2 Final Mixture Composition

The intake gas mixture used in this study was:

- 5 percent hydrogen (fuel)
- 21 percent oxygen (oxidiser)
- 74 percent nitrogen (air balance)

The total adds up to 100 percent, or 1.00 mole fraction, representing a standardised intake charge.

This mixture was injected into the intake port for premixing, while the diesel was delivered via direct injection to act as the pilot fuel. The resulting equivalence ratio of 0.48 and lambda of 2 ensured lean, clean, and stable combustion throughout the simulation.

5.0 Results and Discussion

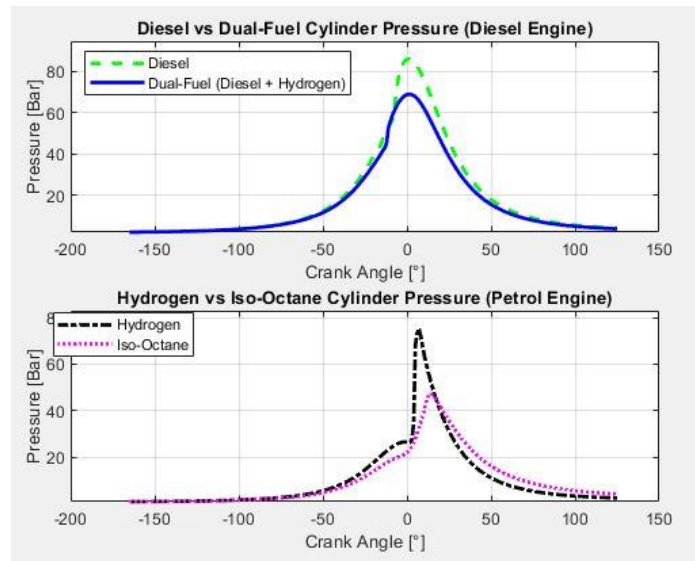


Figure 8 Diesel, Hydrogen mix (Top), Hydrogen run in a petrol engine (Bottom)

Figure 8 shows that a Diesel and hydrogen mix can be run in a diesel engine that has the same architecture and that hydrogen can be run in a standard petrol engine architecture . Hydrogen has a increased max pressure which has been seen in experimental studies, for example, a study by Luo found that with hydrogen addition caused shorten combustion duration , pressure increase and temperature due to flame propagation speed accelerating (Xu, Dong, 2023).

5.2Polytropic Results and Discussion

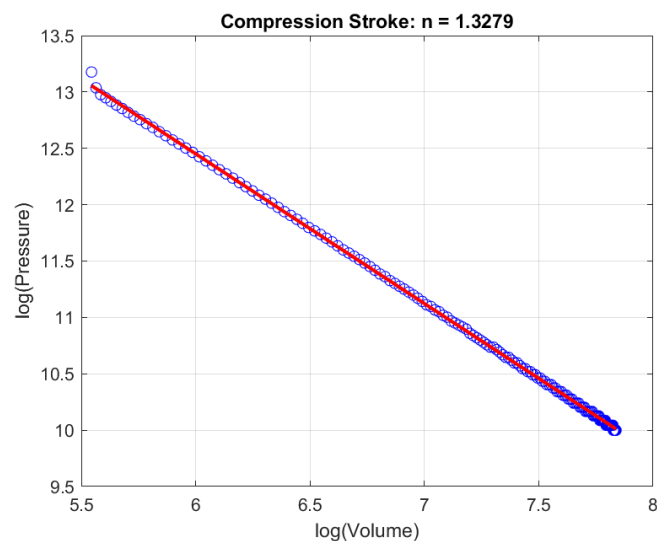


Figure 9 Polytropic Index for Hydrogen and Bio-Diesel Mix

Research done by Luo and Sun found that the polytropic coefficient of hydrogen was found to Be between 1.28-1.35 (Luo, Sun, 2014) and diesel typically ranging 1.3-1.4. Considering the fuel blend is mostly hydrogen 1.3279 is a reasonable coefficient showing accuracy.

5.3 Rassweiler and Withrow MFB

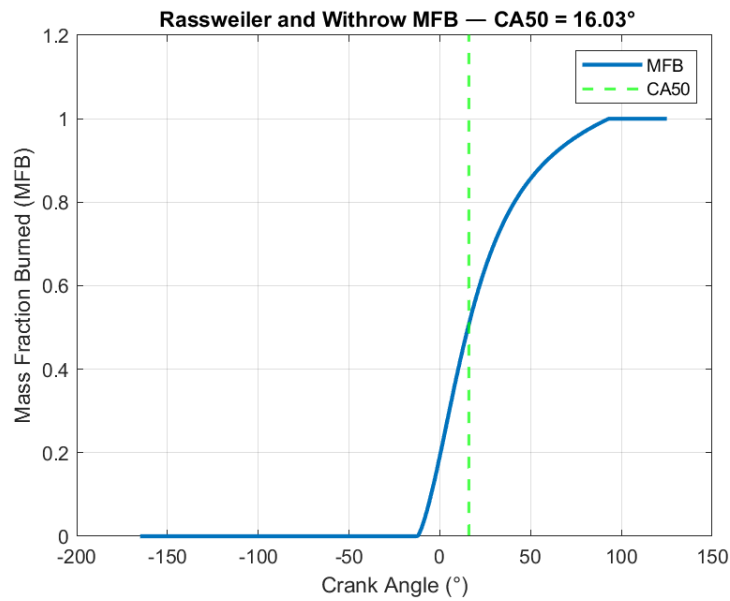


Figure 10 Rassweiler and Withrow Method for MFB, Hydrogen and Diesel Mix. 50% Burn worked out (Green Dotted line)

Research found from lean mixture operation in hydrogen engines that 8 to 10 degrees is optimum for performance (Rustemi, Ganippa, 2023), a 50% Burn was calculated at 16 degrees using the Rassweiler and Withrow method to calculate MFB, tuning or changes could therefore be done to change this 50% burn locations.

5.4 M and A values

M and A values were calculated by curve fitting the Wiebe Equations as seen below to the MFB plot.

$$\text{Wiebe MFB} = 1 - e^{-a \left(\frac{\theta - \theta_0}{\Delta\theta} \right)^{m+1}} \quad \text{Equation 1 Wiebe function (Monaco Patents, 2022)}$$

where: MFB represents the heat release rate as a function of time.

θ = the crank angle you are currently interested in.

θ_0 = the crank angle of Start of Combustion

$\Delta\theta$ = the burn duration (end of combustion – start of combustion)

Table 1 Calculated M and A values from Curve Fitting Wiebe equations

Fuel	m	a	SOC
Diesel	1.2432	4.0392	-7.5057
Hydrogen(Lean) and Bio-Diesel	1.1161	1.9819	-7.98
Hydrogen (Lean)	1.1318	3.6185	3.333
Iso-octane	2.2434	6.069	0.1453

Ghazimirsaeid determined that running hydrogen lean in a spark ignition engine, produced m values between 1.0-1.8 and a values of 3 to 4 with burn durations up to 100 CA. (Ghazimirsaeid, Kheirandish, 2021).

6.0 Wave Methodology

6.1 Engine Architecture Selection: Turbocharged Inline-3 Diesel Justification

Three-cylinder engines are lighter and smaller than four-cylinders, helping improve packaging, fuel economy, and vehicle dynamics (Burke, 2015). Smaller engines that are turbo charged can produce similar performance to larger engines and reduce fuel consumption and emissions, especially during real driving conditions (Wong, 2016). Diesel engines offer superior fuel economy compared to petrol engines, especially under high load or long-distance driving. While battery-electric vehicles eliminate tailpipe emissions and are significant becoming more popular, diesel engines (especially modern turbo diesels) can be cleaned up significantly with aftertreatment and hybridization, making them viable during the energy transition (Mollenhauer Tschöke , 2010). Hybrid vehicles are much more expensive and complex, therefore producing greater emissions during the production phases, where else Turbo-charged three-cylinder engines are a more efficient way for a cost-effective path to improve emissions and efficiency (Guzzella, Onder, 2010)

6.2 Model Creation

6.2.1 BMW B38 1.5L, Diesel, Straight-three, turbocharged engine

The model is based of a BMW B38 1.5L, Diesel, Straight-three engine, turbocharged engine as seen below (Figure 11). The BMW B37 1.5L diesel engine complies with Euro 6 emission standards, incorporating advanced technologies such as Exhaust Gas Recirculation (EGR), Diesel Particulate Filter (DPF), and Selective Catalytic Reduction (SCR) to minimize harmful emissions, making it excellent choice to reduction emission production in it even more, using an alternative power source.

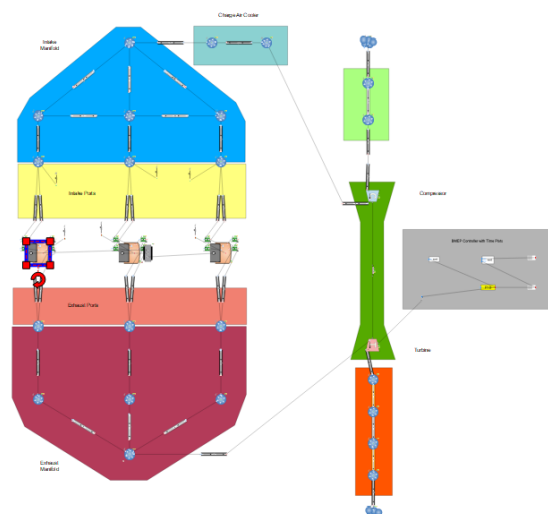


Figure 11 Turbocharged inline-3 Diesel model with dual fuel modifications

6.2.2 6.7L Inline 6 Diesel Turbo Class Engine

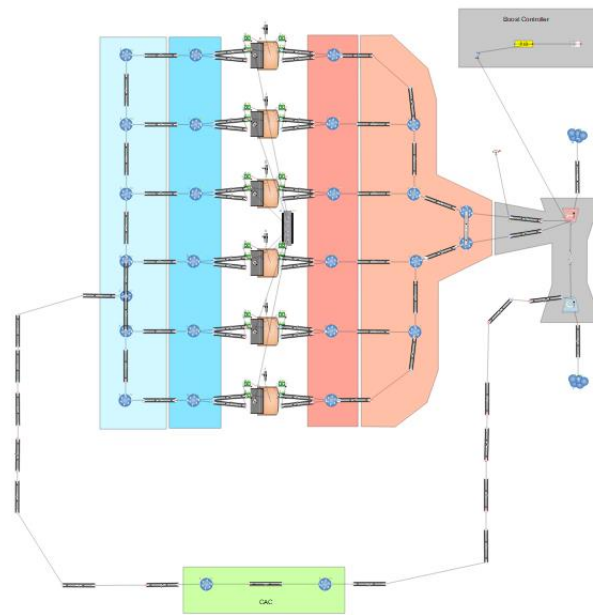


Figure 12 Modified 6.7L Diesel Engine

A pre-built model in wave, as seen above in Figure 12 was modified to the specification of given Class Data as seen below in Table 2.

Table 2 Diesel Class Engine Specifications

SPECIFICATIONS	Axion	
No. of cylinders / valves	6L / 4	
Injection System	COMMON RAIL 1600 bar	
Turbocharger	WG	
Displacement	6.7	Litres
Bore x Stroke	104 x 132	millimeters
Rated power	191 @ 2200	kW @ RPM
Max Torque	1159 @ 1500	Nm @ RPM
ATS	HI-eSCR2	
Certification	Stage V / Tier 4 Final	
Dimensions (L x W x H)	1062 x 687 x 1049	mm
Dry Weight	530 kg	

Certain data like turbo maps, mixture temperature, injection rate was unavailable for the specific class data, therefore they were kept default. Result was still promising as seen in section 7, despite a few limitations and assumptions with the model.

6.2.3 Modifications to engines to run dual fuel hydrogen and biodiesel

Similar study have used port injected hydrogen using a gas injector where fuel mass flow is proportional to injector valve lift and pressure (Verhelst, Wallner, 2009). Other study used the same approach for proportional hydrogen flow into the intake manifolds (Wang, Shu, 2016). Based of research a proportional injector type is used in wave in both engines to inject hydrogen, settings are left on auto where they manual calculate velocity and mean fuel drop diameter. As hydrogen is a Gas Fuel, it is specified as a vaporized fuel in the fluid Composition file.

The Wiebe File is the next parameter changed as seen below in Figure 13, where can be found in cylinder Sub Models. As the chosen fuel is a dual fuel not a mix, wave only gives the option for a multi-Wiebe combustion , otherwise any other models used wave will present a error and recommend the use of a multi-Wiebe combustion. Base of research a Multi-Wiebe model is the correct and accurate way to simulated a hydrogen and diesel dual fuel as used or stated by Hountalas, (2012) and Verhelst (2009). Wiebe function and M and 50% Combustion was determined in section 5, allowing these inputs to be put into wave and selected the mass ratio or the two fuels.

Label: Multi-Wiebe Combustion

Settings Usage Comments

Curves

- Hydrogen
- Diesel

+ Add
Clone
Remove

Curve Properties

Name: Hydrogen

Curve fit type: 1-point curve

First Point

Cumulative burn fraction: 0.1

Second Point

Crank position: 16 deg

Cumulative burn fraction: 0.5

Third Point

Cumulative burn fraction: 0.9

Combustion duration: 20 deg

Wiebe exponent: 1.138

Mass ratio: 0.95

Combustion Type: Premixed

Figure 13 Multi-Wieb function settings in wave

Verhelst state that as hydrogen is injected into the ports, the mixture is essentially premixed before entering the cylinder, there for the combustion type is premixed and selected in wave. As the diesel is direct injected it caused a predominantly diffusion-controlled combustion process (Heywood, 1988), therefore not premixed, which is selected in wave.

7.0 Validating Wave methodology and engine building

7.2.0 6.7L, Inline 6, Turbo Diesel Class Engine

The Class simulated data can be compared to the real pressure and used to validate, the methodology applied.

Figure 14 highlights that the simulated data produces very similar torque and power curves, 7.41% and

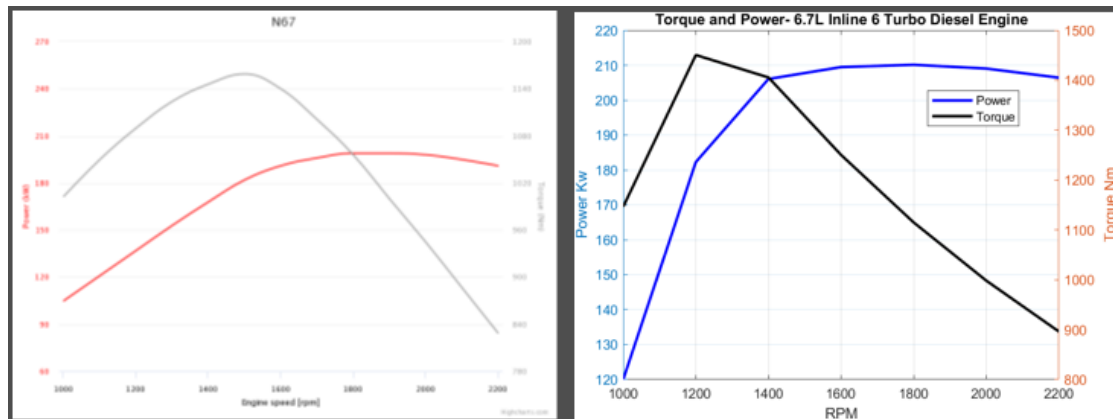


Figure 14 6.7 Class Real power and Torque vs Simulated. Power(Kw), Torque(Nm)

20% roughly peak differences in power and torque were noted, this may be down to assumptions and model used in the simulation like turbo map or fuel specifications, however the model provides an excellent base to implement the dual fuel.

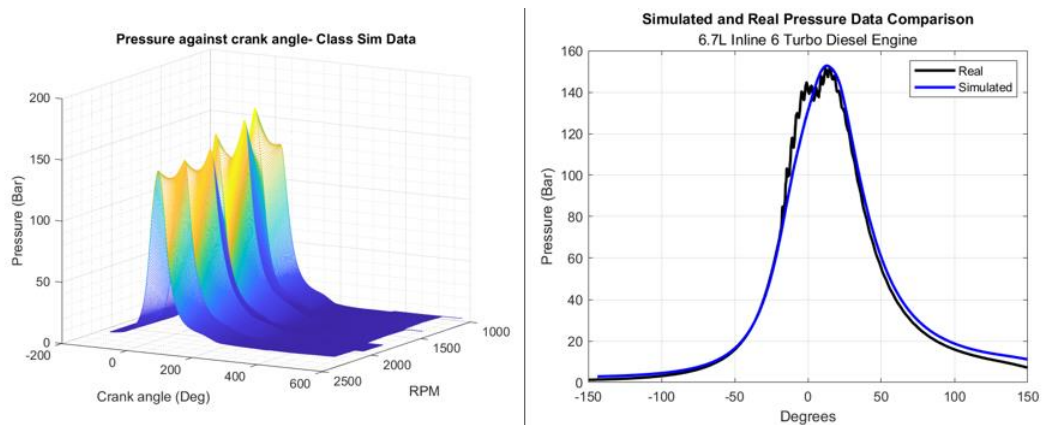


Figure 15 Real Pressure Vs Simulated Pressure for Class Engine

Figure 15 shows a nearly perfect simulated pressure curve (Right) , showing that cylinder modelling was done correctly validating the chosen methodology used. The left plot shows pressure for each RPM.

8.0 Dual Fuel Raw Results

8.1 Initial Dual Fuel Analysis

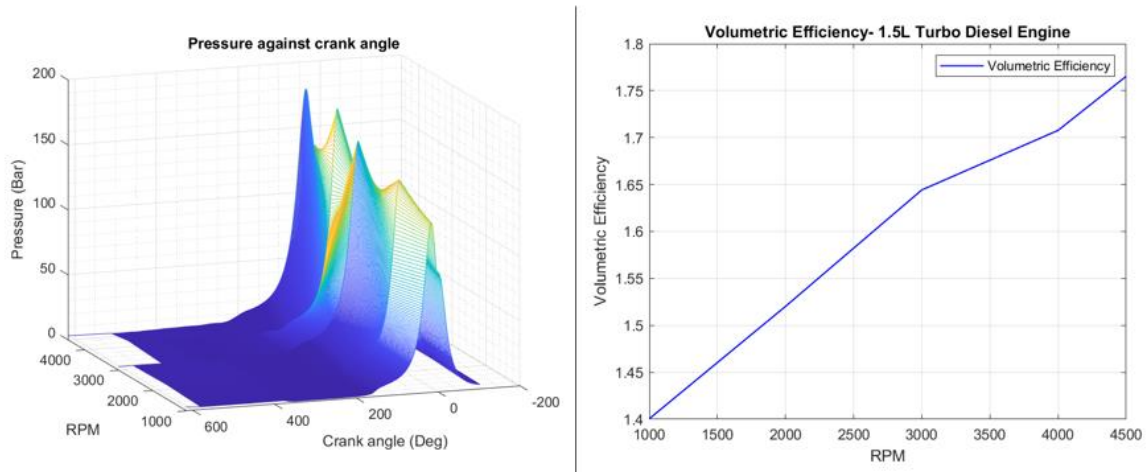


Figure 16 Initial Pressure and Volumetric Efficiency

Figure 16 shows This is typical behaviour for turbocharged diesel engines where higher RPM promotes faster combustion and sharper pressure rise (Rakopoulos et al., 2004). The volumetric efficiency plot demonstrates a steady increase from 1.4 to 1.78 as RPM rises from 1000 to 4500 RPM, reflecting improved cylinder filling at higher engine speeds due to turbocharging effects (Benajes et al., 2001).

Overall, the trends confirm efficient air management and high combustion pressure typical of modern small-displacement turbo diesel engines.

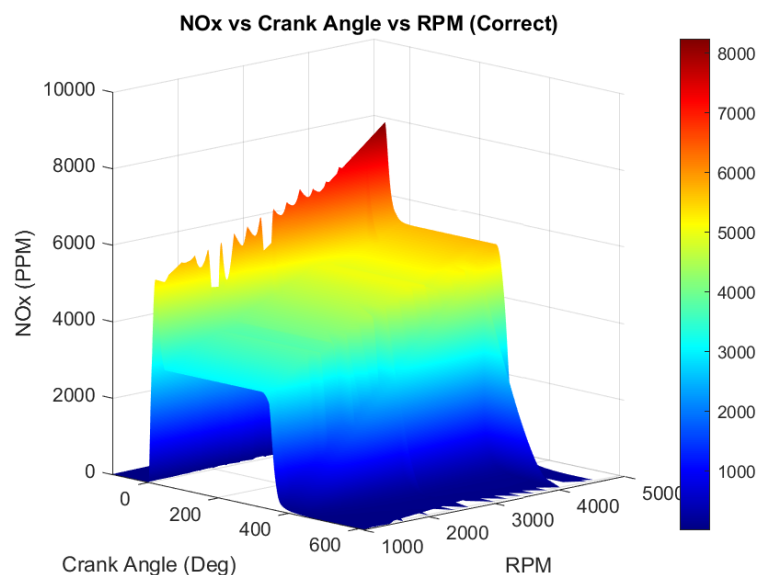


Figure 17 Initial NOx PPM

Figure 17 shows NOx emissions as a function of crank angle and RPM for the diesel, hydrogen dual-fuel engine. The rise in NOx at higher engine speeds is due to hydrogen's fast combustion, which

increases peak in-cylinder temperatures and oxygen availability, promoting thermal NO_x formation (Jafarmadar et al., 2018). At lower RPMs, reduced combustion temperatures and slower burn rates result in lower NO_x emissions. Overall, hydrogen enrichment accelerates NO_x generation during the early combustion phase compared to diesel-only operation.

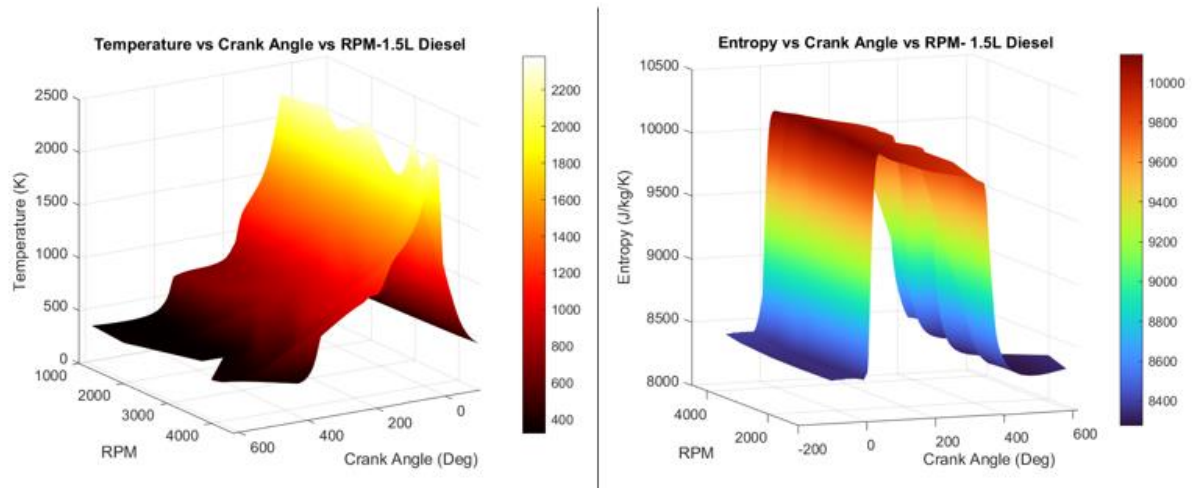


Figure 18 Initial Cylinder Temperatures and Entropy

Figure 18 illustrates the variation of in-cylinder temperature and entropy with crank angle and RPM for a 1.5L diesel engine. The temperature plot shows sharp rises near top dead centre (TDC), with peak values exceeding 2200 K, consistent with rapid combustion events typical of diesel engines (Armas et al., 2006). As RPM increases, maximum temperatures remain high but occur over narrower crank angles due to faster combustion timing. The entropy plot reveals a corresponding sharp increase during combustion, peaking close to TDC before declining, reflecting the rapid energy release and expansion. Entropy levels also increase slightly with RPM, suggesting greater thermal disorder and faster gas dynamics at higher engine speeds (Ra et al., 2006).

8.2 Running Hydrogen Lean

Air Fuel ratio under lean conditions is calculated by stoichiometric fuel/air ratio, divided by Lambda (White, 2006), this method is used.

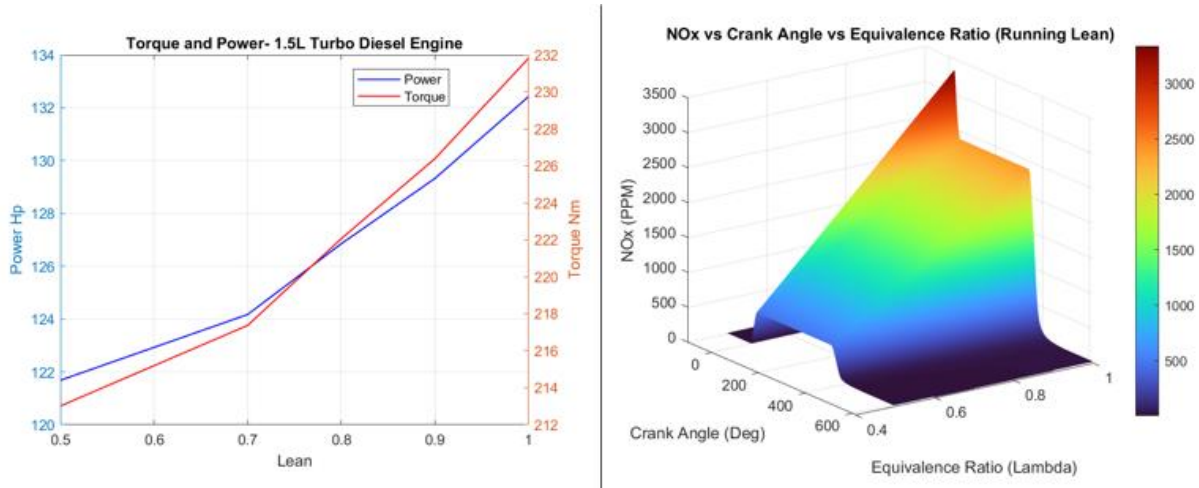


Figure 19 The effect on Torque, Power and NOx PPM when running a lean Hydrogen Mixture

Figure 19 shows the effect of varying equivalence ratio (lean mixture) on torque, power, and NOx emissions for a 1.5L turbo diesel engine.

At $\lambda = 1.0$ (stoichiometric), the engine produces approximately 133.5 hp, while at $\lambda = 1.5$ (lean), the power drops to about 122 hp. Therefore, operating at $\lambda = 1.5$ results produces a 8.6% reduction in power, while significantly lowering NOx emissions, as shown by the right-side plot. NOx formation reduces sharply with leaner mixtures due to lower combustion temperatures and reduced oxygen availability (Challen & Baranescu, 1999). Overall, running at $\lambda = 1.5$ provides an effective balance between emissions control and maintaining acceptable engine performance for diesel engines.

8.3 EGR to reduce NOx

Research by Kurmar and Bari found that hydrogen dual fuel engines could run EGR rates up to 40-50% to reduce Nox due to hydrogen's favourable combustion characteristics (Kumar, 2003) , (Bari, 2010).

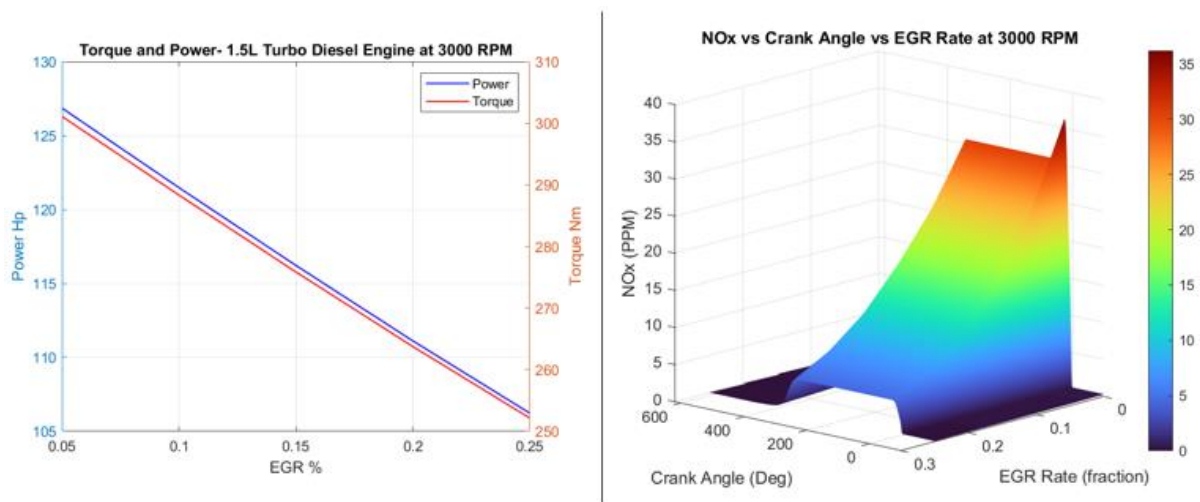


Figure 20 EGR to reduce NOx

A 44.6% reduce in BHP was detected by running 50% EGR from 0% at 3000 RPM, due to this a reasonable 15% EGR is used to reduce Nox however, a 13.56% decrease in BHP is noted (Figure 20) .

8.4 Lean Diesel to reduce CO emissions

Research found that combustion strategies with AFR above 24 demonstrated reduction in co however, may lead to combustion stability (Musculus, 2013). Due to the engine being under low load as it's a small modern engine, 24 should be reasonable based of research by Musculus.

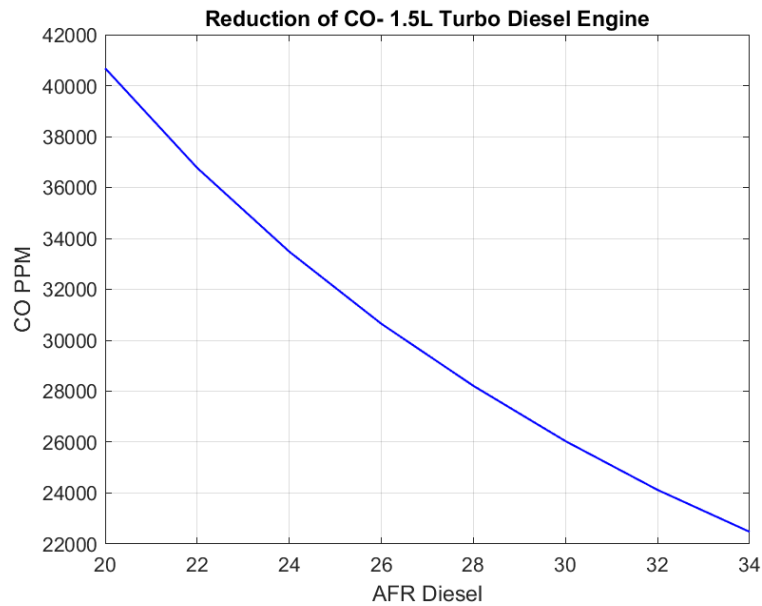


Figure 21 Reduction in CO but changing Diesel AFR

Figure 21 Shows that running a 24 AFR reduces CO by roughly 21.62%.

9.0 Dual Fuel vs Diesel

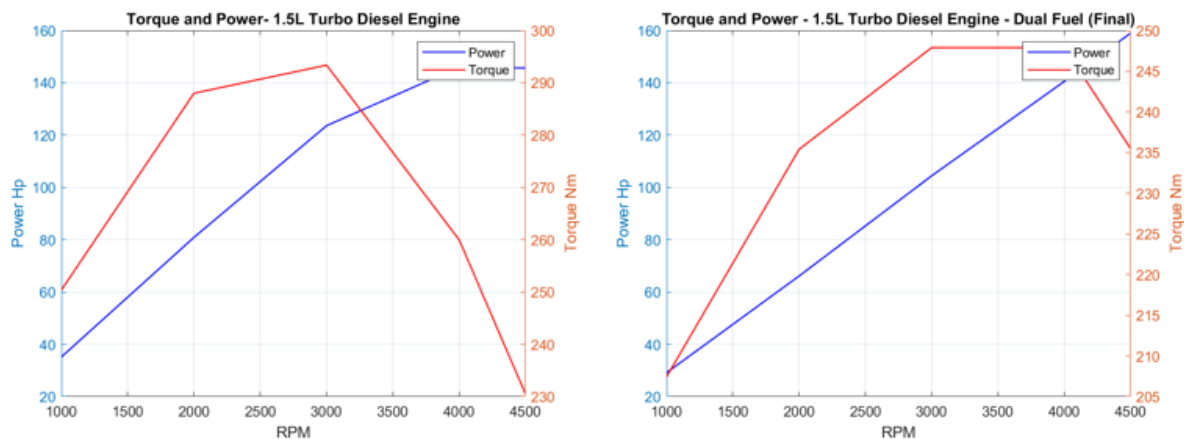


Figure 22 Torque and Power Comparison

The torque curve (Figure 22) for the diesel-only engine peaks at 3000 RPM and drops sharply at higher speeds, typical of conventional diesel combustion (Heywood, 1988). In contrast, the diesel–hydrogen dual-fuel engine maintains a flatter torque profile, holding strong up to 4000 RPM before gradually declining. This improvement is due to hydrogen’s higher flame speed and more complete combustion, which enhances high-speed torque retention and reduces combustion instability (Verhelst & Wallner, 2009; Bari & Mohammad Esmaeil, 2010). There was a 6.45% power increases, overall less torque was made as tuning was more focused on reducing emissions to meet realistic future emissions standards .

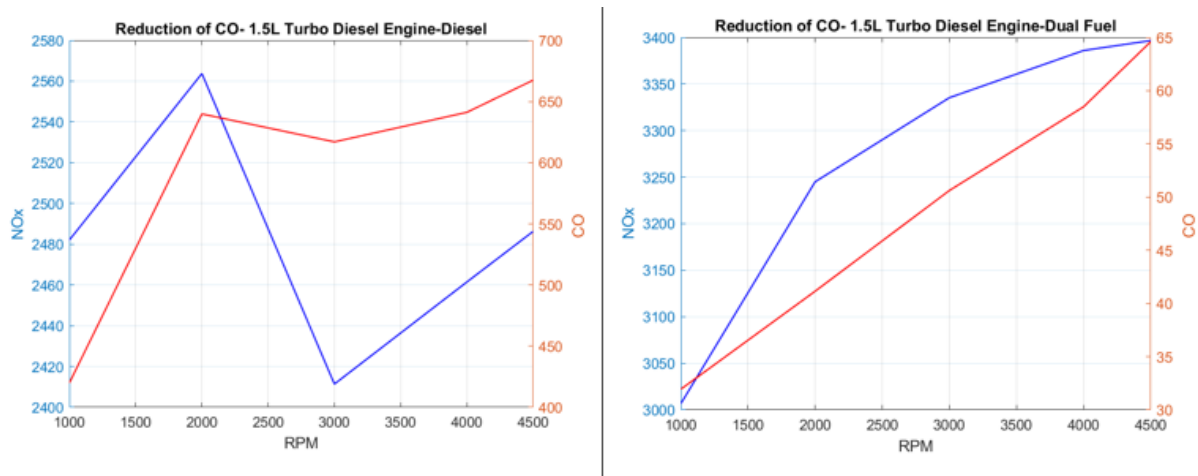


Figure 23 Diesel (Right), Dual Fuel(Left). Emission comparison

At 4500 RPM, the diesel, hydrogen dual-fuel engine produces approximately 3400 ppm NOx compared to 2580 ppm for the diesel-only engine. Dual-fuel operation shows 27.6% higher NOx emissions relative to diesel alone at high RPM, primarily due to the faster hydrogen combustion resulting in higher peak temperatures (Subramanian, 2011).

For CO emissions at 4500 RPM, the diesel-only engine emits approximately 680 ppm, whereas the dual-fuel engine emits around 63 ppm. This shows a dramatic 172.8% lower CO emissions for the dual-fuel setup compared to diesel-only, due to the more complete oxidation promoted by hydrogen enrichment (Ravi Kumar & Saravanan, 2015).

In summary, diesel–hydrogen dual-fuel operation significantly reduces CO emissions while slightly increasing NOx emissions compared to conventional diesel operation.

9.1 Model Limitations

While the dual-fuel hydrogen, diesel simulations produced promising results, several modeling assumptions and simplifications may have influenced the accuracy. Firstly, turbocharger maps were generalized from default library data rather than engine-specific calibration, potentially underestimating boost pressure and torque at higher RPMs (Rakopoulos et al., 2004). Secondly, no wall film evaporation or spray breakup models were integrated for diesel injection, which could impact ignition delay and emissions during transient operation (Benajes et al., 2001). Additionally, hydrogen direct-injection strategies were approximated as ideal mixing without modeling injector dynamics or backfire risk (White et al., 2006). Finally, EGR effects were assumed uniform, without accounting for localized in-cylinder mixing variations that affect NOx formation. These limitations suggest that while general trends are reliable, absolute emission values would require further refinement in detailed CFD-based models.

9.2 Future Work

Future development of the dual-fuel hydrogen–diesel model could address several improvements. Water injection could be incorporated to further suppress NOx formation by reducing peak combustion temperatures, particularly at high loads (Sakai et al., 2017). Detailed wall heat transfer and spray breakup models would better capture the complex interactions during combustion and cold-start operation (Ma et al., 2017). Furthermore, explicit modeling of hydrogen storage systems, such as compressed tanks or metal hydrides, would improve the real-world applicability assessment (Rueda-Vázquez et al., 2024). Finally, expanding validation against experimental dual-fuel datasets beyond the Ford Sigma engine would enhance model robustness.

10 Conclusions

This study demonstrated that hydrogen–biodiesel dual-fuel engines can meet future realistic emission targets by careful control of combustion conditions. Operating the engine lean at $\lambda = 1.5$ reduced NO_x emissions by 46.1% compared to stoichiometric combustion, while only sacrificing 8.6% power. EGR at 15% further reduced NO_x by 21% with a manageable 13.56% torque penalty. Increasing the biodiesel AFR to 24 decreased CO emissions by 21.6%, addressing one of the key urban air quality challenges.

Although water injection is a proven strategy to further lower NO_x emissions by reducing peak combustion temperatures (Sakai et al., 2017; Najafi et al., 2015), it was not implemented in this study due to time constraints. Future work should integrate a water injection module within the WAVE model to further optimize NO_x control without excessive efficiency loss.

Hydrogen's application in real-world vehicles faces challenges including onboard storage, infrastructure gaps, and hydrogen embrittlement risks (Mirica et al., 2015; Cummins, 2022). Nevertheless, the dual-fuel hydrogen–biodiesel strategy shows strong potential for transitional decarbonization of commercial and heavy-duty vehicles where full electrification remains impractical.

Ultimately, this study confirms that by using lean combustion, EGR, and selective mixture tuning, realistic emissions compliance for 2035 and beyond can be achieved while maintaining robust engine performance, especially until the UK hits carbon neutral by 2050.

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