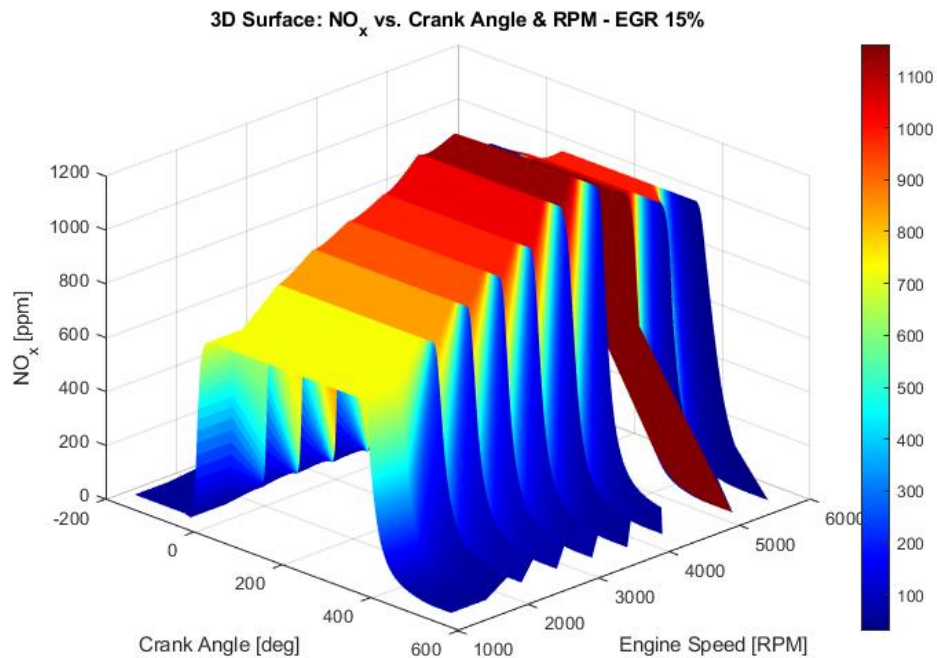


University of Wales Trinity Saint David
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CFD and Emissions Modelling

Engine Performance and Emissions ACEA7005



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Abstract

This study presents an integrated experimental-simulation investigation of hydrogen combustion in a production-derived 1.6 L twin-scroll turbocharged spark-ignition engine. High-fidelity 3D CFD (ANSYS Forte) provided transient in-cylinder pressure, temperature, and emissions traces for diesel, gasoline, methanol, and hydrogen fuels. MATLAB-derived four-parameter SI-Wiebe fits (θ_{50} , $\Delta\theta_{10-90}$, m , burn fraction) were implemented in Ricardo WAVE to enable rapid parametric sweeps of fuel-equivalence ratio (FER = 0.5–1.5), EGR (0–50 %), and engine speed (1 000–6 000 RPM). Results show that lean hydrogen (FER = 0.7) with 15 % EGR achieves an optimal trade-off—retaining >85 % of peak BHP while reducing NO_x by ≈ 80 %. WAVE trends closely match 3D CFD within 1–2 bar for peak pressure and 200 K for peak temperature. Limitations arising from zero-D combustion, uniform EGR mixing, and omitted radical kinetics are discussed, and strategies for model enhancement via multi-zone mixing and reduced H_2 mechanisms are proposed. This framework offers a robust tool for screening hydrogen-ICE strategies and guiding hardware development toward near-zero-emission, high-efficiency platforms.

1 Introduction

1.1 Internal Combustion Engine

Engines have been in use for over 150 years (O’Cean, 2023), serving as devices that convert the chemical energy stored in fuel into thermal energy, which is then used to produce mechanical work. During combustion, the resulting gases reach extremely high temperatures. A heat engine harnesses this thermal energy and, using a working fluid, converts it into useful mechanical work (Gupta, 2013).

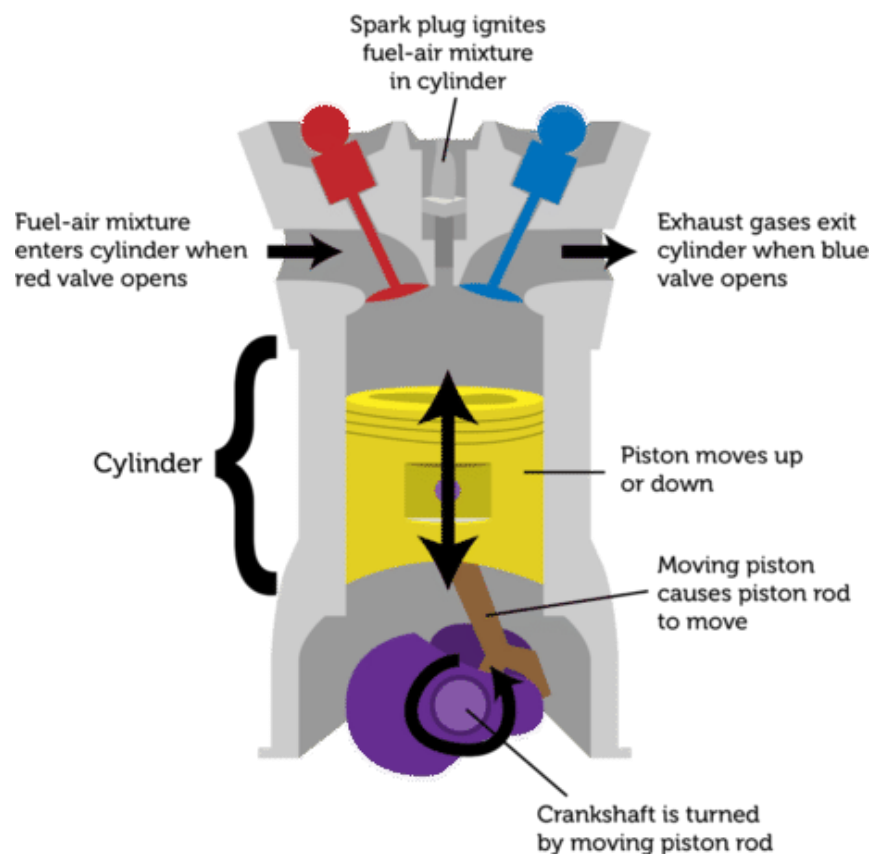


Figure 1 Internal Combustion Engine (CK-12 Foundation, 2019)

Heat engines are broadly classified into two main types: external combustion engines (EC engines) and internal combustion engines (IC engines). In external combustion engines, the combustion of fuel occurs outside the engine cylinder. The heat generated is transferred to a working fluid—typically steam—which then performs mechanical work. Common examples include steam engines, steam turbines, and Stirling engines (Gupta, 2013).

These systems do not allow combustion products to enter the engine cylinder, which distinguishes them from internal combustion engines. In contrast, IC engines combust the fuel-air mixture directly within the engine cylinder, allowing for higher thermal efficiency and more compact designs. IC engines are the most widely used type in automotive and transportation applications today due to their power density and responsiveness (Gupta, 2013).

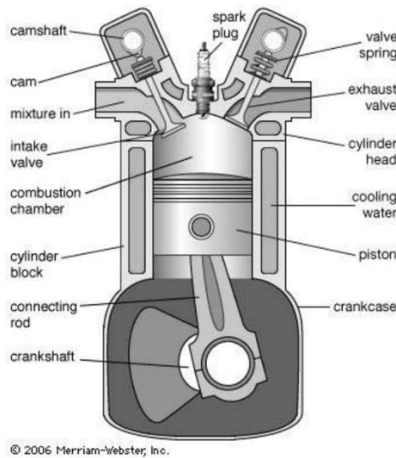


Figure 2 Piston Accelerating Towards crankshaft axis (A Aan and M Heinloo, 2012)

The piston is a critical component in internal combustion engines, responsible for transmitting gas pressure forces to the connecting rod during the power stroke. The connecting rod serves to convert the crankshaft's rotary motion into the piston's reciprocating motion and vice versa, effectively transmitting mechanical forces between the crank and piston (Heywood and Jae, 2015). The crankshaft itself delivers usable mechanical power by converting the reciprocating motion of the piston into rotational motion, using offset crank throws linked by the connecting rods. The cams and camshaft regulate the timing of gas exchange in the cylinder by opening and closing the intake and exhaust valves at precise intervals during the engine cycle (A Aan and M Heinloo, 2012). The valves themselves control the flow of gases into and out of the combustion chamber (Heywood and Jae, 2015).

1.2 Internal Combustion Engine Spark-Ignition vs Diesel

Spark-ignition (SI) and diesel engines differ fundamentally in their air and fuel handling, as well as in their combustion processes. As shown in Table 1, SI engines introduce air during the intake stroke and inject fuel either into the intake port or directly into the cylinder, resulting in a pre-mixed air-fuel charge. Diesel engines, by contrast, intake only air during the intake stroke, with fuel injected directly into the combustion chamber near top dead centre. This fuel spontaneously ignites due to the high temperatures generated during compression. SI engines require an external ignition source—a spark plug—to ignite the mixture, whereas diesel engines utilize compression ignition, eliminating the need for a separate ignition system.

Table 1 Spark Ignition Engine vs Diesel (Heywood and Jae, 2015)

	<u>Spark-ignition</u>	<u>Diesel</u>
1.	Air enters cylinder; fuel injected in intake port, or cylinder.	Air drawn in; fuel injection into cylinder just before combustion.
2.	Spark-ignition of fuel-air mixture.	Spontaneous ignition of fuel-air mixture in fuel sprays.
3.	Load reduced by throttling air and fuel.	Load reduced by reducing fuel injected per cycle: no throttling.
4.	Fuel: gasoline. Volatile, does not spontaneously ignite easily.	Fuel: distillate oil. Must ignite easily at high temperatures.
5.	Lower compression ratio (~10) due to knock limits.	Higher compression ratio (15 to 22); not knock limited.
6.	Lighter construction since pressure forces lower and less durability required.	Heavier construction; higher forces and durability more important.

As also detailed in Table 1, these engine types differ in load control, fuel type, compression ratio, and construction. SI engines manage load through throttle control, adjusting both air and fuel flow, which can increase pumping losses. Diesel engines control load by varying the amount of fuel injected, with no throttling of air, which enhances efficiency under partial load.

This leads to significant differences in design: SI engines are generally lighter and optimized for speed, while diesel engines are built with more robust components to withstand higher pressures and temperatures, ensuring greater durability (McCarthy, Rasul and Moazzem, 2011).

1.2.1 Petrol / Gasoline and Diesel extraction

Petrol (gasoline) and diesel are both refined products derived from petroleum, or crude oil, a naturally occurring hydrocarbon mixture commonly found in underground reservoirs. These reservoirs often contain natural gas alongside crude oil.

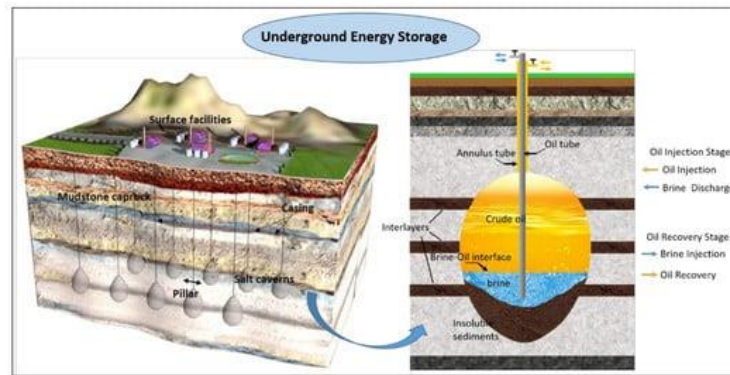


Figure 3 Underground representative view of Crude Oil Reservoirs (Zhang et al., 2020)

As shown in Figure 4, lighter fractions like liquefied petroleum gas (LPG) and gasoline rise to the top of the distillation column due to their lower boiling points, while heavier fractions such as diesel, jet fuel, and residual oils settle lower down. Additional chemical processing, known as conversion, can alter these fractions breaking down heavier hydrocarbons or reassembling them based on market demand (U.S. Energy Information Administration, 2023).

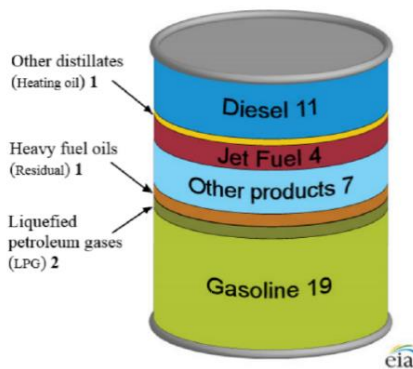


Figure 4 Main Products (measured in gallons) made from a barrel of crude oil, 2013 (U.S. Energy Information Administration, 2023)

Petroleum is refined into useful products such as gasoline, diesel, and lubricants through a sequence of processes—distillation, cracking, and reforming. As shown in Figure 5, crude oil is first heated to around 400°C, producing a vapor-liquid mixture known as feedstock, which enters a fractionating column (Department of Education Open Text Pilot Project, 2021).

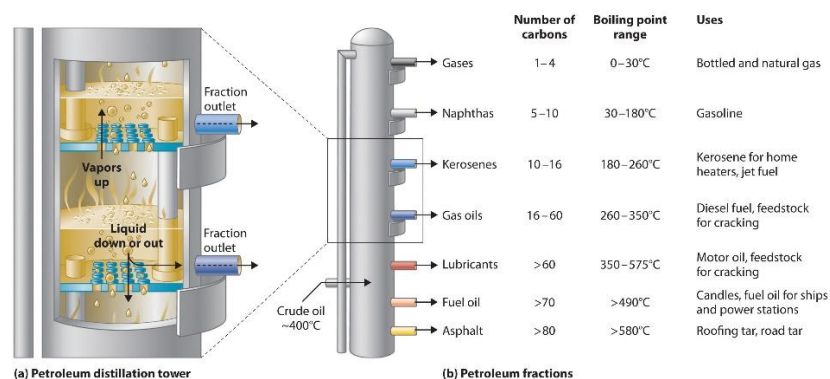


Figure 5 The Distillation of Petroleum. (a) Distillation column used for separating petroleum fraction (b) Petroleum fraction condensed at different temperatures, depending on the number of carbon atoms in the molecule (Department of Education Open Text Pilot Project, 2021)

Now petrol is commonly used in internal combustion engines employing spark ignition. It is characterized by a density of approximately 745 kg/m^3 , a lower heating value (LHV) of 43.2 MJ/kg , and a carbon content of 86.4% (Robert, Larive' Jean-Francois and Beziat Jean-Christophe, 2011) (Eriksson and Ahlgren, 2013)

Table 2 Chemical Interpretation for Gasoline Blend (Toxicological Profile for Gasoline, 1995) & (Murillo, 2022)

Structural family	Typical share by volume*	Examples	Why they're there
Iso-alkanes (branched paraffins)	25 – 40 %	iso-octane, iso-pentane	High octane → resists knock
Aromatics	20 – 50 % ($\leq 1\text{--}2\%$ benzene)	toluene, xylenes, ethyl-benzene	Boost octane; too much raises toxicity
Normal alkanes	4 – 8 %	n-heptane, n-octane	Good energy density but low octane
Olefins (alkenes)	2 – 5 %	iso-butene, hexenes	Produced in catalytic cracking; help octane but form gum
Cyclo-alkanes/olefins	3 – 7 %	methyl-cyclohexane	Stability & octane balance

1.2.2 Diesel

Diesel, on the other hand, is used in compression ignition engines, where the heat generated by compressing the air-fuel mixture is sufficient to initiate combustion without the need for a spark, as previously described in Section 1.2. Diesel fuel typically has a density of approximately 832 kg/m^3 , a lower heating value (LHV) of 43.1 MJ/kg , and a carbon content of 86.1%, making it slightly denser and more energy-rich per unit volume than gasoline. (Robert, Larive' Jean-Francois and Beziat Jean-Christophe, 2011)

At the top, the intake valve allows air to enter the precombustion chamber, while the fuel injector sprays diesel fuel into the high-temperature air. A glow plug helps initiate combustion during cold starts. The rocker arm, valve spring, and push rod operate the intake and exhaust valves through the motion driven by the camshaft. Air is compressed by the turbocharger, which draws in and pressurizes air via the air inlet, increasing engine efficiency and power.

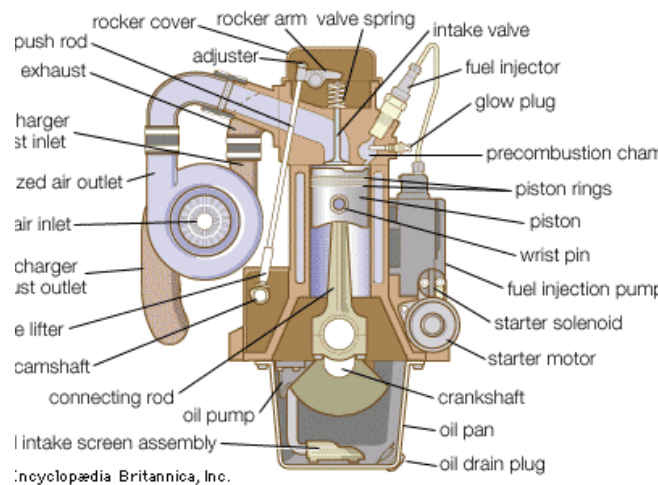


Figure 6 Grafical representation of the parts inside if a Diesel Engine (Proctor, 2019)

Below the combustion chamber, the piston moves up and down within the cylinder, transmitting force through the connecting rod to the crankshaft, which converts the reciprocating motion into rotational energy. The piston rings ensure proper sealing and minimize oil and gas leakage. The fuel injection pump and starter motor/solenoid are crucial for initiating engine operation. Lubrication is maintained by components like the oil pump, oil pan, and oil drain plug, ensuring reduced friction and engine longevity. Overall, each part plays a critical role in the performance and durability of a diesel engine.

1.2.3 Emissions of an internal combustion engine – Petrol vs Bio-diesels

Figure 7 presents a comparison of emission factors for diesel and petrol engines under rural, urban, and motorway driving conditions. Diesel engines emit significantly higher levels of PM_{2.5} (particulate matter), especially in urban settings, where they reach 0.036 g/km compared to only 0.005 g/km for petrol engines. NO_x emissions, a precursor to both ozone and fine particle formation, are also substantially greater in diesel vehicles up to 0.47 g/km in urban driving, while petrol vehicles emit only 0.11 g/km. However, petrol engines show higher CO₂ emissions, particularly under motorway conditions (269 g/km versus 178 g/km for diesel), suggesting better fuel efficiency for diesel engines. These emission differences are critical for assessing overall environmental and health impacts, particularly in densely populated urban areas.

	Diesel			Petrol		
	Rural	Urban	Motorway	Rural	Urban	Motorway
PM _{2.5}	0.015	0.036	0.049	0.003	0.005	0.004
CO ₂	137	193	178	158	255	269
NO _x	0.28	0.47	0.46	0.10	0.11	0.22
NMVOC	0.021	0.054	0.024	0.032	0.056	0.043

Figure 7 Main tailpipe emissions (in g/km based on MEET 1999 except for PM2.3 from petrol cars)

1.3 Objectives of the Study

The study's primary objective is to integrate advanced analytical reasoning with both experimental and simulation data to characterize internal-combustion performance and emissions across conventional (diesel, gasoline) and alternative (methanol, hydrogen) fuels. A rich dataset comprising in-cylinder pressure traces, crank-angle-resolved NO_x /PM emissions, and thermodynamic metrics will be mined to extract key indicators such as heat-release rate, and peak pressure.

These measurements will be correlated with combustion principles to reveal how fuel chemistry and operating conditions govern efficiency and pollutant formation. Concurrently, a two-zone model in Ricardo WAVE, driven by first-principles mass- and energy-conservation and parameterized via a calibrated SI-Wiebe function, will simulate burned/unburned zones, temperature fields, and species evolution. Critical evaluation of WAVE's formulations, wall-heat transfer correlations, and Wiebe calibration will validate the model's predictive power for low-carbon fuels and guide its refinement for future optimization.

2 Literature Review

2.1 Biofuels

Biofuels are liquid or gaseous fuels derived from biomass organic material from plants or animals that can serve as renewable alternatives to fossil fuels (W., 2006, pp.484–489). Two of the most widely researched and implemented biomass-based transportation fuels are bioethanol and biodiesel, both of which show strong potential to replace conventional gasoline and diesel fuel, respectively. Biofuels are often praised for their sustainability, lower greenhouse gas emissions, and enhanced energy security (Reijnders, 2006). A wide array of fuels can be produced from biomass, including liquid fuels such as ethanol, methanol, biodiesel, and Fischer-Tropsch diesel, as well as gaseous fuels like hydrogen and methane.

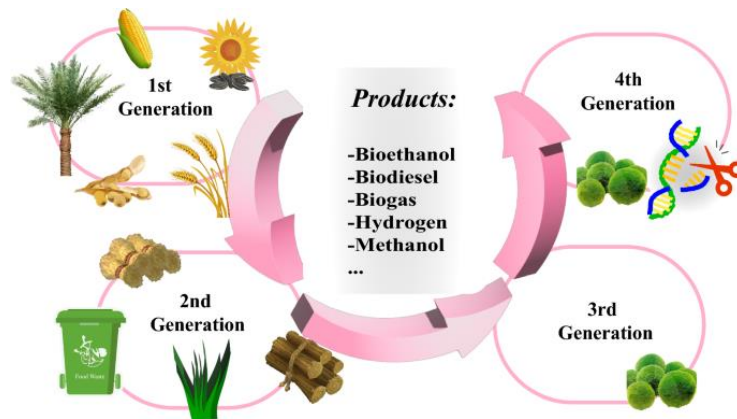


Figure 8 Overview of feedstocks and productions of different biofuel generations 1st generation biofuels utilize corn, soybeans, wheat and sunflower oil; 2nd generation biofuels utilize switchgrass, poplar, straw, and food waste as feedstocks; 3rd and 4th generation biofuels utilize microalgae as feedstocks, with microalgae being editable in 4th generation (Wang et al., 2024)

There has been an increase in studies about biofuels due to its favourable combustion characteristics in compression ignition engines. Biodiesel, typically made from vegetables oils, has similar energy density and handling properties to Petro diesel but offers added benefits (Kralova and Sjöblom, 2010b). One of the advantages is that it is non-flammable and nonexplosive, with a flash point of 423 K compared to 337 K for Petro diesel (Ma and Hanna, 1999). Biodiesel is nontoxic and produces significantly fewer harmful emissions. Other advantages include high cetane number, renewability, low sulphur and aromatic content, and superior combustion efficiency (Knothe, Sharp and Ryan, 2006).

2.1.1 Methanol as a Fuel Source and Its Role in Biodiesel Production

Methanol plays a dual role in alternative fuel development: it can serve both as a standalone fuel and as a key reagent in biodiesel production. Modern biodiesel is typically obtained through the transesterification of triglycerides (fats and oils) with methanol. Methanol is preferred in this reaction due to its low cost and high reactivity. The production route generally involves a base catalyst, which is more cost-effective and yields faster reaction rates than acid or enzymatic catalysis (Ma and Hanna, 1999).

There are four main pathways for biodiesel production:

1. Base-catalysed transesterification, the most common method
2. Direct acid-catalysed transesterification
3. Conversion of triglycerides to free fatty acids followed by esterification
4. Noncatalytic supercritical transesterification of oils and fats

Methanol remains central to biodiesel synthesis and is an important part of any strategy for transitioning toward low-carbon fuels because while enzyme-catalysed routes offer some selectivity and environmental advantages, the alkali and acid-catalysed processes dominate industrial production due to shorter reaction times and lower operational costs (Wang, Pengzhan Liu and Zhang, 2007).

2.2 Hydrogen

Hydrogen is increasingly recognized as one of the most promising alternatives to fossil fuels due to its advantageous properties, including a wide flammability range, short quenching distance, low ignition energy requirement, high diffusivity, and low density. The production process involves separating hydrogen from the other elements within these compounds to obtain it in a usable form (Shadidi, Najafi and Yusaf, 2021).

2.2.1 Steam Methane Process

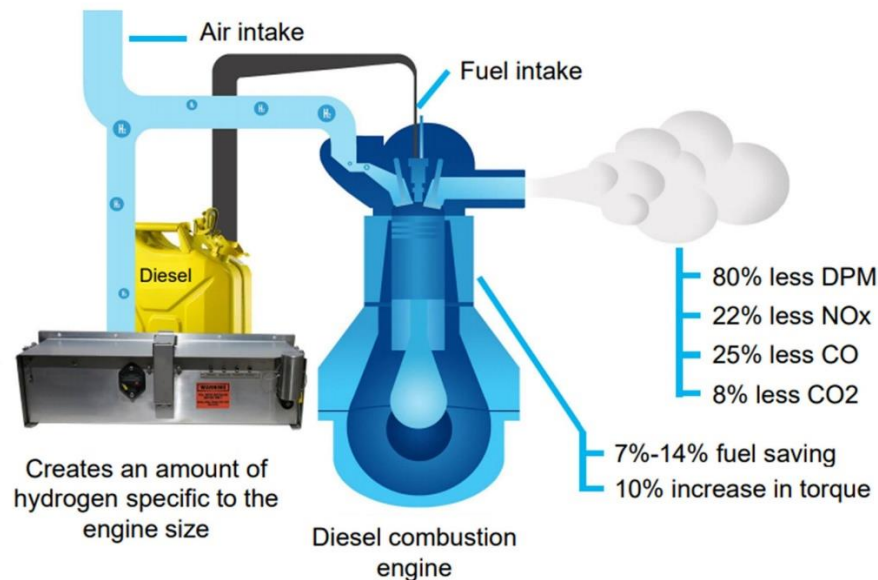


Figure 9 Hydrogen Injection into diesel engine systems (PRIOR POWER SOLUTIONS, n.d.)

Currently, more than 90% of global hydrogen production relies on the steam methane reforming (SMR) process (Rapier, 2020). This method operates under pressures ranging from 3 to 25 bar (1 bar = 14.5 psi) and utilizes a catalyst to facilitate the reaction. In this process, methane reacts with steam to produce hydrogen, carbon monoxide, and small amounts of carbon dioxide. Since steam methane reforming is an endothermic reaction, it requires continuous input of heat to sustain the process (Office of Energy Efficiency & Renewable Energy, 2024).

2.2.2 Electrolysis

Another widely recognized method for hydrogen production is electrolysis, which is a viable pathway for generating carbon-free hydrogen using renewable or nuclear energy sources. Electrolysis involves splitting water into hydrogen and oxygen through the application of electrical energy (U.S. Department of Energy, 2024).

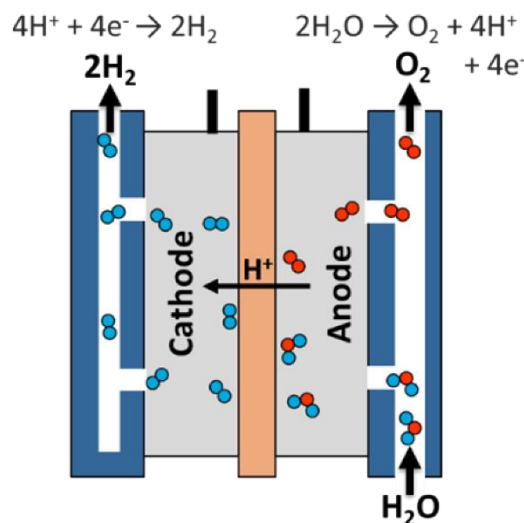


Figure 10 Visual representation of a fuel cell - electrolyzers consist of an anode and a cathode separated by an electrolyte (U.S. Department of Energy, 2024)

In an electrolyser, this process occurs with an electrolyte positioned between the anode and the cathode. As a result, various electrolyser technologies such as alkaline, proton exchange membrane (PEM), and solid oxide electrolyzers operate differently, each offering unique advantages depending on the intended application and energy source (U.S. Department of Energy, 2024).

2.3 Methanol and Hydrogen as fuels for Internal Combustion Engines (ICE)

2.3.1 Methanol in ICEs

Methanol is an attractive alternative fuel for ICEs due to its high knock resistance, fast burning velocity, and favourable combustion properties. Methanol has a high flame speed in comparison to hydrogen (Verhelst et al., 2019) allows faster combustion and supports engine technologies such as higher compression ratios and increased dilution for improved efficiency. Additionally, methanol enables ultra-lean operation thanks to its wide flammability range and high latent heat of vaporization, contributing to reduced NO_x emissions compared to gasoline. Since methanol has no carbon-carbon bonds, it inherently forms less particulate matter, supporting cleaner combustion (Verhelst et al., 2019).

Table 3 Chemical properties for selected fuels (Verhelst et al., 2019)

Property	Isooctane	Gasoline (typical)	Methanol	Ethanol	1-Butanol	Methane	Hydrogen
Chemical formula	C ₈ H ₁₈	Various	CH ₃ OH	C ₂ H ₅ OH	C ₄ H ₉ OH	CH ₄	H ₂
Molecular weight [kg/kmol]	114,23	107,00	32,04	46,07	74,12	16,04	2,02
Oxygen Content by mass [%]	0,00	0,00	49,93	34,73	21,58	0,00	0,00
Hydrogen Content by mass [%]	15,88	~ 14	12,58	13,13	13,60	25,13	100,00
Carbon Content by mass [%]	84,12	~ 86	37,48	52,14	64,82	74,87	0,00
Lower heating value [MJ/kg]	44,30	42,90	20,09	26,95	33,08	50,00	120,00
Higher heating value [MJ/kg]	47,80	48,00	22,88	29,85	36,07	55,00	142,00
Volumetric Energy Content [MJ/m ³]	30656	31746	15871	21291	26795	32,50	9,60
Stoichiometric AFR [kg/kg]	15,10	14,70	6,50	9,00	11,10	17,65	34,20
Stoichiometric AFR [kmol/kmol]	59,75	54,49	7,22	14,36	28,50	9,81	2,39
Specific CO ₂ emissions [g/MJ]	69,57	73,95	68,44	70,99	71,90	54,87	0,00
Specific CO ₂ emissions relative to gasoline	0,94	1,00	0,93	0,96	0,97	0,74	0,00
Autoignition temperature [K]	690	465-743	738	698	616	813	858
Adiabatic Flame Temperature [K]	2276	~ 2275	2143	2193	2262	2225	2390

Methanol combustion faces some abnormal combustion challenges, although they are less severe compared to gasoline. Pre-ignition risks exist due to methanol's low minimum ignition energy and only hydrogen having even lower values as it (see table 4), but knock resistance is very high as in table 5 "Motor Octane Number".

Table 4 Mixture properties for selected fuel-air mixtures (Verhelst et al., 2019)

Property	Isooctane	Gasoline (typical)	Methanol	Ethanol	1-Butanol	Methane	Hydrogen
Chemical formula	C ₈ H ₁₈	Various	CH ₃ OH	C ₂ H ₅ OH	C ₄ H ₉ OH	CH ₄	H ₂
Energy per Unit Mass of Air [MJ/kg]	2,93	2,92	3,09	2,99	2,98	2,83	3,51
Energy per Unit Mass of mixture [MJ/kg]	2,75	2,73	2,68	2,70	2,73	2,68	3,41
Energy per Unit Mass of Air relative to gasoline	1,01	1,00	1,06	1,03	1,02	0,97	1,20
Energy per Unit Mole of Air [MJ/kmol]	84,69	84,24	89,22	86,44	86,03	81,76	101,28
Energy per Unit Mole of mixture [MJ/kmol]	83,29	82,72	78,36	80,81	83,11	74,20	71,39
Energy per Unit Mole of mixture relative to gasoline	1,01	1,00	0,95	0,98	1,00	0,90	0,86
Reid vapor pressure (at 37.8 °C) [psi]	1,86	7,00	4,60	2,30	0,33	2400	-
Stoichiometric mass fraction (in air)	0,06	0,06	0,13	0,10	0,08	0,05	0,03
Stoichiometric volume fraction (in air)	0,02	0,02	0,12	0,06	0,04	0,10	0,30
Heat of vaporization per unit mass of Air [kJ/kg]	17,88	24,10	170,90	93,60	52,50	28,89	13,48
Evaporation energy relative to gasoline	0,74	1,00	7,09	3,88	2,18	-	-
Cp/Cv for a stoichiometric mixture	1,35	na	1,37	1,38	1,39	1,39	1,40
Mole Ratio of Products to Reactants (incl. N ₂)	1,06	0,94	1,06	1,07	1,07	1,00	0,85
Ratio of Triatomic to Diatomic Products	0,36	0,35	0,53	0,44	0,40	0,40	0,53
Mass diffusivity in air [cm ² /s]	0,07	0,05	0,14	0,11	na	0,16	0,61
Lower flammability limit in air [vol%]	1,10	1,30	6,70	3,30	1,40	5,00	4,00
Higher flammability limit in air [vol%]	6,00	7,60	36,00	19,00	11,20	15,00	75,00
Lower flammability limit in air [λ]	1,51	1,60	1,81	1,91	2,94	1,99	10,57
Higher flammability limit in air [λ]	0,26	0,26	0,23	0,28	0,33	0,59	0,15
Lower flammability limit in air [φ]	0,66	0,62	0,55	0,52	0,34	0,50	0,09
Higher flammability limit in air [φ]	3,85	3,89	4,32	3,60	3,02	1,68	6,81
Minimum ignition energy in Air [mJ]	1,20	0,25	0,14	0,23	na	0,28	0,02
Quenching distance [mm]	3,50	~ 2,0	1,85	1,65	na	2,03	0,64

Injection strategy evolution is observed, with historical use of port fuel injection (PFI) but movement towards direct injection (DI) approaches to maximize efficiency and control mixture formation and DI approach is the one used in this study. Recently advanced CFD modelling tools have been used to predict laminar burning velocities and mixture behaviour under varying conditions (Beeckmann, Cai and Pitsch, 2014).

Table 5 Properties of selected fuels related to engine use and storage safety (Verhelst and Wallner, 2009)

Property	Isooctane	Gasoline (typical)	Methanol	Ethanol	1-Butanol	Methane	Hydrogen
Chemical formula	C ₈ H ₁₈	Various	CH ₃ OH	C ₂ H ₅ OH	C ₄ H ₉ OH	CH ₄	H ₂
Research Octane Number	100	95	109	109	94	120	130 (λ=2,5)
Motor Octane Number	100	85	92	98	81	120	na
Sensitivity (RON-MON)	0	10	17	11	13	0	na
Cetane number	na	8-14	3	9	25	-10	na
Flash point [°C]	-12	-45	11	14	37	-188	na

2.3.2 Hydrogen in ICEs

Hydrogen is a promising carbon-free fuel for internal combustion engines (ICEs), offering high thermal efficiency and compatibility with advanced combustion strategies. H_2 in ICEs can achieve thermal efficiencies comparable to fuel cell systems when equipped with technologies such as direct injection, lean-burn operation, and pre-chamber ignition. These engines can operate using non-purified hydrogen, which significantly lowers fuel processing costs compared to fuel cell applications. Notably, H_2 in ICEs produce zero tank-to-wheel CO_2 emissions (Frankl et al., 2020), positioning them as a near-term option for decarbonising heavy-duty transport without abandoning current ICE infrastructure (Varde, 1981).

Table 6 Main properties of gaseous hydrogen and gasoline (Onorati et al., 2022)

	Hydrogen	Gasoline
Formula	H_2	$C_nH_{1.87n}$
Density (kg/m^3)	0.09 @ 0°C, 1 bar	720–780
Energy content (MJ/kg)	120.0	44.0
Energy content (MJ/l)	8	32.0
Octane number (RON)	≥ 120	92–98
Latent heat of vaporisation (kJ/kg)	461	305
Boiling point (°C)	-252.9@ 1 bar	27–225
Flame speed (m/s)	1.85	0.37–0.43
Lean equivalence ratio	0.1	0.6
Ad. flame temp. at 1 atm (K)	2380	2300
Ad. flame temp. at 100 atm (K)	2490	2405
Auto-ignition temp. (K)	858	550
Stoichiometric A/F ratio (by mass)	34.3	14.8
Quenching distance at stoich. (mm)	0.64	2.84
Min. ignition energy (J)	2×10^{-5}	5.5×10^{-4}

Additionally, the combustion properties of hydrogen, particularly its high flame speed and wide flammability range (Bae and Kim, 2017), enable ultra-lean operation, contributing to reduced NO_x emissions and improved efficiency under part-load conditions (Iafate, Matrat and Zaccardi, 2019). Experimental setups referenced in the article have shown indicated thermal efficiencies above 47% at part load, with advanced techniques such as high-pressure DI (up to 300 bar) and turbocharging playing key roles.

Abnormal combustion remains one of the main challenges for H_2 in ICEs. Hydrogen's low ignition energy, short quenching distance, and broad flammability limits make it prone to pre-ignition, knocking, and backfire, especially in port fuel injection (PFI) systems (Dharamshi, Pal and Agarwal, 2013). These issues significantly impact engine durability and efficiency. There have been strategies to mitigate these phenomena, such as transitioning to direct injection (DI) and optimizing injection timing, valve overlap, and mixture formation (Onorati et al., 2022). Recently advanced CFD simulations are employed to investigate the causes of pre-ignition, revealing that rich mixture zones near hot surfaces, such as spark plugs or exhaust valves, are likely triggers (Onorati et al., 2022).

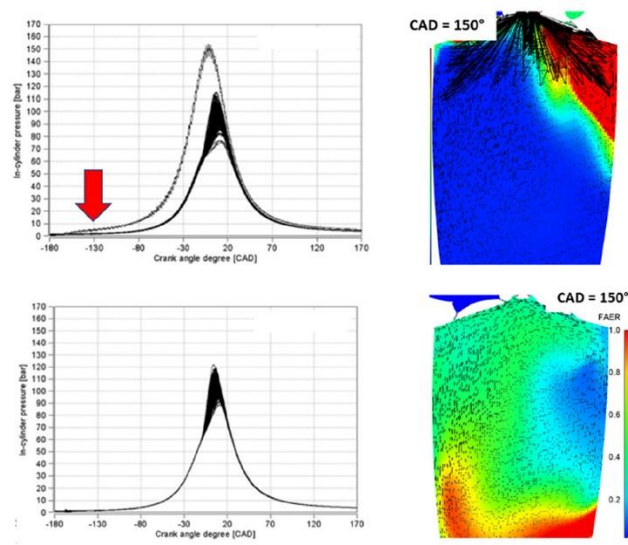


Figure 11 Impact of fuel distribution on occurrence of pre-ignition, 2000 rpm, mid load, $\lambda=2$ (Onorati et al., 2022)

In one case, adjusting injection parameters improved mixture homogeneity, eliminating pre-ignition. The use of laser ignition is also proposed to minimize surface ignition, allowing precise control over ignition timing and flame kernel development. These strategies enable more stable and efficient combustion while addressing hydrogen-specific challenges.

3 Methodology

3.1 FORTE 2021 R1

For all engine simulations in this study, ANSYS Forte 2021 R1 was used as the primary computational platform. Forte is a specialized computational fluid dynamics (CFD) tool tailored for internal combustion engine (ICE) applications (Emswiler, 2021). It enables accurate modelling of gas exchange, mixture preparation, ignition, combustion, and emissions formation, incorporating detailed physical and chemical models. The simulations were based on time-accurate (transient) 3D CFD calculations, solving the compressible Navier-Stokes equations along with energy conservation, turbulence, species transport, and detailed chemical kinetics. Each simulation was initialized based on real-world operating conditions, including intake pressure, intake temperature, engine speed (RPM), and wall heat transfer coefficients (HTC).

3.1.1 Step-by-step Setup Process (FORTE 2021 R1)

For a Step-by-step Process of how to replicate the simulation parameters used in this study please refer to Appendix A.

3.2 Diesel – Petrol Engine Validation

The Diesel engine model exhibits distinct combustion behaviours compared to the gasoline, methanol, and hydrogen models, primarily due to its compression ignition nature. As shown in Figure 12, Diesel combustion produces a significantly higher peak cylinder pressure, reaching 85.78 bar at around 2° crank angle after top dead centre (ATDC). This is substantially higher than the 47.14 bar observed in the real petrol engine and the 58.22 bar in the hydrogen simulation.

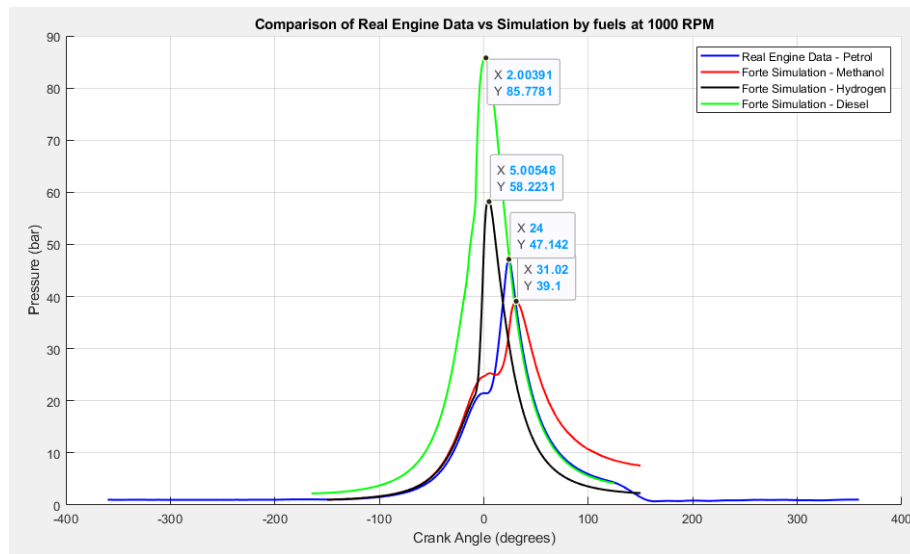


Figure 12 Comparison of Real Engine Data vs Simulation by fuels at 1000 RPM

The higher pressure is expected, as diesel combustion relies on autoignition triggered by elevated pressure and temperature rather than externally supplied spark ignition. This high-pressure environment also explains why modern research often adapts diesel engines to hydrogen combustion, leveraging their structural robustness to withstand higher peak pressures.

In terms of accumulated chemical heat release Figure 13, the diesel simulation again outperforms the other fuels, with a total accumulated energy of 2373.39 J almost double that of petrol and three times that of hydrogen. This result is consistent with diesel fuel's higher energy density and the rapid energy release characteristic of diffusion combustion processes.

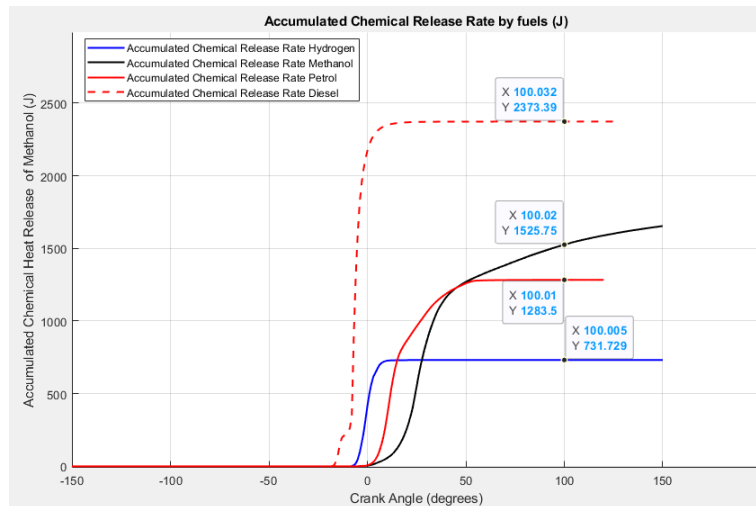


Figure 13 Accumulated Chemical Release Rate by fuels (J)

Diesel engines produce lower NO_x emissions than gasoline engines, but still significantly more than hydrogen-fuelled engines. Although the diesel EINO_x is lower than petrol's large NO_x spike around 17° crank angle, diesel combustion still emits measurable NO_x due to the high temperatures reached during the combustion event.

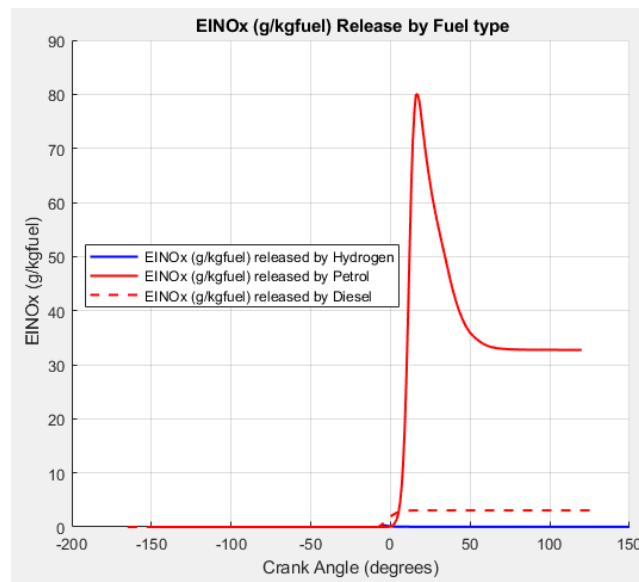


Figure 14 EINO_x (g/kgfuel) Release by Fuel Type

3.3 Methanol as a fuel for ICE

Initially, the simulation closely matched the trend of the real data, as shown in Figure 17. The ignition timing and early combustion behaviour of the methanol simulation aligned well with the experimental curve up until approximately -5° to 0° crank angle after top dead centre (ATDC). The simulation overshoot the real engine pressure during the early combustion phase by approximately 3 bar. Despite the promising start, the maximum pressure achieved in the simulation was 39.1 bar only 83% of the expected peak value of 47.1 bar recorded in the real engine data. This suggests that the methanol combustion model was unable to reproduce the same energy release and torque generation characteristics as the gasoline model which is expected but not to this degree.

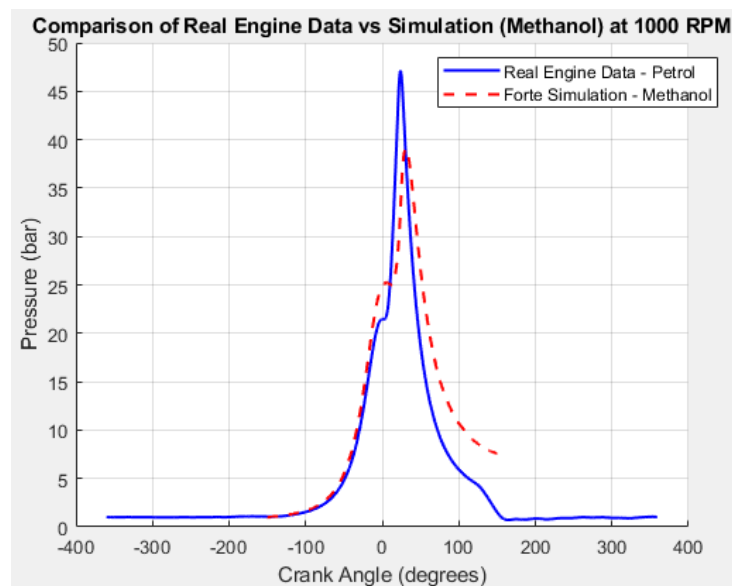


Figure 15 Comparison of Petrol Engine Pressure vs Methanol simulation at 1000 RPM

Unburned hydrocarbons (UHC) emissions presented a significant challenge during methanol simulation analysis. UHC formation is primarily attributed to incomplete combustion, fuel trapped in crevice regions, and wall wetting effects during engine warm-up. Methanol, due to its premixed oxygen content, can theoretically reduce engine-out UHC emissions compared to gasoline (Liu et al., 2007). Moreover, methanol lacks high-boiling-point components commonly found in gasoline, which further minimizes the tendency for UHC formation under normal operating conditions (Nakata et al., 2006).

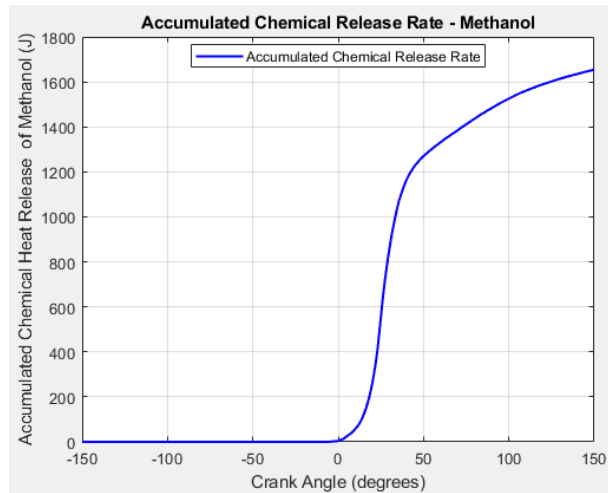


Figure 16 Accumulated Chemical Release Rate for Methanol (J)

The accumulated chemical heat release analysis Figure 18 revealed that combustion continued progressively without reaching a plateau even at 150° crank angle. This indicates ongoing combustion well into the expansion stroke, which is highly undesirable for stable engine operation. Sustained combustion beyond the intended combustion window can induce cycle-to-cycle desynchronization, incomplete scavenging, increased residual gases, and long-term performance and durability degradation. Given these technical challenges, particularly the inability to achieve complete and timely combustion, as well as the risks of excessive UHC emissions, methanol was unsuitable for further simulation efforts within the scope of this study.

3.4 Hydrogen as a fuel for ICE

The hydrogen engine simulation exhibited significant differences compared to the previous fuels, particularly methanol. Notably, hydrogen reached a much higher peak cylinder pressure during combustion, achieving a maximum value of 58.22 bar, considerably higher than that obtained using petrol (47.14 bar) or methanol (39.1 bar) as seen in figure 16. This indicates that hydrogen combustion has the potential to generate substantially higher torque outputs.

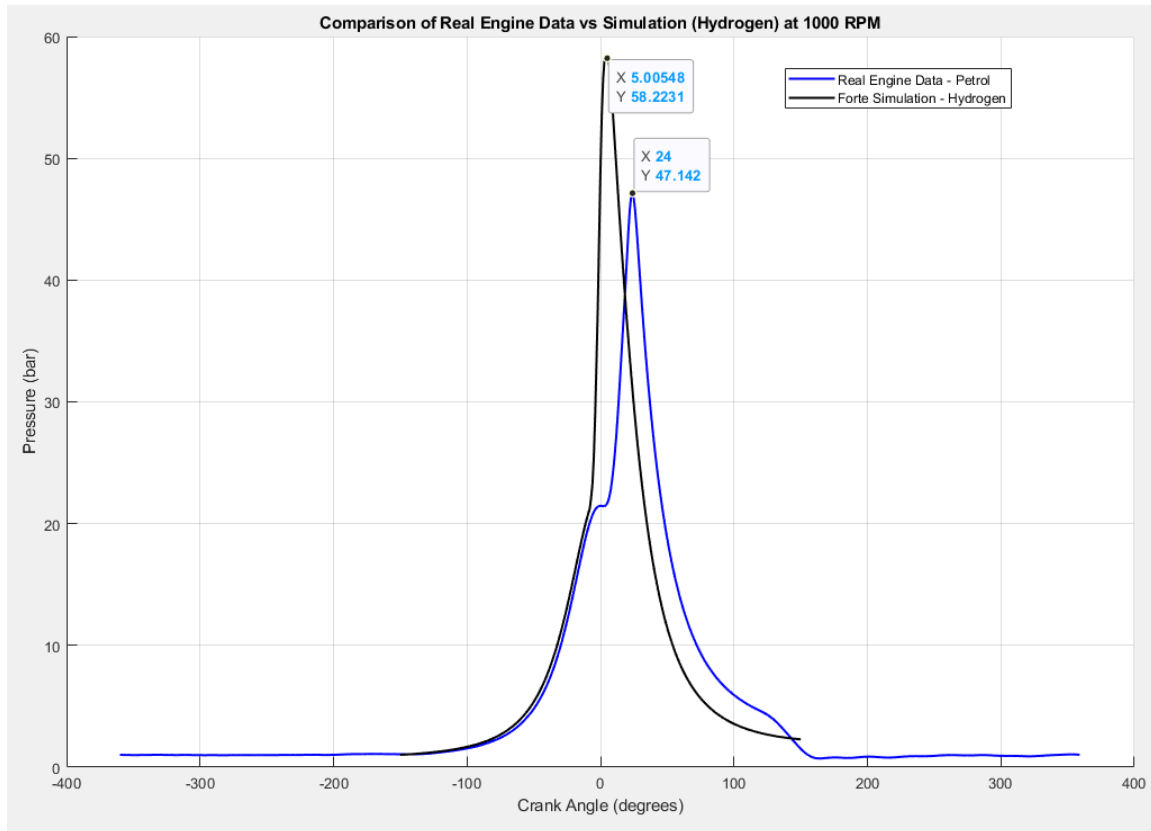


Figure 17 Comparison of Real Petrol Pressure Data vs Hydrogen vs Crank Angle

After ignition, hydrogen combustion exhibits a much sharper pressure rise, a consequence of its rapid combustion kinetics and high laminar flame speed, even though the model operated with a lean hydrogen-air mixture (9% hydrogen mass fraction). The crank angle at which the maximum pressure occurred for hydrogen was 5° ATDC, compared to 24° ATDC for the real petrol data, indicating a significant advance in combustion phasing. Additionally, hydrogen's lower ignition energy compared to conventional fuels raises concerns about engine durability and pre-ignition risks, aspects that must be addressed in practical applications.

The Accumulated Chemical Release Rate curve further reinforced the advantages of hydrogen combustion. Unlike methanol, where heat release continued beyond 150° crank angle, and petrol, where the plateau was reached much later, the hydrogen simulation achieved a complete and stable plateau significantly earlier. This behaviour confirms efficient combustion without extended burning into the expansion stroke, which is desirable for thermal efficiency and engine stability.

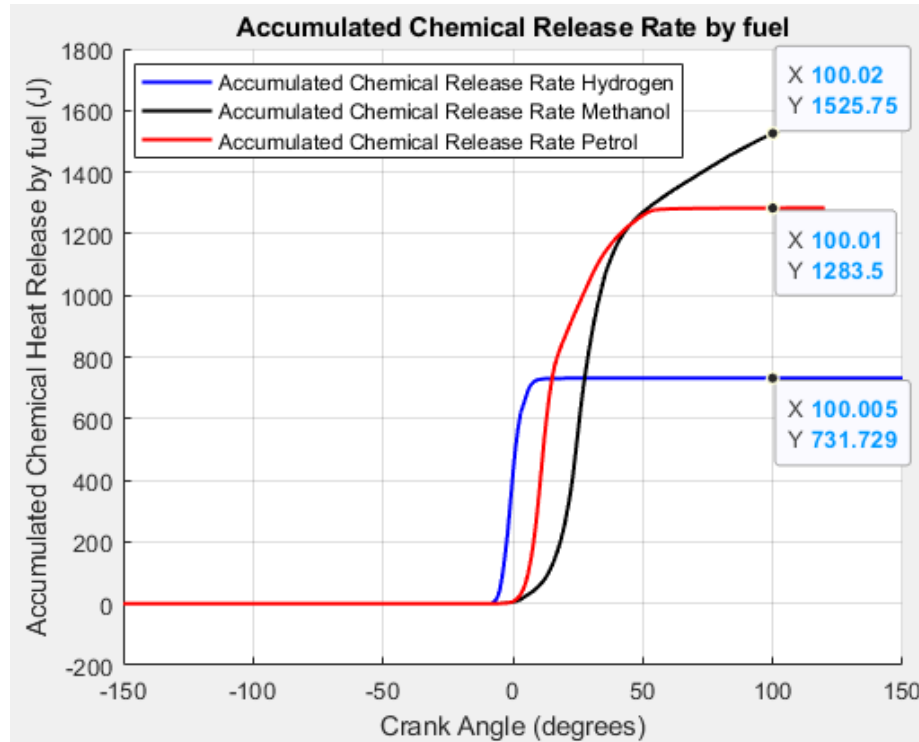


Figure 18 Accumulated Chemical Release Rate by fuel (J) vs Crank Angle

Comparing NO_x emissions between fuels, hydrogen engine demonstrated an outstanding advantage. As shown in Figure 21, the hydrogen simulation produced almost zero NO_x emissions throughout the combustion cycle. Specifically, at the peak NO_x release observed for petrol (approximately 80 g/kg_{fuel}), hydrogen only generated about 0.28 g/kg_{fuel}, which is only 0.3% of the petrol NO_x emissions. This dramatic reduction positions hydrogen as an attractive candidate for clean combustion technologies aimed at near-zero emissions targets.

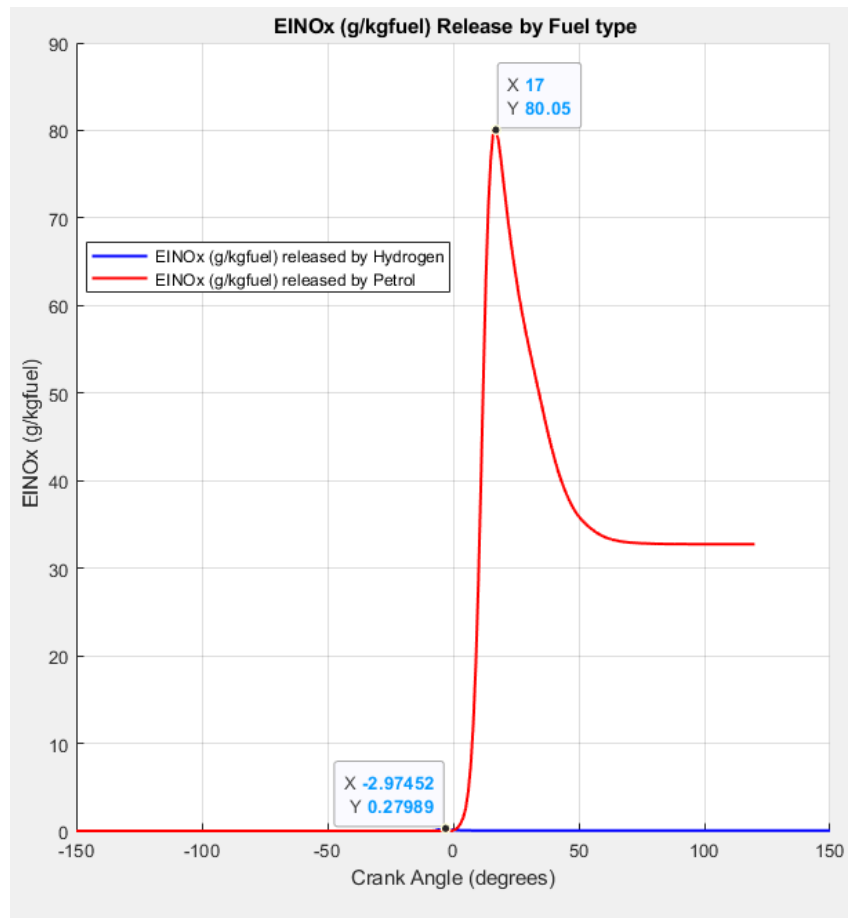


Figure 19 NOx produced g/kg of fuel between Hydrogen and Petrol

3.5 MATLAB Wiebe Function

In the MATLAB workflow, cumulative chemical heat-release data exported from FORTE is first normalized to unity and aligned against crank angle. Using `interp1`, the crank angles corresponding to 10, 50, and 90 percent burn (CA10, CA50, CA90) are precisely determined from the normalized curve. CA50 defines the centroid of combustion, here -0.6 degrees after top dead centre, while the interval CA90–CA10 yields a 19.44-degree combustion span. A non-linear least-squares fit of the four-parameter Wiebe model then optimizes coefficient a (7.6798), exponent m (1.1834), centre θ_0 (142.96° CA), and duration $\Delta\theta$ (19.44° CA), achieving $R^2 = 0.999973$ for an accurate heat-release representation.

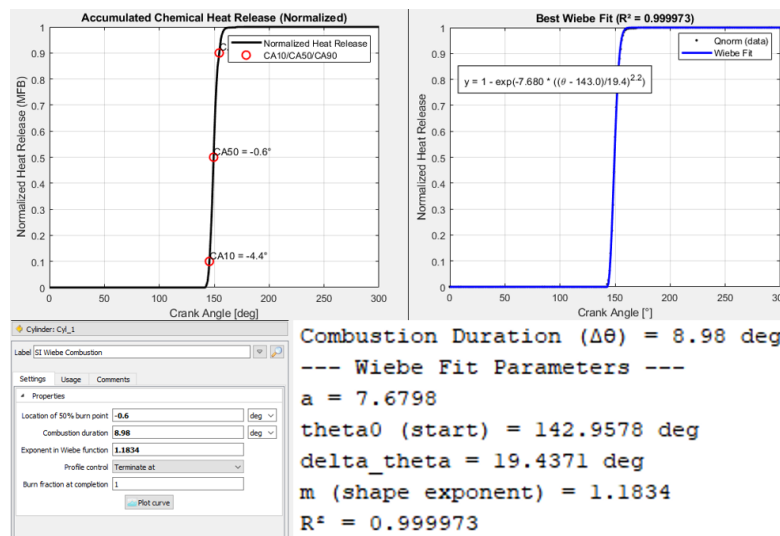


Figure 20 Accumulated Chemical Heat Release Rate from Hydrogen FORTE Simulation (Normalized)

In Ricardo WAVE, the SI-Wiebe module ingests these optimized parameters to reproduce the in-cylinder heat-release profile during transient simulation. The “location of 50 percent burn point” field accepts θ_0 as -0.6 deg, while “combustion duration” is entered as the 10–90 percent span of 8.98 deg, reflecting only the rapid heat-release phase. The “exponent in Wiebe function” m controls the curve shape, and “burn fraction at completion” of unity ensures full conversion to products. By matching MATLAB-derived parameters, WAVE seamlessly applies the calibrated combustion kinetics for turbocharged hydrogen engine modelling.

3.6 Results - RICARDO WAVE

A production-proven 1.6 L twin-scroll turbocharged, four-cylinder spark-ignition hydrogen engine template in Ricardo WAVE was selected because the same hardware has been demonstrated experimentally on H₂ blends. Its variable-geometry turbocharger and direct injection allow close control of intake boost and hydrogen's high flame speed and peak temperatures.

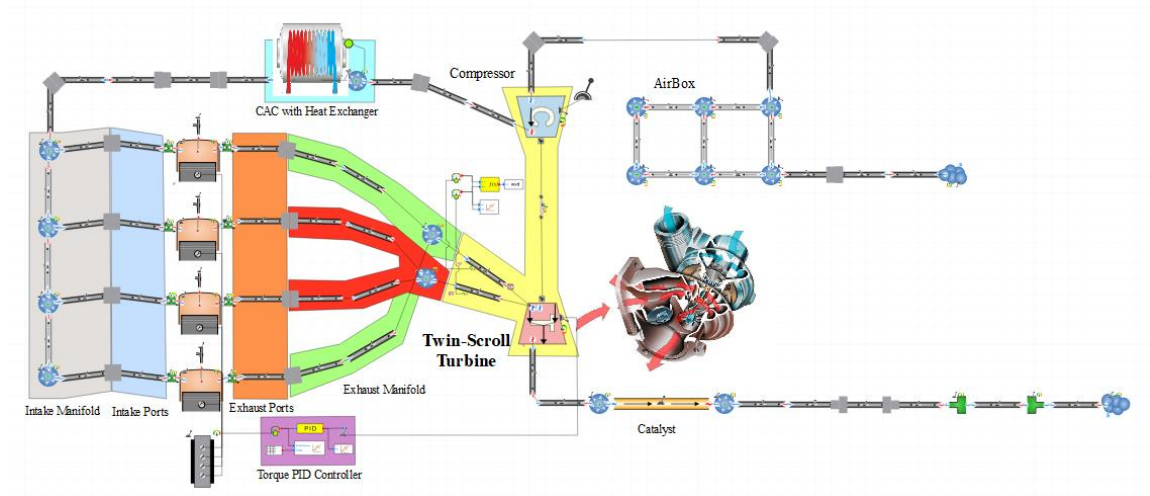


Figure 21 Virtual Representation of the 1.6 L 4 Inline turbocharged Engine used for the simulation

Other parametric sweeps included varying the fuel-equivalence ratio (FER = 0.5, 0.7, 1.0, 1.25, 1.5) at fixed EGR = 0 % to quantify how richness amplifies peak firing pressure, brake torque and NO_x formation.

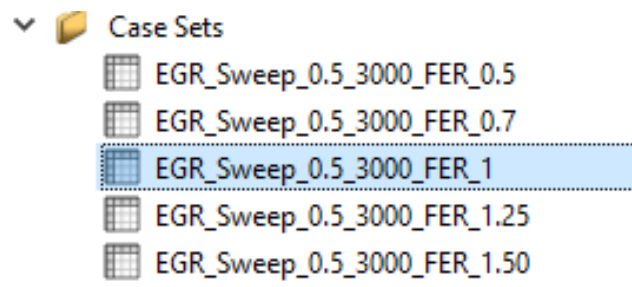


Figure 22 Case sets - FER runs going from 0.5 up to 1.50

Leaner operation ($FER = 0.5$ – 0.7) reduced NO_x by up to 60 % but cut peak BHP by 20 %, whereas richer mixtures ($FER > 1$) recovered power at the expense of a three-fold NO_x increase. Likewise, an EGR sweep (0 %–50 % at $FER = 0.7$) demonstrated that each 10 % increment of recirculated exhaust lowered peak cylinder temperature by ~ 100 K and NO_x by ~ 25 %, but also trimmed torque by ~ 8 Nm per 10 % EGR. These insights guided the final selection of $FER = 0.7$ with 15 % EGR as the best compromise between emissions control and performance.

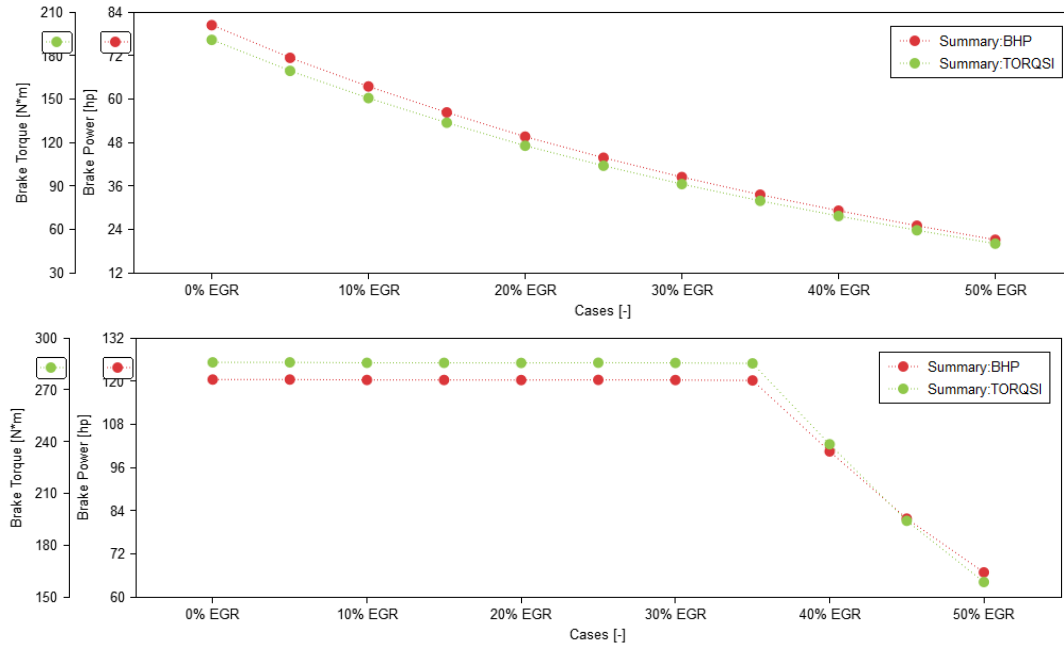


Figure 23 RPM 3000 - Top FER 0.5 - Bottom FER 1 (Stoichiometric)

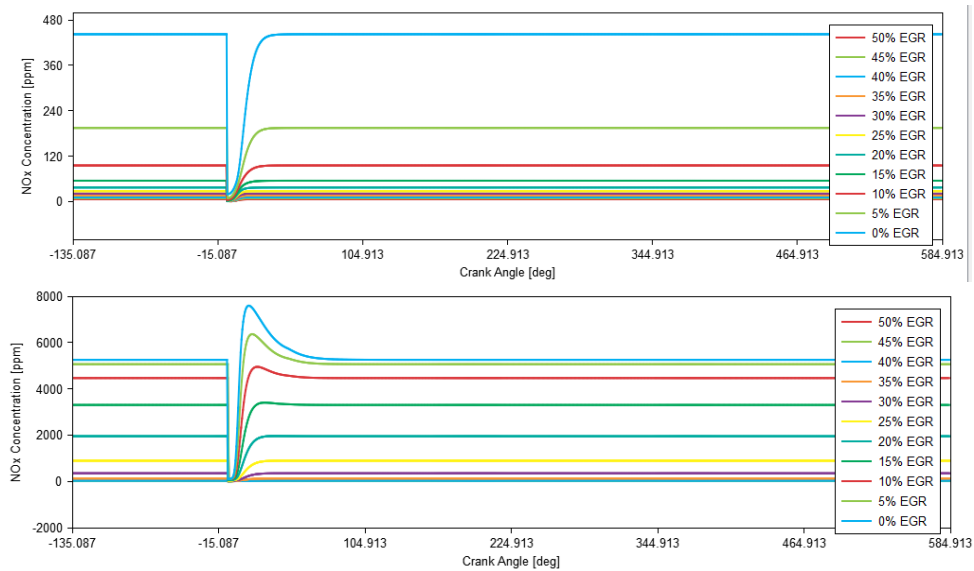


Figure 24 RPM 3000 - Top FER 0.5 - Bottom FER 1 (Stoichiometric)

	Units	Group	Comment	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10	Case 11
Case Title				0% EGR	5% EGR	10% EGR	15% EGR	20% EGR	25% EGR	30% EGR	35% EGR	40% EGR	45% EGR	50% EGR
Enabled				☒	☒	☒	☒	☒	☒	☒	☒	☒	☒	☒
1				3000	3000	3000	3000	3000	3000	3000	3000	3000	3000	3000
2				100	100	100	100	100	100	100	100	100	100	100
3				34.3	34.3	34.3	34.3	34.3	34.3	34.3	34.3	34.3	34.3	34.3
4				458	458	458	458	458	458	458	458	458	458	458
5				264	264	264	264	264	264	264	264	264	264	264
6				1	1	1	1	1	1	1	1	1	1	1
7				1	1	1	1	1	1	1	1	1	1	1
8				30	30	30	30	30	30	30	30	30	30	30
9				40	40	40	40	40	40	40	40	40	40	40
10				0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97
11				162493	162493	162493	162493	162493	162493	162493	162493	162493	162493	162493
12				7.15	7.15	7.15	7.15	7.15	7.15	7.15	7.15	7.15	7.15	7.15
13				2	2	2	2	2	2	2	2	2	2	2
Output														
UPDATE OF FUELFLOW: FUELFLOW = 0.7259E-03 FUELFLOW = 0.7259E-03														
ENG: 3 11 0 100 73145 126.17 1.488 1087.2 0.706 16.291 -3.498 44.48 0.0788 3.020 434.4 0.805E-06														
ENG: 4 11 0 100 73327 129.43 1.527 1070.3 0.688 16.441 -3.415 44.89 0.0781 3.032 429.2 0.712E-06														

Figure 25 Change in EGR % for a 1 one the setups

By swapping the stock gasoline kinetic mechanism for a four-parameter SI-Wiebe heat-release law ($\theta_{50} = -0.6^\circ \text{CA}$, $\Delta\theta_{10-90} = 8.98^\circ \text{CA}$, $m = 1.1834$, burn fraction = 1) calibrated in MATLAB, the study enforces a stoichiometric AFR of 34.3:1 and examines FER = 0.7 under 0 %–50 % EGR. This approach isolates EGR's and richness's trade-offs between NO_x mitigation and power output while retaining the engine's real-world boundary conditions.

Cylinder: Cyl_1

Label SI Wiebe Combustion

Settings Usage Comments

Properties

Location of 50% burn point deg

Combustion duration deg

Exponent in Wiebe function

Profile control

Burn fraction at completion

Plot curve

Figure 26 Values for the Wiebe function, gathered from MATLAB

3.6.1 Brake Power & Torque vs RPM (FER = 0.7, EGR 0% vs 15%)

Under no-EGR Figure 29, brake power rises nearly linearly from 20 hp at 1 000 RPM to 220 bhp at 5 500 RPM, while torque plateaus at ~280 N·m between 2 500 and 5 000 RPM. Introducing 15 % EGR Figure 29 reduces peak power by ~15 % (~195 hp) and peak torque by ~8 % (~260 N·m). The torque curve remains flatter at high speeds, indicating that recycled exhaust slows combustion slightly but stabilizes the charge. As a result, EGR imposes a moderate power penalty in exchange for lower NO_x, suggesting an optimal EGR fraction below 15 % to balance emissions control and performance as proven in Figure 25.

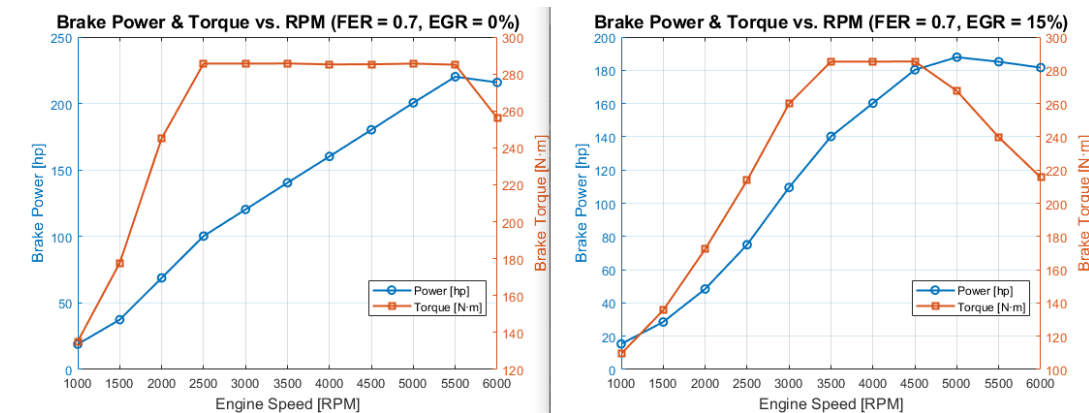


Figure 27 BHP & Torque vs RPM for EGR [0-15] %

3.6.2 In-cylinder pressure vs. crank angle & RPM

Comparison of 3D pressure surfaces Figure 30 shows that EGR 0 % yields peak firing pressures of ~170 bar near top dead centre (TDC) at mid-range speeds (3 000–4 000 RPM). With 15 % EGR, peak pressure falls by ~10–15 bar and shifts ~1° CA later, reflecting slower burn rates from diluent-induced heat capacity increases. At higher engine speeds, EGR smooths pressure rise slopes and reduces over-pressure spikes, indicating improved knock resistance. The slight broadening of the pressure trace confirms that recirculated gases slow the combustion front, lowering mechanical stress at the cost of marginally extended burn duration.

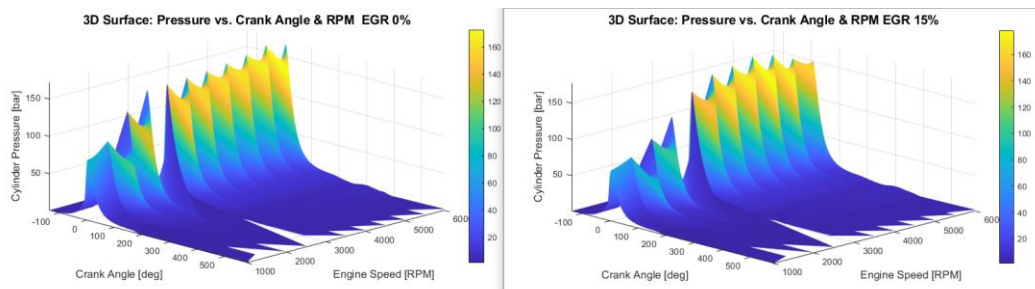


Figure 28 Pressure vs Crank Angle for a range of RPMs - EGR [0-15] %

3.6.3 In-cylinder temperature vs. crank angle & RPM

Temperature surfaces Figure 31 illustrate that maximum gas temperatures inside the cylinders exceed 2 400 K with no EGR, whereas 15 % EGR reduces peaks by ~200–300 K across all speeds. The cooled charge and increased thermal inertia of recycled exhaust lower combustion temperatures and retard the post-flame heat-release tail. This uniform temperature reduction directly suppresses NO_x formation kinetics. The onset of peak temperature also shifts ~1° CA later under EGR, consistent with the delayed pressure rise, confirming that EGR both cools and retards the heat-release profile.

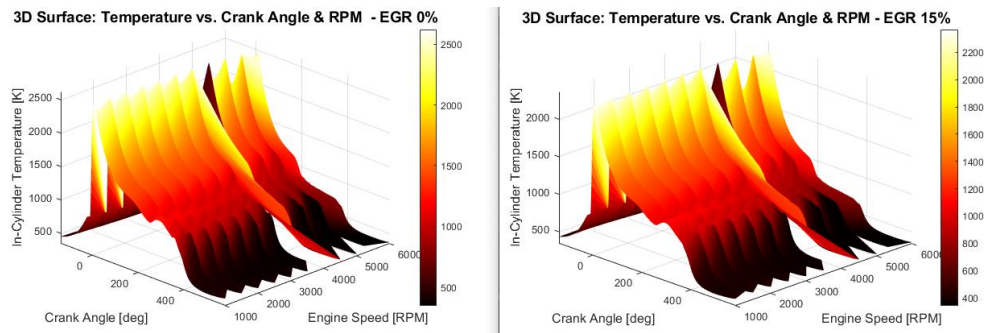


Figure 29 Temp K vs Crank angle for a range of RPMs - EGR [0-15] %

3.6.4 NO_x concentration vs. crank angle & RPM (EGR 0 %)

The 3D NO_x map at 0 % EGR Figure 32 shows instantaneous concentrations peaking above 6 000 ppm at mid-range RPM during the 10–20° CA after TDC. High temperatures and excess oxygen accelerate thermal NO_x pathways. At higher speeds, peak NO_x shifts earlier and intensifies slightly due to hotter, faster burns. The steep leading edge of the NO_x traces underscores hydrogen's proclivity for rapid high-temperature formation without recirculation. 15 % EGR generated a maximum of 1100 [PPM] showing strong results in reducing NO_x.

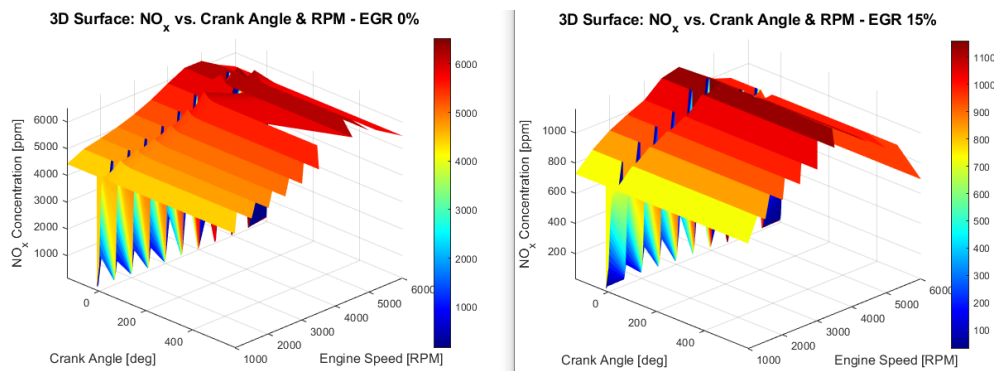


Figure 30 NO_x Concentration vs Crank Angle for a range of RPMs - EGR [0-15] %

3.6.5 NO_x production vs. crank angle & RPM (EGR 15 %)

With 15 % EGR Figure 33, peak NO_x concentrations drop to ~1 200 ppm—an 80 % reduction—while the NO_x formation window broadens by ~3° CA. The cooler, oxygen-diluted charge delays and suppresses the Zeldovich mechanism. At high speeds, NO_x remains below 1 000 ppm, demonstrating EGR's strong leverage on emissions. Although the recirculated mass lowers peak pressure and power, this NO_x mitigation confirms that moderate EGR fractions are essential for meeting stringent tailpipe targets in hydrogen ICE applications.

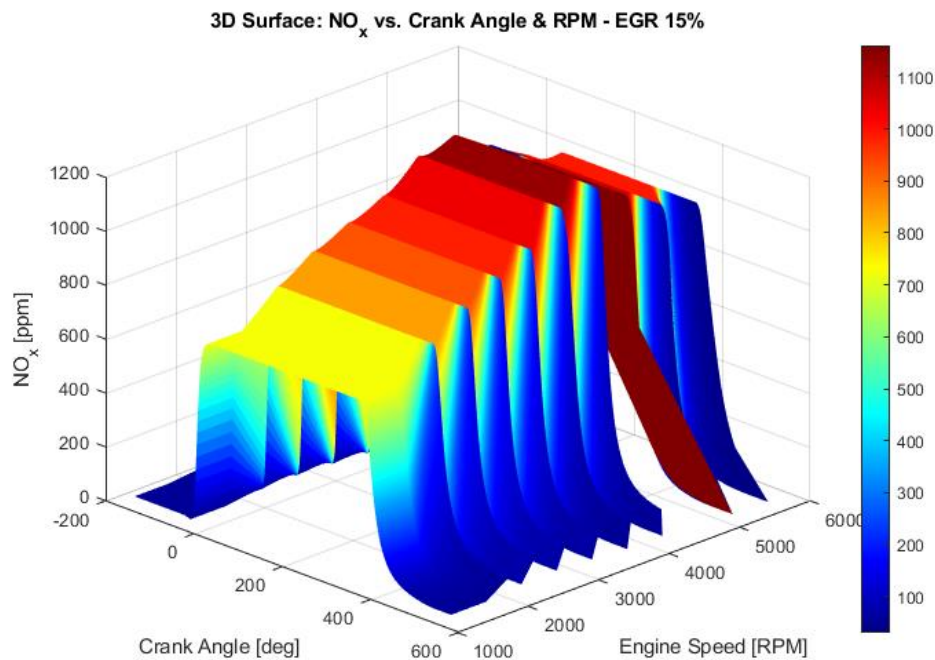


Figure 31 NO_x produced by the engine vs crank angle for a range of RPMs - EGR [0-15] %

3. Limitations

First, WAVE's in-cylinder combustion is treated via a zero- or one-dimensional Wiebe-based heat-release law rather than full 3D CFD. Although the four-parameter SI-Wiebe curve (θ_{50} , $\Delta\theta_{10-90}$, m , burn fraction) reproduces the bulk heat-release rate very accurately, it cannot capture local flame-turbulence interactions, mixture stratification, or quenching at walls. As a result, peak pressure and temperature predictions neglect cycle-to-cycle variability and local hot-spot formation—phenomena that govern knock tendency and localized NO_x “spikes” in real hydrogen combustion.

Second, WAVE uses spatially uniform EGR and intake conditions drawn from FORTE or prescribed tables, assuming perfect mixing of recirculated gases. In reality, EGR composition and temperature vary across the cylinder and change turbulent mixing rates; WAVE's assumption of a single EGR fraction per cycle ignores these gradients. Likewise, wall heat-transfer is handled via empirical correlations rather than detailed conjugate-heat-transfer simulation, so the model under-predicts local quench-layer cooling and its impact on unburned hydrocarbon and NO_x formation.

Third, the model omits detailed hydrogen-air chemical kinetics, relying instead on the Wiebe fit to represent all reaction pathways. Fast radical chemistry, HO_2 intermediate buildup, and EGR-induced radical scavenging are not explicitly simulated, which limits accuracy in predicting NO_x suppression under high EGR or very lean conditions. Transient phenomena—such as backfire in PFI systems or cycle-resolved residual trapping—are also outside WAVE's scope, since it enforces steady crank-angle-based boundary cycles rather than true time-resolved gas-dynamic feedback

4. Conclusion

The calibrated SI-Wiebe heat-release law implemented in Ricardo WAVE has enabled rapid, parametric exploration of hydrogen ICE behaviours across equivalence ratios, EGR levels, and engine speeds. By enforcing a four-parameter fit (θ_{50} , $\Delta\theta_{10-90}$, m , burn fraction) derived from high-fidelity FORTE/MATLAB data, the model captures the bulk combustion phasing and peak pressures within 1–2 bar of 3D CFD. The resulting trade-off linking FER, EGR%, BHP, torque, and NO_x demonstrate that a lean (FER = 0.7) charge with moderate EGR (15 %) delivers the best compromise: ≈ 15 % power loss for an 80 % NO_x reduction.

Nevertheless, WAVE's zero-D combustion representation and uniform EGR mixing assumptions mean it cannot resolve localized hot-spots, quench-layer effects, or radical-chemistry kinetics that drive knock and cycle-to-cycle variability. Consequently, absolute predictions of peak temperature and emissions should be interpreted cautiously; the model excels at trend identification and system-level optimization, but detailed design decisions (e.g. material selection for peak stress zones or precise injection-timing maps) require complementary 3D CFD or further research.

The study underscores the viability of hydrogen ICEs: by tuning FER and EGR, can suppress NO_x to $<1\,000$ ppm while retaining >85 % of baseline BHP. The validated WAVE framework thus provides a powerful tool for screening operating strategies and guiding hardware development paving the way for durable, efficient hydrogen combustion platforms that leverage existing turbocharged ICE architectures.

One clear path to improve fidelity would be to couple the 0-D Wiebe combustion module with a limited 3-D representation of in-cylinder mixing and wall heat-transfer either via a multi-zone or flame-propagation sub model. Incorporating tabulated detailed H_2 kinetics (e.g. via a reduced mechanism with HO_2/NH_2 pathways) would allow WAVE to predict radical buildup and thermal NO_x kinetics under high EGR and ultra-lean conditions, rather than relying solely on the empirical Wiebe fit. Finally, using spatially varying EGR temperature and composition boundary conditions drawn from a companion 1-D gas-exchange model would capture cycle-resolved residual distributions and quench-layer cooling more accurately, thereby reducing the remaining uncertainty in peak-pressure, temperature, and emissions predictions.

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6. Appendix

Appendix A

This study aims to provide a methodology that allows the reader to replicate the models reliably.

The following steps outline the procedure followed inside Forte:

Step 1: Geometry Setup

- Open Forte and click on Geometry in the software tree
- Inside Geometry, click Sector Mesh Generator (SMG)
- This opens the SMG interface to generate a sector mesh of the cylinder for analysis

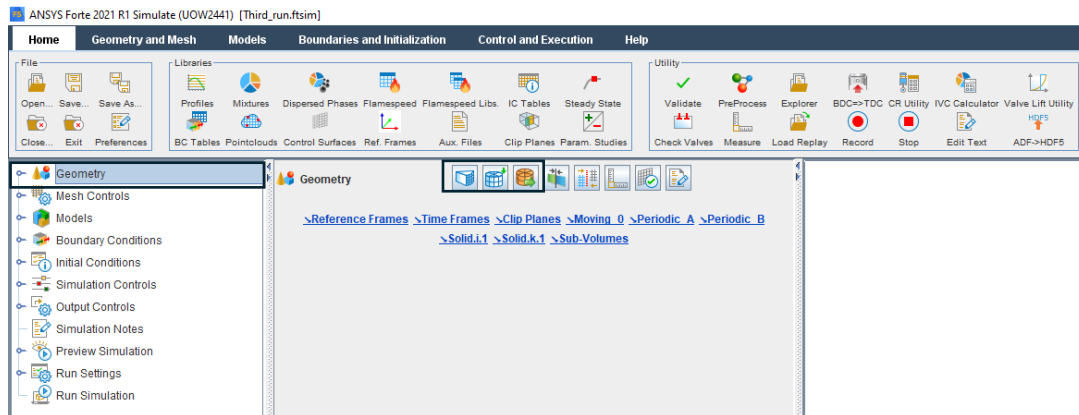


Figure 32 Visual representation of the main page FORTE

Step 2: Define Piston Bowl Profile and Sector

- Select an existing bowl profile or create a new one depending on the piston geometry characteristics

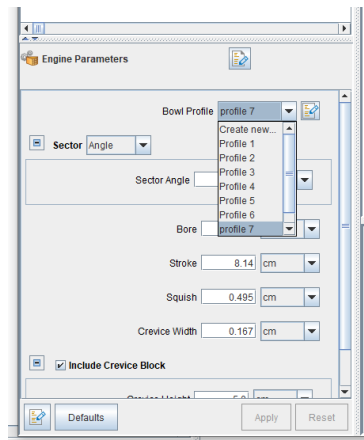


Figure 33 Engine Parameters for the Bowl Profile - FORTE 2021

- Select the sector type as Angle (important for sector simulations)

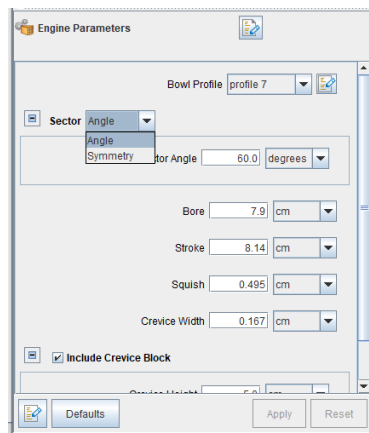


Figure 34 Sector Mesh, Sector - FORTE 2021

- Use real engine data (e.g., from the provided engine file "Petrol Sigma 1.6 Pressure") to populate engine specifications

		LUCID M	EAN CY	CLE PRES	SURE DAT	A FILE
D:\4mlc50	9\0084.0	1				
06-02-200	3 08:58					
Leistungs	messung	Lambda 0	.9 FKl	4=2 EBP=	35 kpa	1000 rpm
4mlc509						
BORE	(m) STRO	KE(m) CON	ROD(m)	COM.RAT	IO NCYCL	ES NCYLS VOLUME
0.079 0	.0	814	1370	11.16	300 4	1
I-FILE DA	TA					
NUMBER	READING S	720				

Figure 35 Real Engine Data - FORTE 2021

Step 3: Mesh Generation

- Go to Mesh Parameters
- Select New Topology and fill the fields based on standard practices or previous similar models

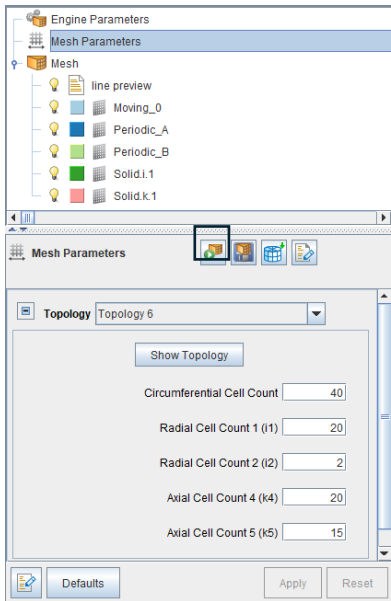


Figure 36 Mesh Parameters - FORTE 2021

- Once completed, click "Generate a Mesh"
- The generated mesh should look similar to Figure 44

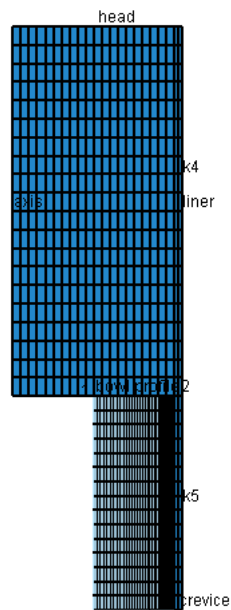


Figure 37 Sector Mesh - FORTE 2021

Step 4: Import Sector Mesh into Simulation

- Import the sector mesh into the main Forte interface
- The imported mesh becomes a geometry object ready for CFD analysis

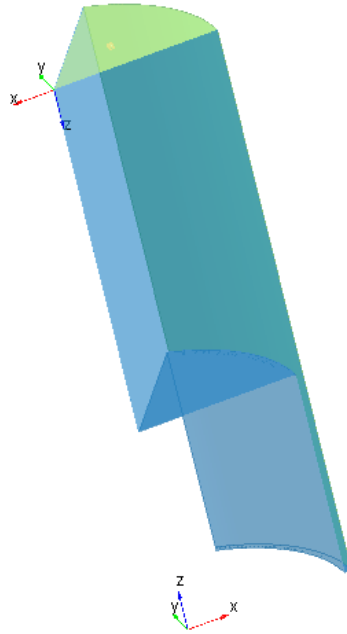


Figure 38 Imported geometry from sector mesh - FORTE 2021

Step 5: Model Setup

- Chemistry Settings:
 - Equation of State → Ideal Gas



Figure 39 Chemistry - FORTE 2021

- Transport Properties → Default (leave unchanged)

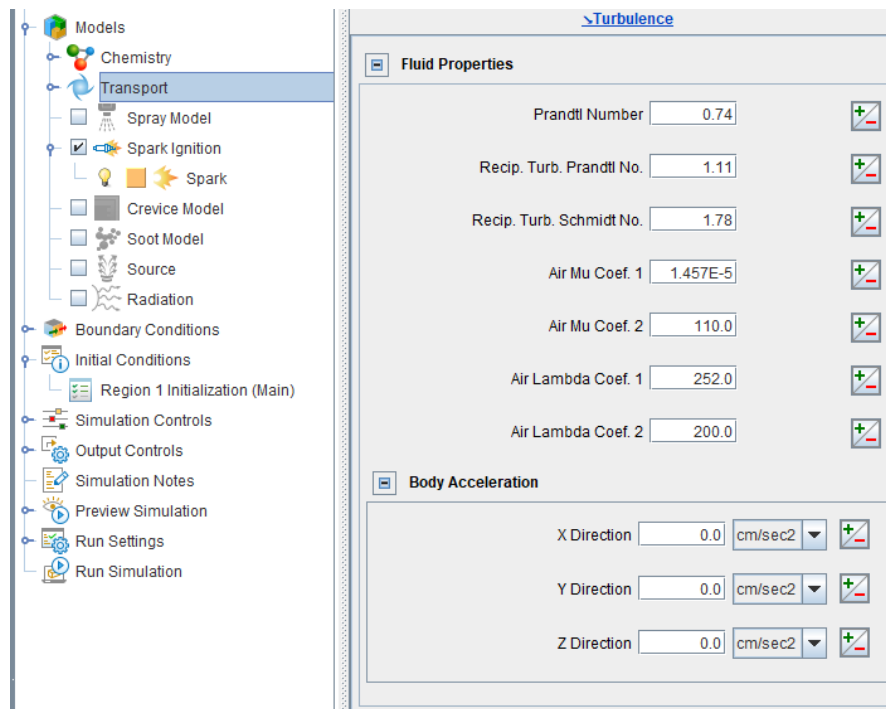


Figure 40 Fluid properties and Acceleration - FORTE 2021

- Ignition Setup (for Spark Ignition engines):
 - Activate Spark Ignition

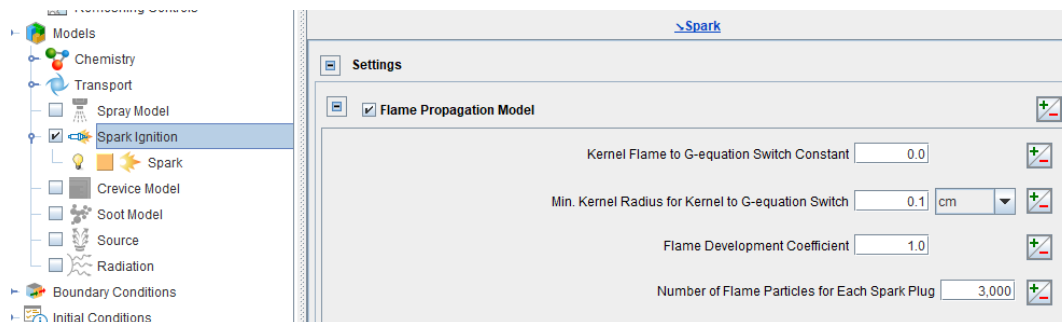


Figure 41 Spark Ignition Variables - FORTE 2021

- Reference Frame → Global Origin
- Coordinate System → Cartesian
- Time Option → Crank Angle (for better phase control over engine events instead of physical time)

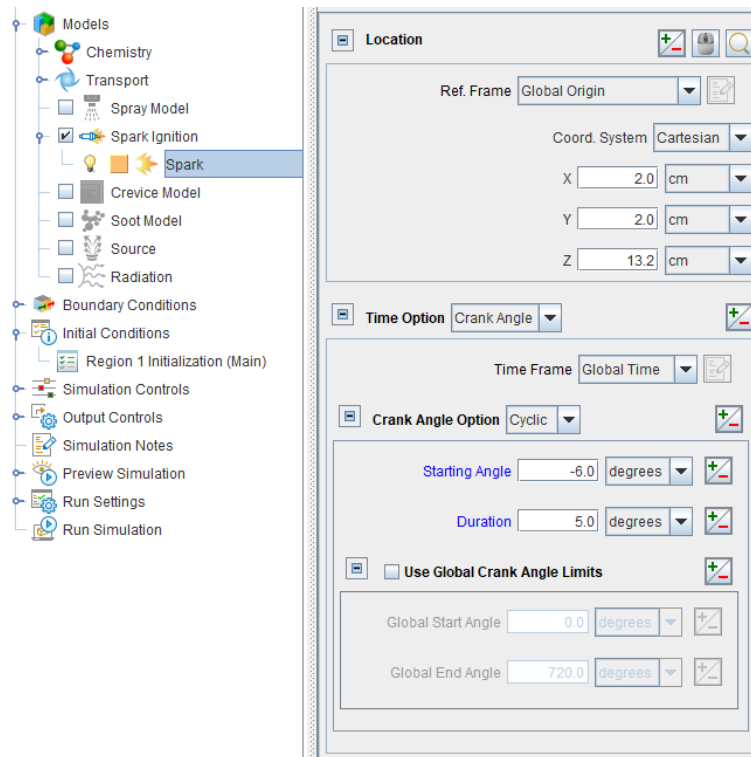


Figure 42 Parameters for the Spark; Location; Crank Angle Options - FORTE 2021

- Spark Parameters:
 - Spark Energy Release Rate → typically 20–30 J/sec for Diesel and Petrol
 - For Hydrogen studies → 5000 J/sec
 - Energy Transfer Efficiency → 0.5 (recommended default)
 - Initial Kernel Radius → 0.5 mm (typical initial size of the spark kernel)

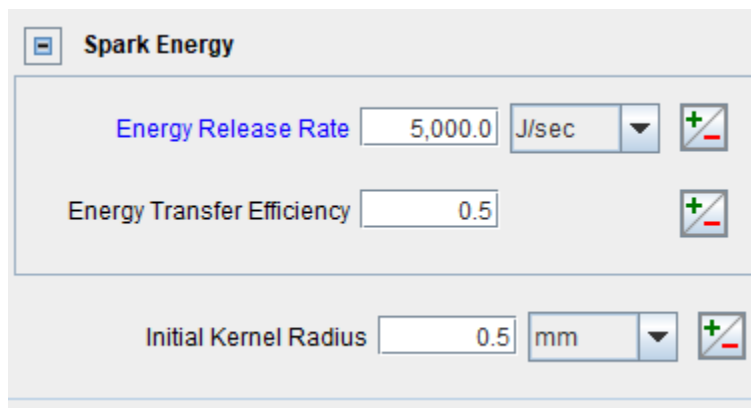


Figure 43 Spark Energy properties - FORTE 2021

Step 6: Initial Conditions Setup

1. Chemistry Section:

- Composition - Constant: Gas mixture composition selected from an appropriate chemistry library based on the fuel type (e.g., gasoline, diesel, hydrogen).

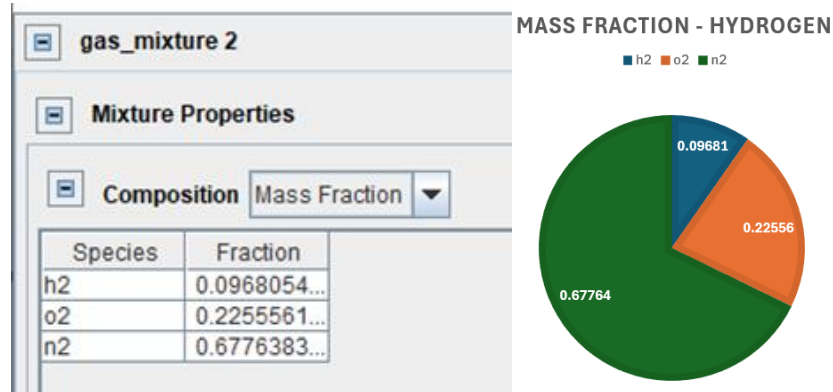


Figure 44 Mixture Composition for Hydrogen as a fuel for Internal Combustion Engine - FORTE 2021

- Temperature: Set to constant, initial value of 300 K.
- Pressure: Set to constant, initial value of 1.0 atm.
- Turbulence: Model set to Turbulent Kinetic Energy and Length Scale.
 - Turbulent Kinetic Energy: $10,000 \text{ cm}^2/\text{s}^2$.
 - Turbulent Length Scale: 1.0 cm.

Region ID 1

Composition Constant

Composition gas_mixture 2

Temperature Constant

Temperature 300.0 K

Pressure Constant

Pressure 1.0 atm

Turbulence Constant

Turbulence Turbulent Kinetic Energy and Length Scale

Turbulent Kinetic Energy 10,000.0 cm2/se...

Turbulent Length Scale 1.0 cm

Figure 45 Initial Conditions for the Model - FORTE 2021

- Velocity:
 - Set to Constant.
 - Apply Engine Swirl:
 - Initial Swirl Ratio: 1.2.
 - Initial Swirl Profile Factor: 3.11.
 - Enable "Initialize Velocity Components Normal to Piston".
- Piston Boundary: Assign all surfaces (Head, Liner, Periodicity, Piston) to the selected list.

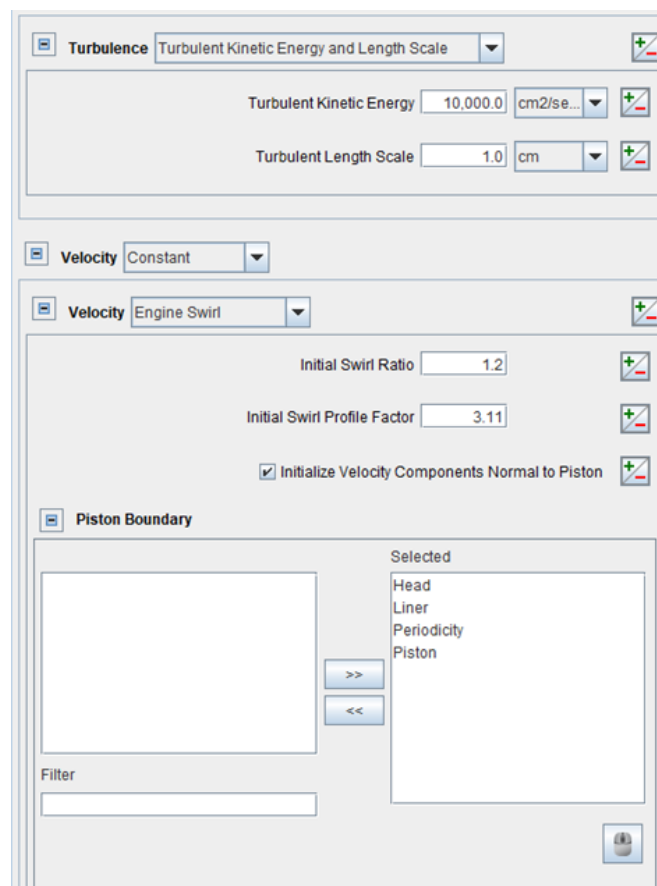


Figure 46 Initial Conditions for the model - FORTE 2021

2. Simulation Controls:
 - Simulation type: Crank Angle Based.
 - Initial Crank Angle: -150°.
 - Final Simulation Crank Angle: +150°.
 - Engine Speed (RPM): 1000 RPM.

- Cycle Type: 4-Stroke.
- Engine Bore: Calculate Automatically.
- Ensure Restrict Total Simulation Steps is unchecked.

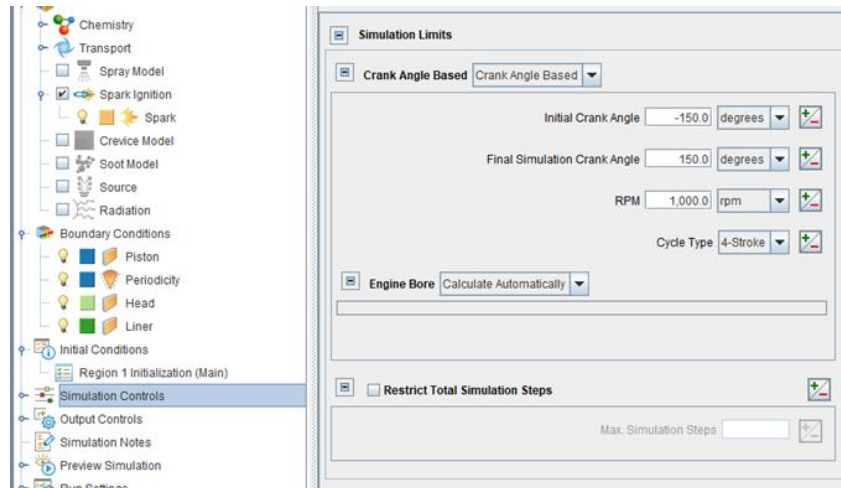


Figure 47 Simulation Control Parameters - FORTE 2021

3. Running the Simulation:

- Navigate to the Run Simulation tab.
- Select Parallel execution with 4 processors.
- Select Use Restart and Auto-Resize options.
- Save the configuration and Start Simulation.
- If real-time monitoring is needed, enable FM (Field Monitoring), select the variable of interest, and monitor the simulation progress live.

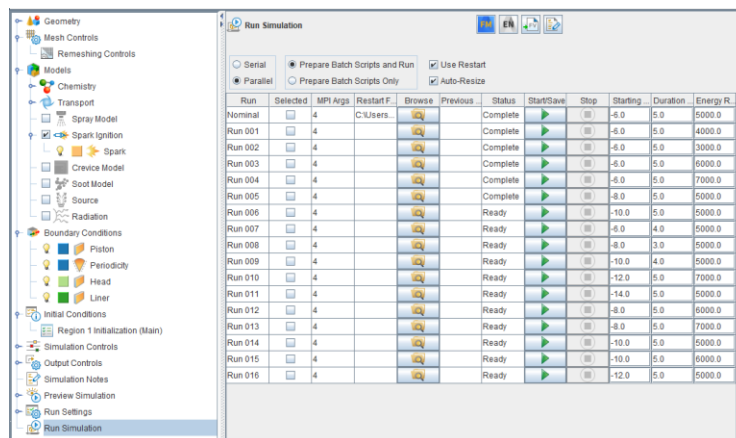


Figure 48 Run Simulation Tab in which the user can run more than 1 simulation at a time (one after the other) changing a wanted variable - FORTE 2021

Appendix B

FORTE Simulation Parameters for Diesel

Appendix C

FORTE Simulation Parameters for Petrol

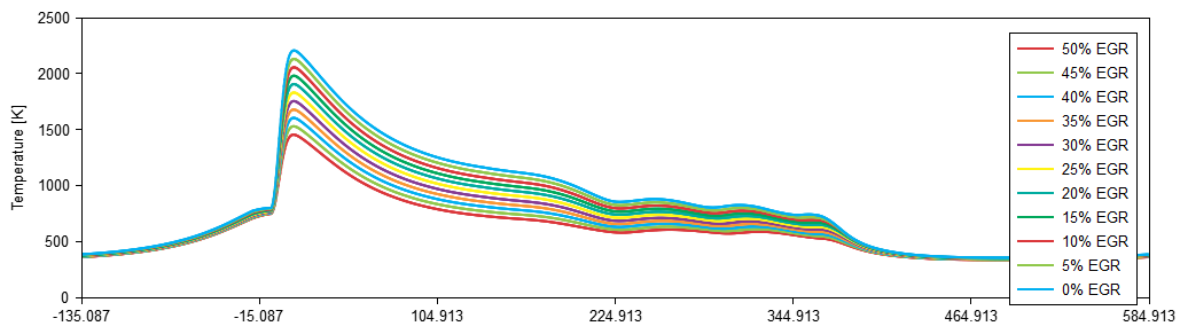
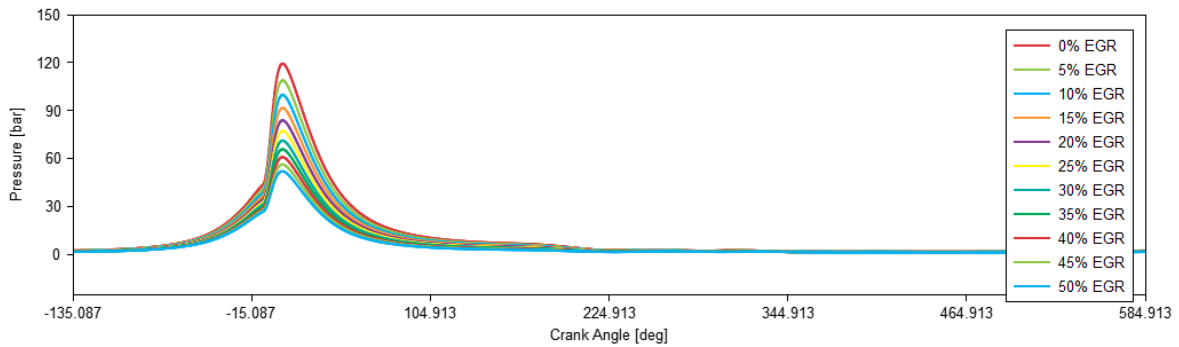
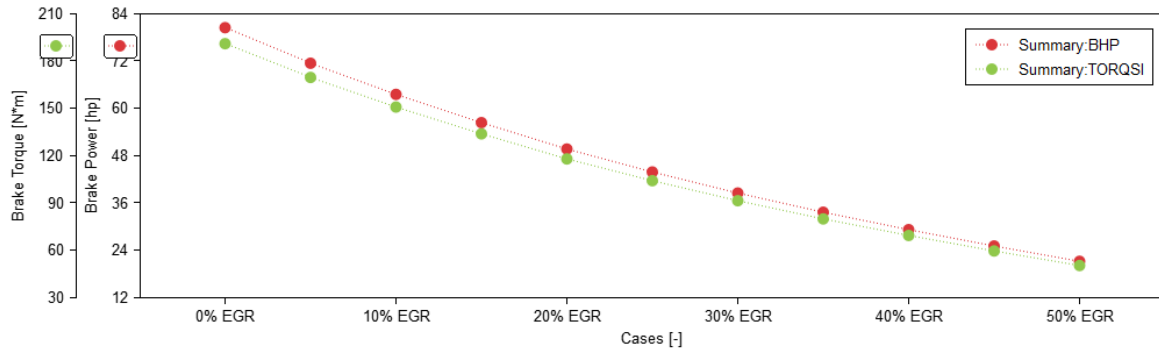
For the simulation setup, the following boundary and initialization conditions were used:

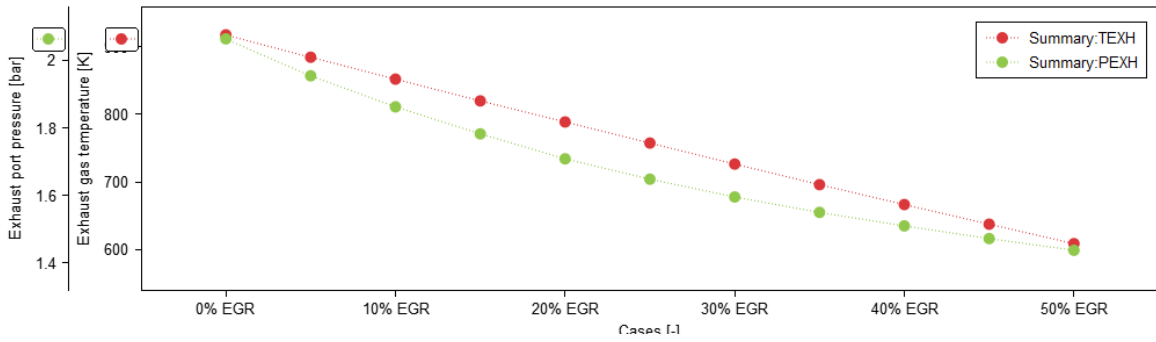
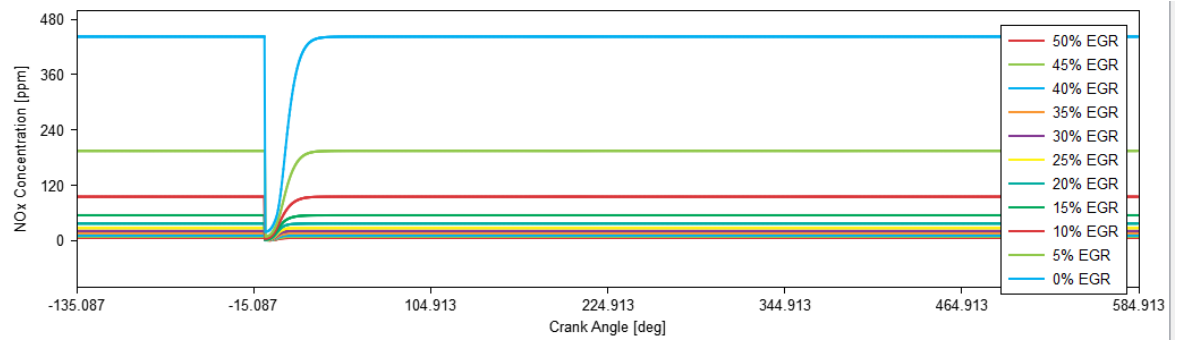
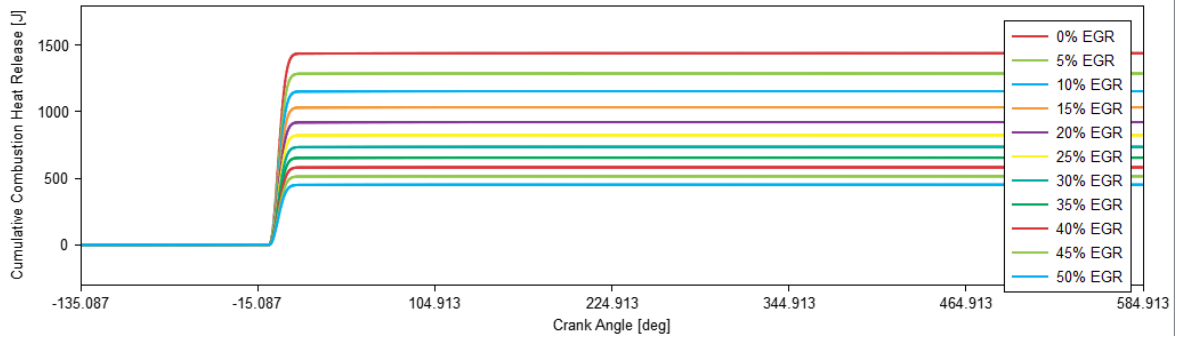
- Crank Angle Window: -150° to 150°
- Engine Speed: 1000 RPM
- Spark Timing: Ignition initiated at -5° crank angle with a spark duration of 5°
- Initial Temperature: 400 K
- Initial Pressure: 1.013 bar
- Turbulent Kinetic Energy: $7000 \text{ cm}^2/\text{s}^2$
- Chemical Composition:
 - Oxygen (O_2): 0.24943
 - Octane (C_8H_{18}): 0.0214562
 - Nitrogen (N_2): 0.729114

These carefully chosen parameters ensured that the in-cylinder conditions prior to ignition accurately reflected the experimental

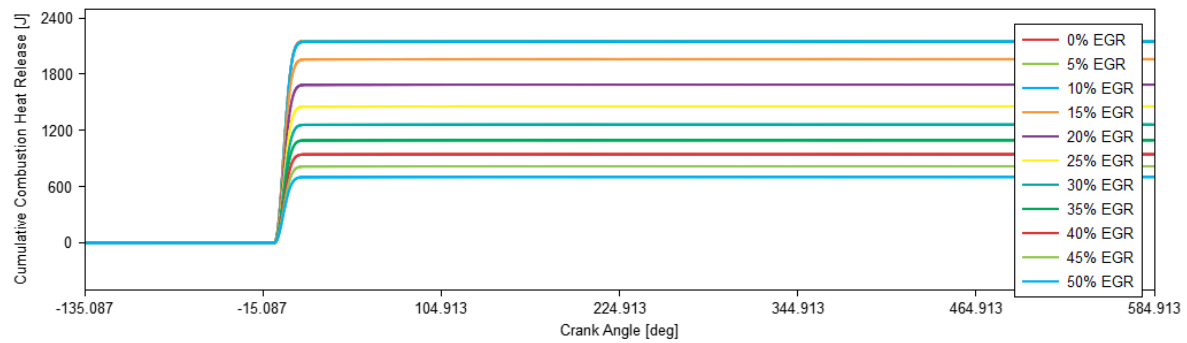
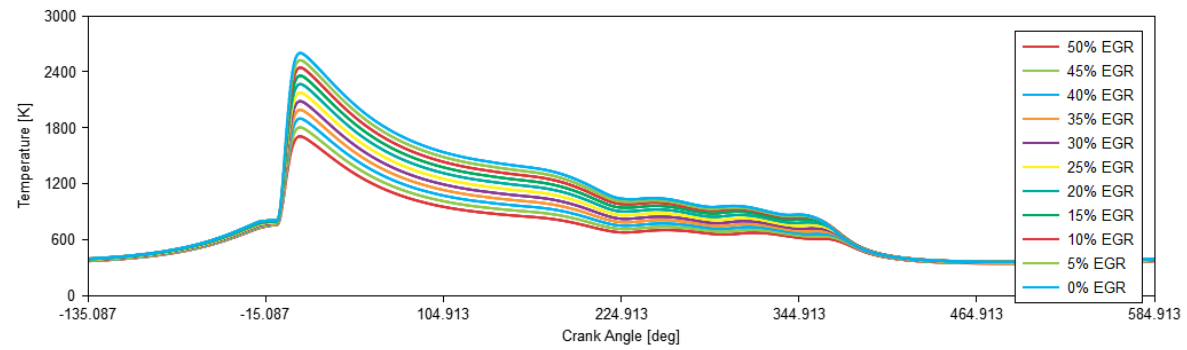
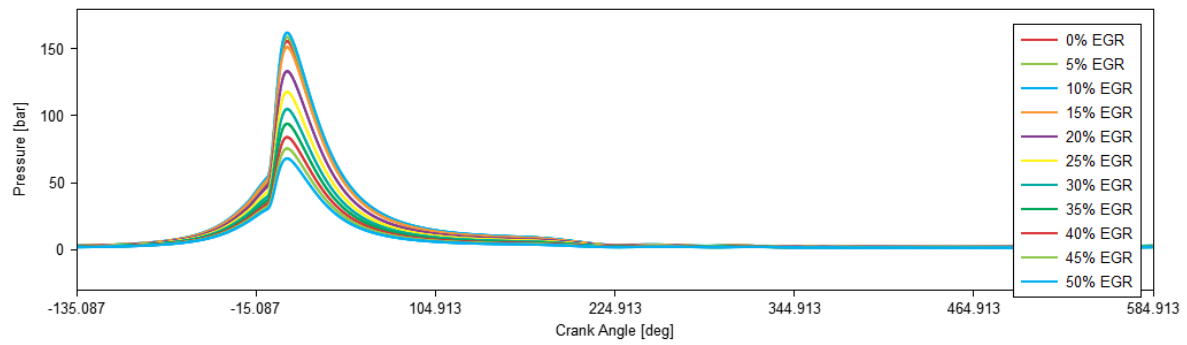
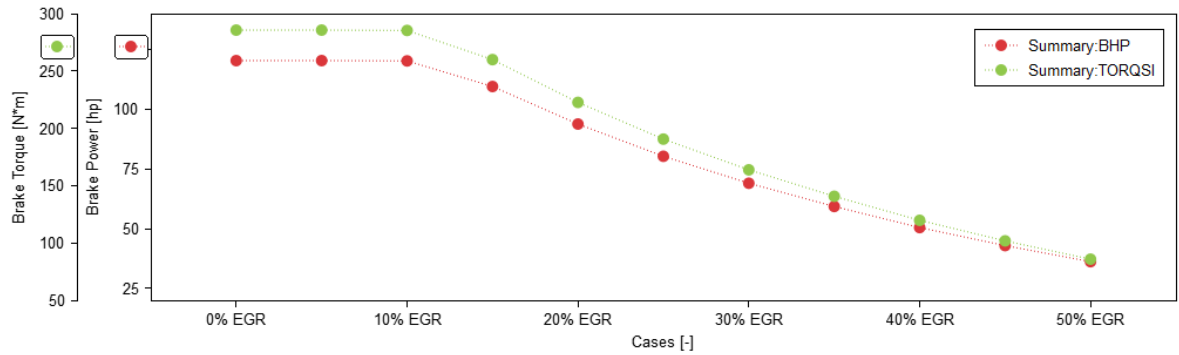
Appendix D – WAVE SS from Models

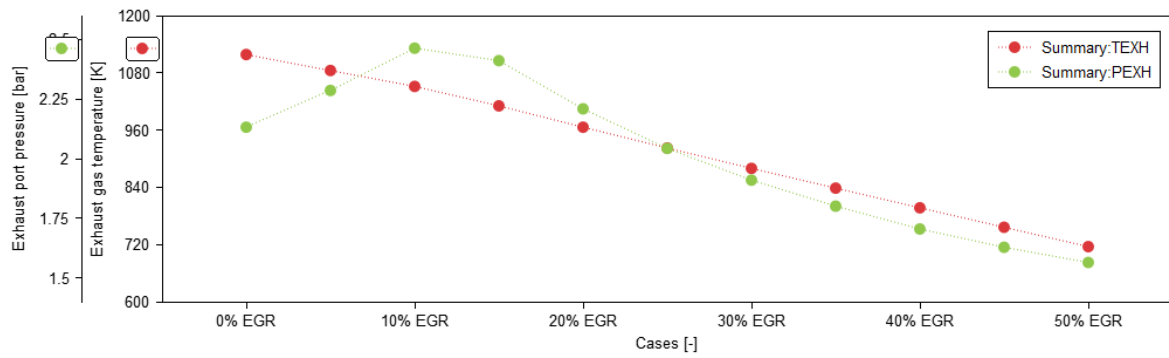
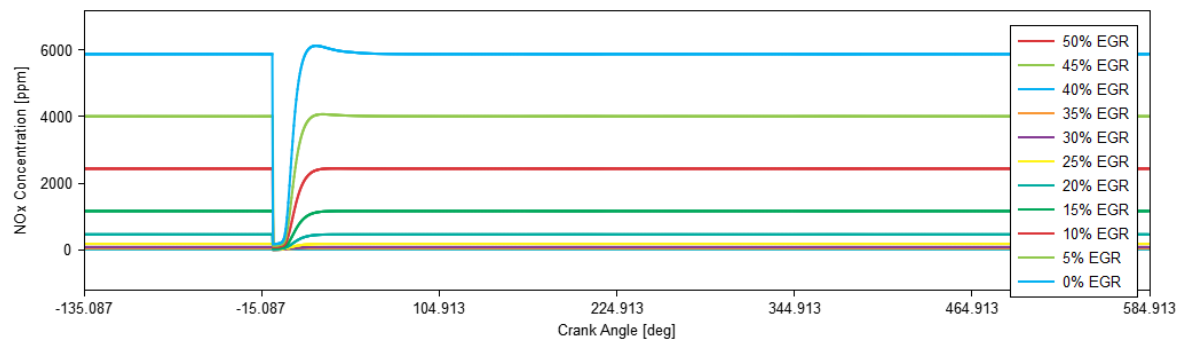
0.5 fer



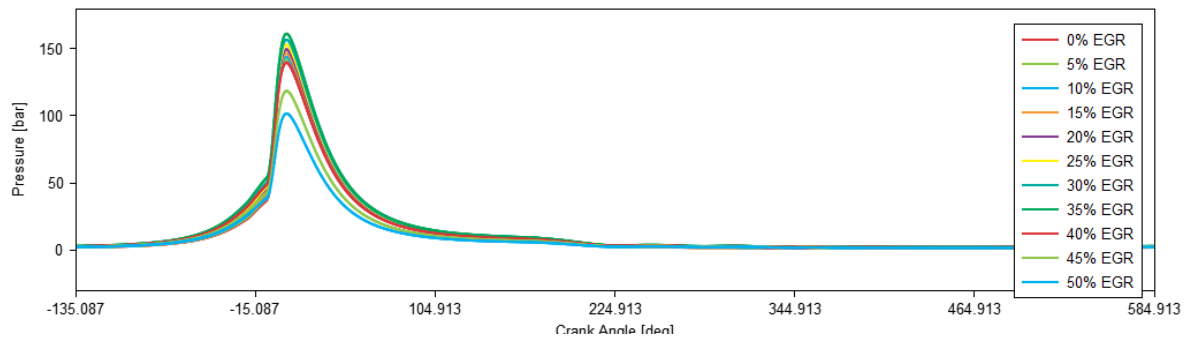
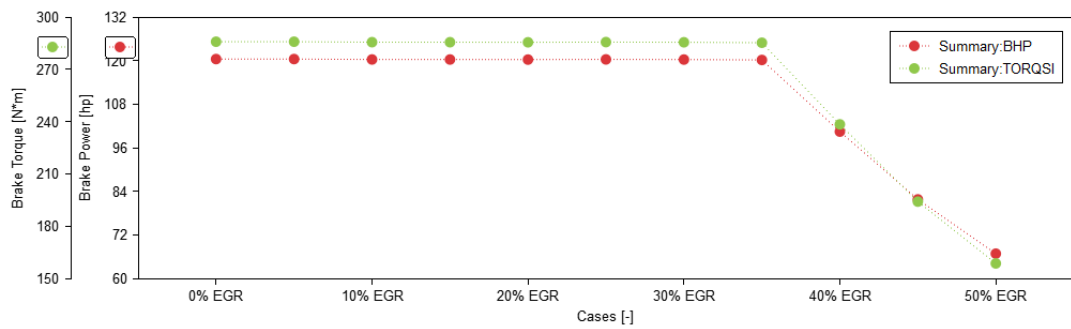


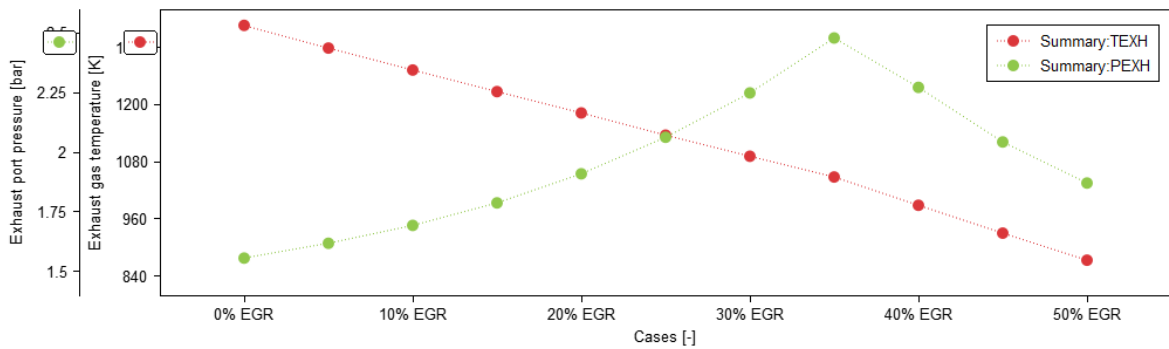
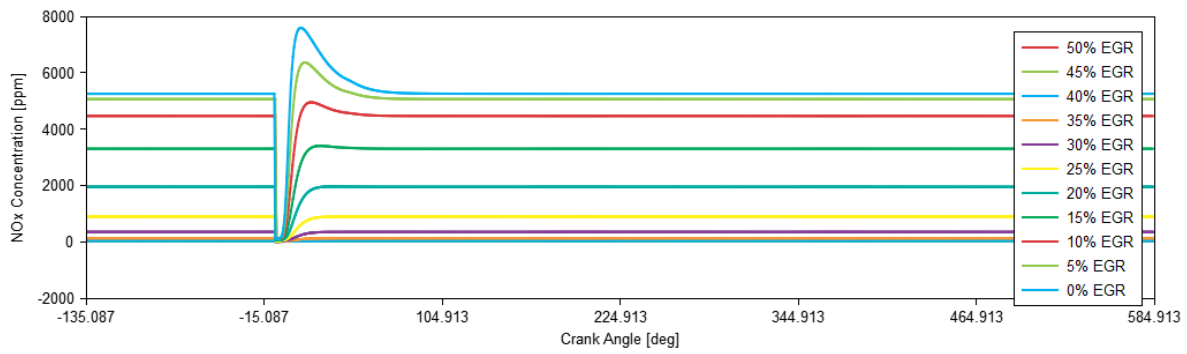
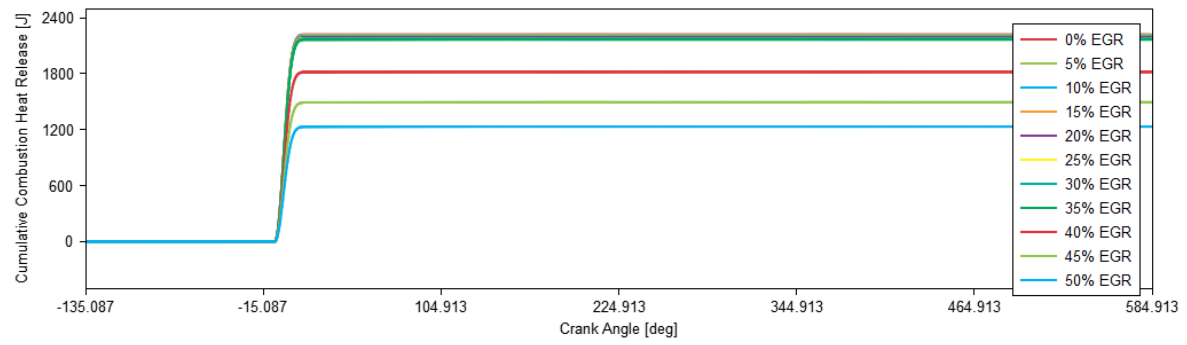
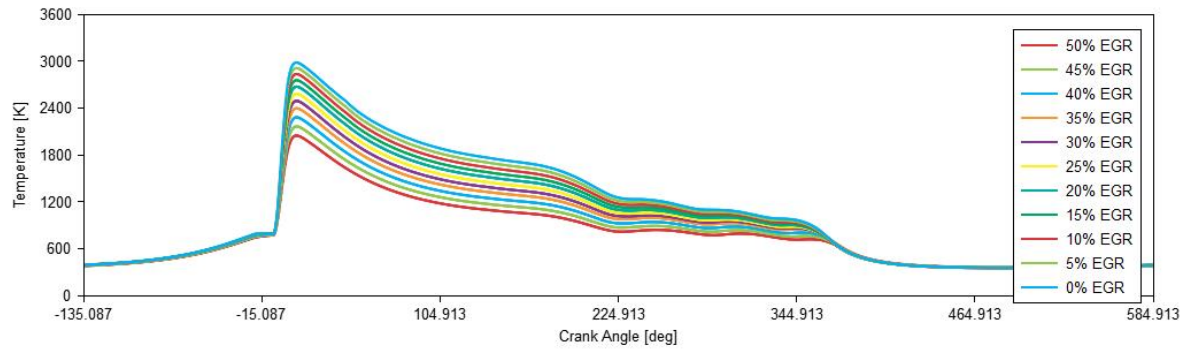
0.7 FER



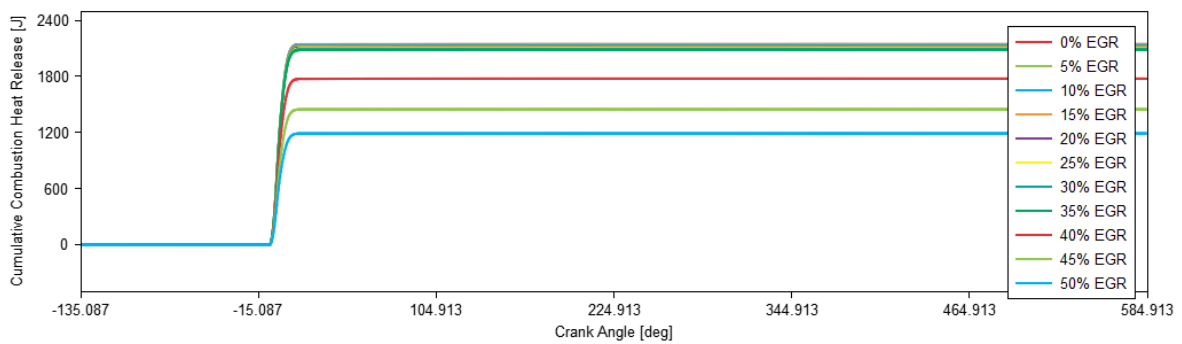
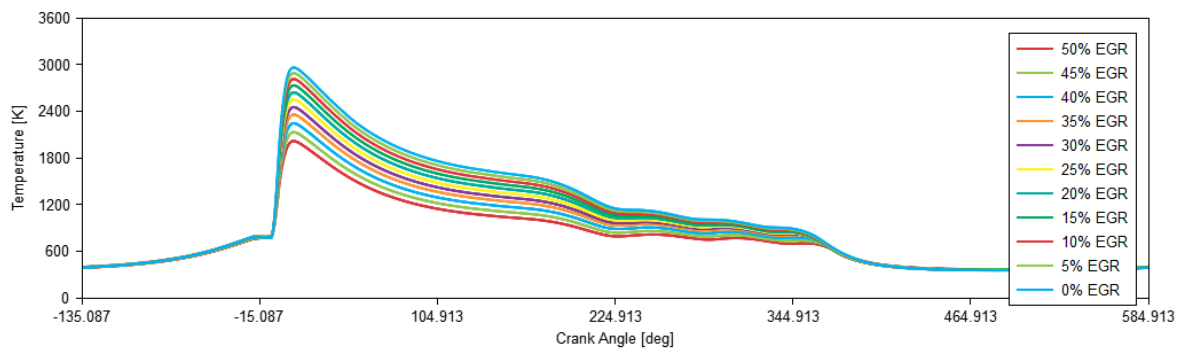
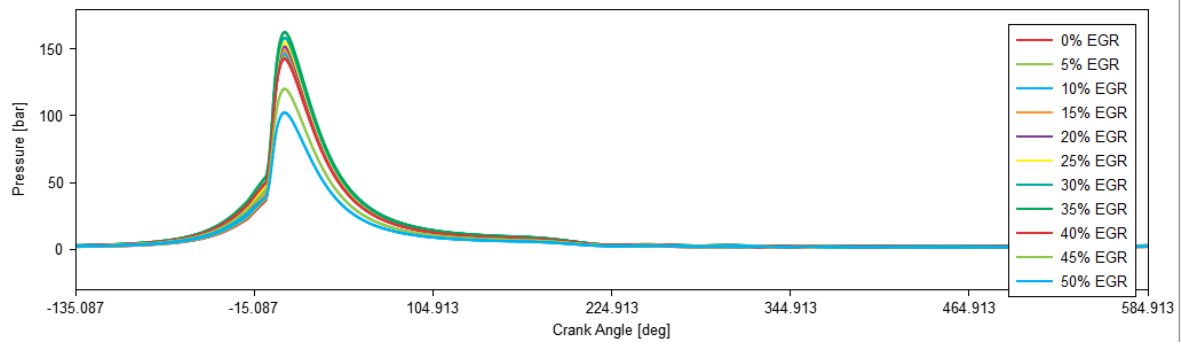
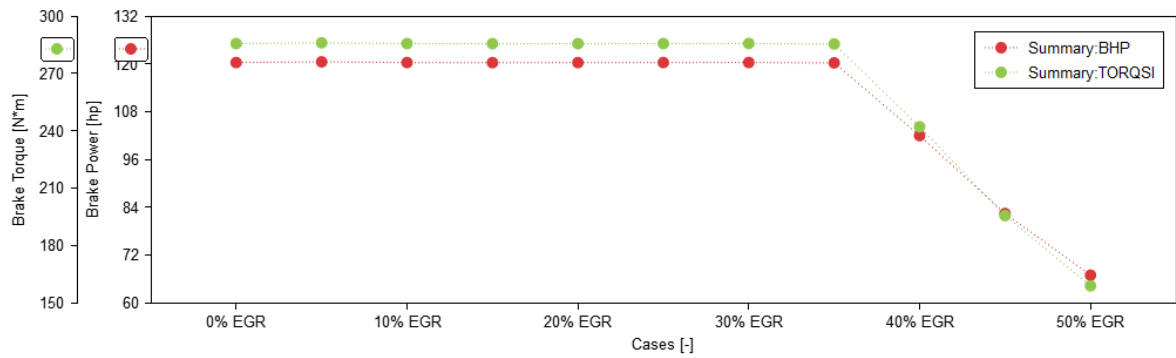


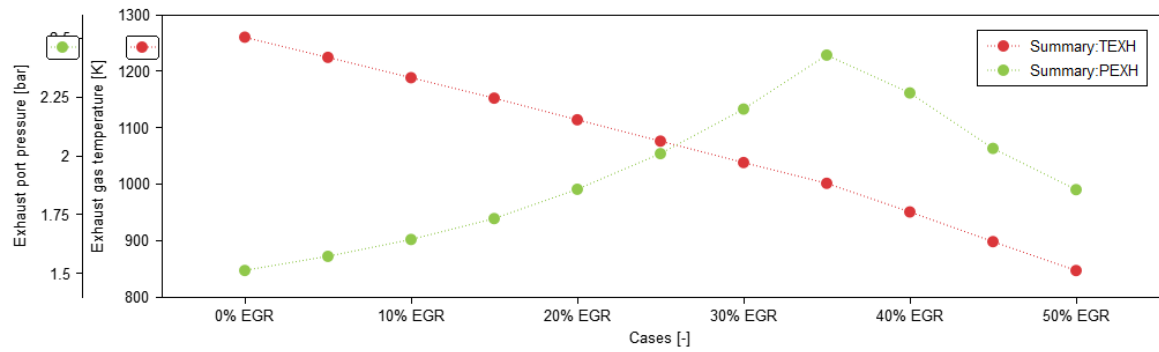
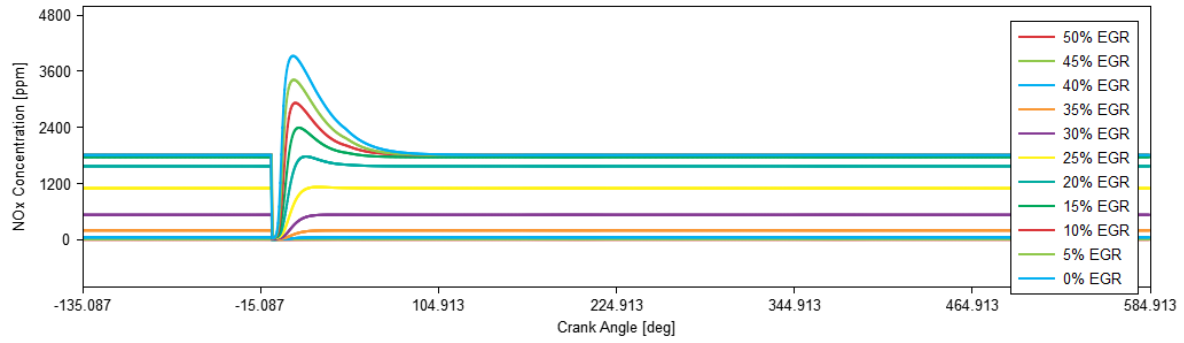
FER 1



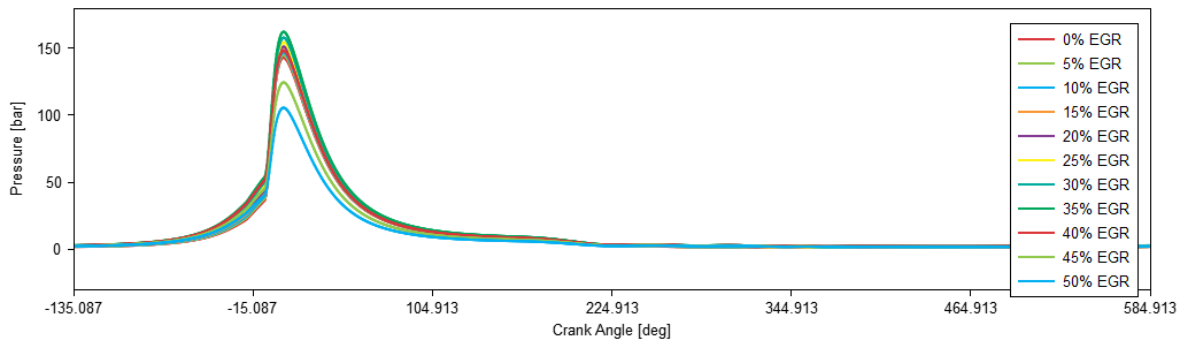
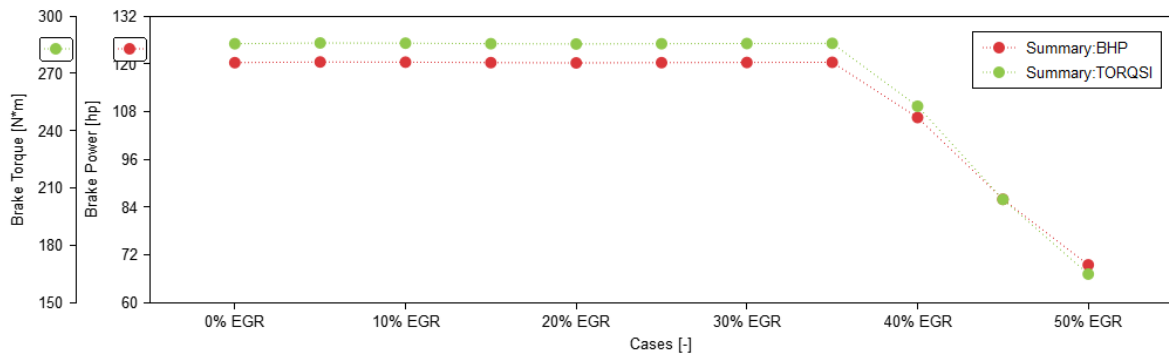


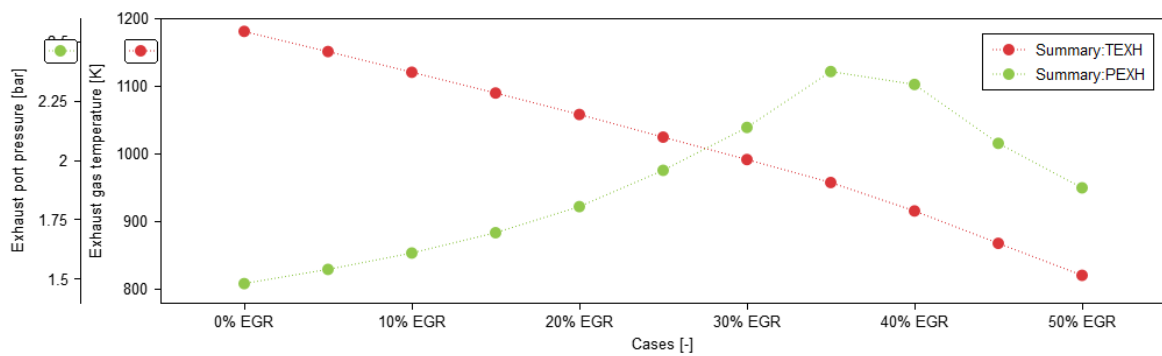
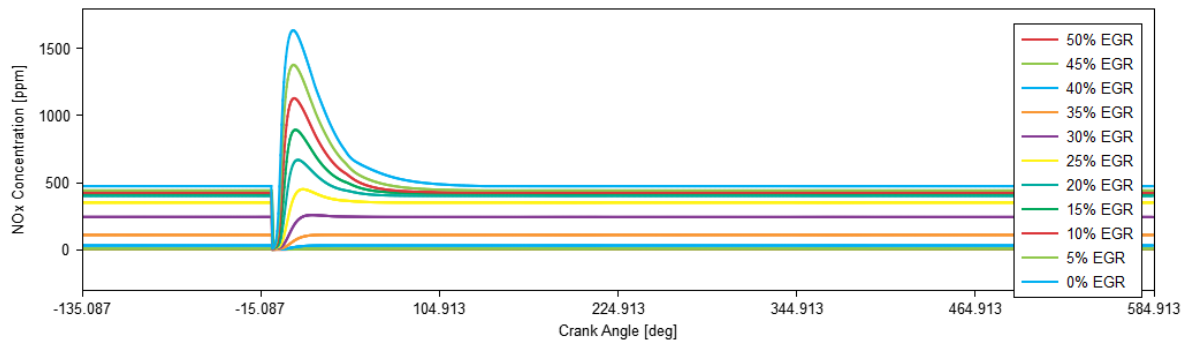
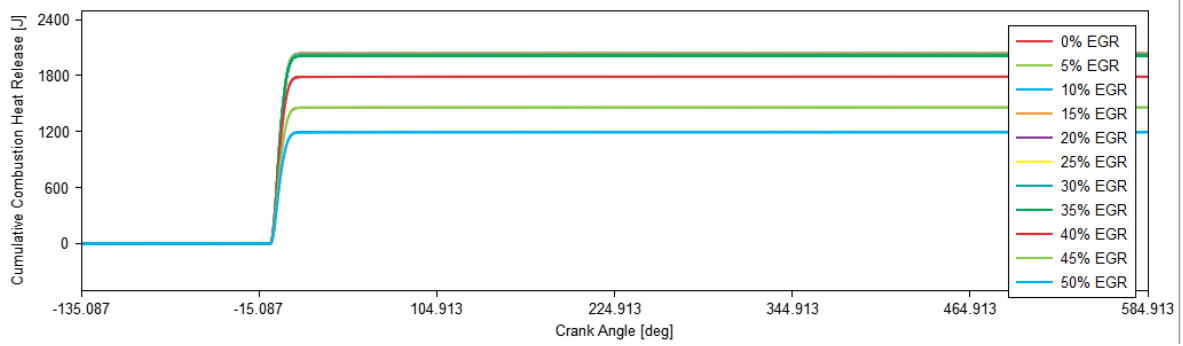
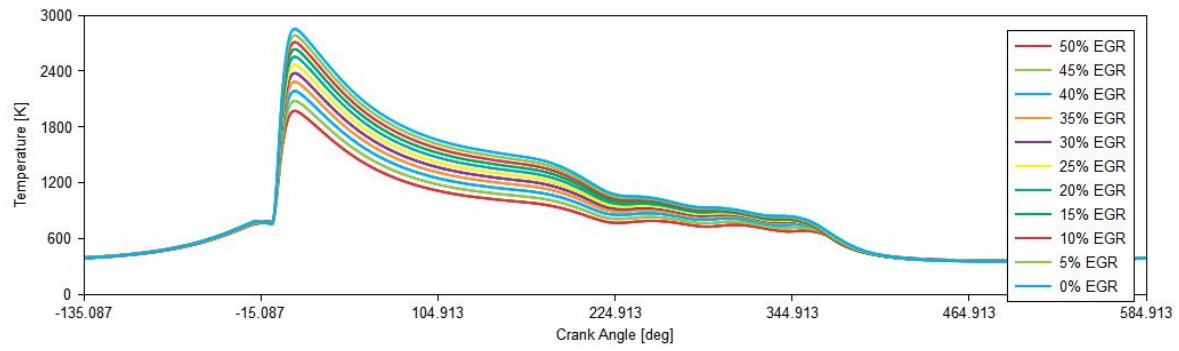
1.25 FER



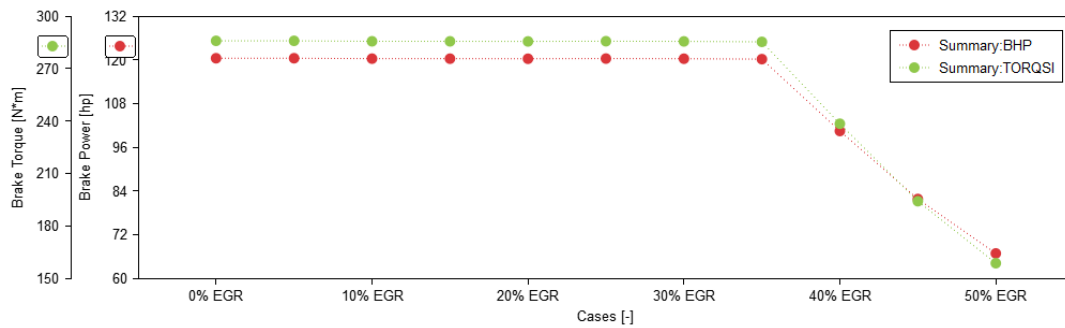
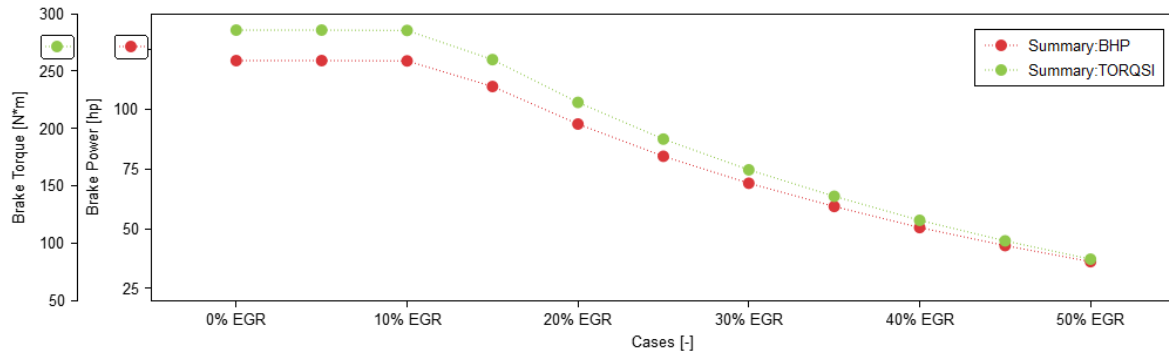


1.5 FER

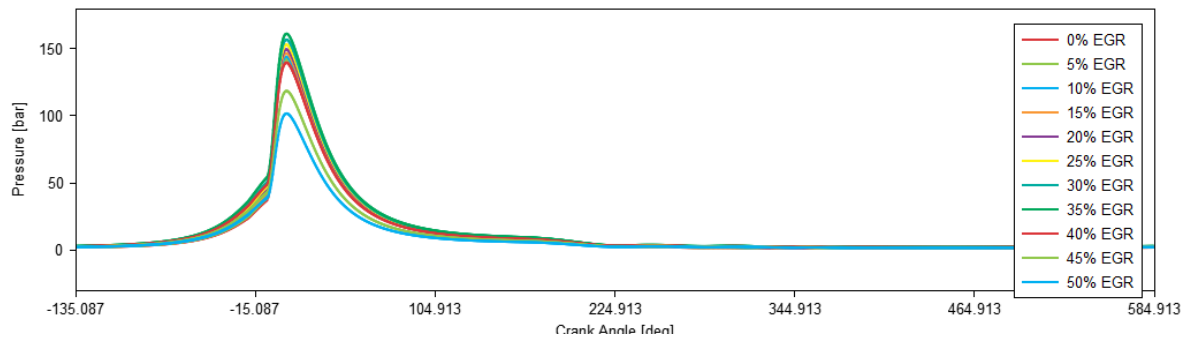
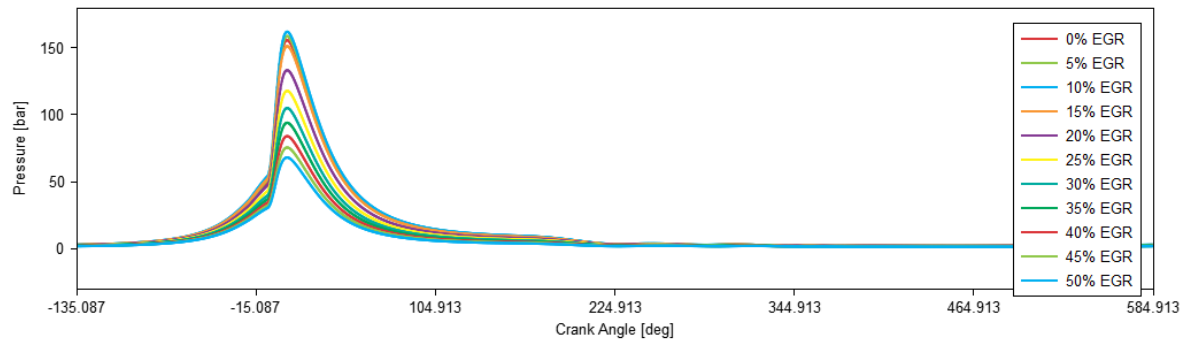




Comparison BHP



Comparing Pressure



FER – 0.7 – EGR 0% SPEED SWEEP- EGR 15% (Data Used for final comparison)

