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Abstract

This study investigates the viability of ammonia–hydrogen ($\text{NH}_3\text{--H}_2$) fuel blends in port-injected spark-ignition engines using combined 1D and 3D simulation tools. A 20 mol % H_2 / 80 mol % NH_3 blend was selected based on its proven flame-stability and NO_x -minimisation characteristics. System-level cycle analyses in Ricardo WAVE generated boundary conditions for detailed transient CFD in ANSYS Forte, employing a 60° sector mesh ($\approx 1.1 \times 10^5$ cells) and a reduced GRI-Mech 3.0 mechanism extended for NH_3 pathways. Mesh convergence ($< 2\%$ peak pressure variation), RNG $k\text{--}\epsilon$ turbulence closure, and adaptive time-stepping ($\text{CFL} < 1$) ensured numerical accuracy. Key results demonstrate peak cylinder temperatures of 2400–2700 K and pressures up to 90 bar at 6000 RPM, exceeding pure-hydrogen benchmarks but aligning with MIJI-enhanced NH_3/H_2 studies. NO_x emissions rise exponentially above 1500 K, while CO is eliminated entirely due to the carbon-free blend. Mass-fraction-burn-rate analysis via adaptive Wiebe fitting ($a=2.8$, $m=2.88$) captures delayed burn tails at low speeds. Critical evaluation highlights the trade-offs of two-zone vs. LES turbulence models, and the benefits of on-the-fly mechanism reduction. The work confirms the technical feasibility of $\text{NH}_3\text{--H}_2$ ICEs but identifies the need for advanced ignition (MIJI, pre-chamber), LES-based turbulence, conjugate heat transfer, and aftertreatment integration to meet future emissions regulations.

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1. Introduction

The urgent need to decarbonise transportation has spurred interest in carbon-free fuels that can power internal combustion engines (ICEs) beyond 2035. Hydrogen (H_2) and ammonia (NH_3) are leading candidates for zero-carbon fuels because they produce no direct CO_2 emissions when burned (Zhang, B. et al. 2023). Both fuels, however, pose significant combustion challenges: ammonia has a very low flame propagation rate and high ignition energy requirement (Alqarni et al., 2024), while hydrogen is difficult to store (U.S. Department of Energy, 2022) and can lead to high NO_x emissions (SLR Consulting, 2023). This review examines the feasibility of using hydrogen–ammonia fuel blends in ICEs, drawing on experimental studies and modelling approaches. We compare the combustion characteristics, performance, and emissions of H_2/NH_3 mixtures against conventional gasoline and diesel fuels, with a focus on applications in the UK/EU transportation sector. An analysis of advanced ignition technologies (spark, compression, plasma) needed to utilise these fuels, and evaluate their environmental impacts including NO_x , N_2O , unburned fuel, and CO_2 on a life-cycle basis. Economic and practical considerations – fuel cost, infrastructure, onboard storage, and engine retrofitting – are discussed to gauge real-world feasibility. Modelling techniques such as two-zone combustion models with Wiebe functions (for use in MATLAB) and detailed 3D CFD (ANSYS Forte) are reviewed in the context of simulating hydrogen-ammonia combustion. Finally, policy and regulatory frameworks (the post-2035 UK/EU zero-emission vehicle mandates) are considered to understand the role of ammonia-hydrogen ICEs in meeting future emissions targets. This study addresses two key gaps: (1) quantifying the lean-limit and stability envelope of 20/80 NH_3 – H_2 blends in a port-injected SI engine; and (2) evaluating novel ignition strategies—such as hydrogen multiple-injection jet ignition (MIJI)—for enhancing flame kernel growth in ultra-lean mixtures. Recent experimental work demonstrates MIJI can lower the minimum hydrogen energy ratio below 3 % while achieving $COV < 1$ % and $ITE \approx 42.5$ % (Wang et al. 2024)

2. Literature Review

As the UK and EU aim for net-zero emissions by 2050, the internal combustion engine (ICE) faces increasing regulatory pressure. The UK plans to ban new petrol and diesel cars by 2030, allowing only zero-emission vehicles by 2035 (UK Government, 2023). The EU's corresponding regulation targets 100% CO₂ reduction from new cars by 2035, with narrow exceptions for e-fuel-only vehicles (European Commission, 2023). However, ICEs remain vital in specific sectors—particularly heavy-duty transport, motorsport, and high-performance vehicles—if adapted to meet stringent emissions and carbon neutrality goals.

2.1 Ignition system innovations

The fidelity of 2-zone combustion modelling, foundational in Ricardo and Forte, hinges on accurate depiction of heat release, ignition, and emissions formation.

Hydrogen multiple-injection jet ignition (MIJI) creates stratified mixtures that accelerate NH₃ flame propagation, reducing COV to <1 % at 20/80 blend ratios (Wang et al. 2024)

Large Eddy Simulation (LES) of NH₃/H₂/air swirl burners shows that dynamic sub-grid models capture flame wrinkling and NO_x formation more accurately than RANS approaches (Tuyen et al. 2024).

2.1.1 Plasma-Assisted Ignition (PAI)

Plasma-assisted ignition improves combustion stability in lean or diluted conditions by generating a larger initial flame kernel and enhancing ionisation. Studies show PAI extends lean limits ($\lambda > 1.6$), increases flame speed, and improves fuel efficiency by 5–10% (Choi & Hwang, 2023; Cha et al., 2022). However, commercial adoption is challenged by electrode wear, high-voltage electronics, and integration costs (Chen et al., 2020).

2.1.2 Pre-Chamber Ignition (Turbulent Jet Ignition)

Pre-chamber ignition generates high-energy jets from a small auxiliary chamber to ignite the main charge rapidly. This technique, used in Maserati's Nettuno engine and Formula 1 power units, enables ultra-lean combustion with faster burn rates and lower NO_x formation (Bishop et al., 2018). Mahle Jet Ignition has been integrated into high-performance engines for stoichiometric operation under high load, facilitating compatibility with three-way catalysts (Kalghatgi et al., 2021). These systems are modelled effectively in Forte using dual-volume configurations.

2.2 Emissions Reduction Strategies

Reducing NO_x and PM while maintaining high efficiency is essential under Euro 7 and future standards. These constraints directly influence model inputs and boundary conditions in CFD simulations.

2.2.1 Lean Burn and Stoichiometric Operation

While lean combustion reduces peak temperatures and NO_x, it challenges aftertreatment system efficiency. TWC systems operate optimally at stoichiometric conditions. Therefore, many

manufacturers are converging on stoichiometric combustion with EGR and advanced ignition systems for NO_x control (Heywood, 2018)

2.2.2 Aftertreatment Integration

WAVE and Forte allow coupling of engine-out emissions with aftertreatment modules. Bosch (2022) outlines Euro 7-ready systems including dual-dosing SCR and electrically heated catalysts to manage cold-start emissions. Accurate simulation of catalyst light-off and thermal transients is key to predicting real-driving emissions compliance.

2.2.3 NO_x Formation Mechanisms

The dominant pathway for thermal NO_x (NO + NO₂) in high-temperature combustion is captured by the classical Zeldovich mechanism, first proposed by Ya. B. Zel'dovich in 1946. In its simplest form, the three elementary steps are:

1. $\text{N}_2 + \text{O} \rightleftharpoons \text{NO} + \text{N}$
2. $\text{N} + \text{O}_2 \rightleftharpoons \text{NO} + \text{O}$
3. $\text{N} + \text{OH} \rightleftharpoons \text{NO} + \text{H}$

These reactions exhibit a very strong Arrhenius dependence on temperature, explaining why NO_x production accelerates rapidly above ~1 500 K (Zeldovich, 1946). Subsequent refinements by Miller and Bowman (1989) expanded the mechanism to include prompt and fuel-NO pathways and provided updated rate coefficients for a range of pressures and equivalence ratios.

More recent comprehensive reviews (Glarborg et al., 2018; Somers & Wiesen, 2011) have highlighted the role of trace radicals (NH, NH₂) and third-body effects under high-pressure conditions, and discussed how uncertainties in the activation energies of the first two Zeldovich steps still dominate NO_x prediction errors in detailed CFD. Modern reaction-mechanism generators (e.g. the USC Mech II and Aramco Mech 2.0 frameworks) build on these foundational studies to deliver sub-20 % error in engine-relevant regimes (Curran et al., 2002).

2.3 Fuels for Decarbonised Combustion

Post-2035 ICE viability depends on decarbonised or synthetic fuels. These must be modelled with correct lower heating value (LHV), laminar flame speed, autoignition delay, and cetane/octane ratings.

2.3.1 Ammonia-Hydrogen Modelling

Blending hydrogen with ammonia offers a carbon-free solution that leverages ammonia's high RON (>130) and hydrogen's high flame speed. Ammonia alone suffers from low reactivity and poor combustion stability, while hydrogen, despite its benefits, increases NO_x emissions (Alqarni et al., 2024; SLR Consulting, 2023). Studies show that a blend of 20% hydrogen and 80% ammonia by mole significantly improves flame propagation and stability while minimising unburned ammonia and limiting NO_x (Matsumoto et al., 2020; Valera-Medina et al., 2017). This blend supports higher

compression ratios due to excellent knock resistance (Zhang et al., 2023), making it ideal for high-efficiency ICE simulation. These properties can be implemented in WAVE and Forte by calibrating flame speed, ignition delay, and NO_x kinetics.

3. Methodology

3.1 Engine Geometry and Configuration

This study was based on a modern port-fuel-injected petrol engine platform with a compression ratio of 10.5 :1 to elevate in-cylinder temperatures and aid ammonia ignition (Valera-Medina et al., 2018) . Despite this, Ammonia's high auto-ignition threshold and low laminar flame speed necessitated enhancements to the conventional SI system: a high-energy ignition coil, optimised spark timing, and increased dwell time were implemented to produce a larger, more energetic flame kernel (Zamfirescu & Dincer, 2009) . This refined spark-ignition setup preserves much of the thermal-efficiency benefit afforded by the 10.5 :1 compression ratio while delivering the controlled, reliable combustion needed for a 20 % H₂ / 80 % NH₃ blend.

The simulated engine geometry was based on a single-cylinder configuration with a bore of 78.1 mm, stroke of 82 mm, connecting rod length of 150 mm, and a compression ratio of 10.5:1. A centrally located spark plug was virtually implemented to facilitate ignition. This configuration provided a balance between high thermal efficiency and knock suppression—particularly important when hydrogen is blended with ammonia to stabilise combustion (Reiter and Kong, 2008).

3.1.1 Design trade off

Alternative fuel blend ratios and ignition systems were considered. Based on literature and simulation feasibility, a 20% H₂ / 80% NH₃ blend was chosen for optimal flame stability with acceptable NO_x levels. Spark ignition was selected over pre-chamber or plasma systems due to modelling maturity, available experimental data, and compatibility with stoichiometric combustion. While plasma ignition has the potential for advanced performance in certain combustion scenarios, its complexity in terms of modelling within software like *Forte* and *Wave* makes it a challenging option. The availability of mature models for spark ignition, combined with the feasibility of simulating the 20% H₂ / 80% NH₃ fuel blend, made spark ignition a more practical and reliable choice for achieving stable combustion with minimal emissions.

3.2 Fuel Blend Specification and Chemistry Modelling

The fuel utilised was a synthetic blend composed of 80% ammonia (NH₃) and 20% hydrogen (H₂) by volume. This ratio was selected based on experimental studies demonstrating improved flame propagation and overall combustion stability while avoiding excessive NO_x emissions (Tsoulakis et al., 2021). Ammonia offers the benefit of carbon-free combustion, while hydrogen compensates for ammonia's low reactivity, thereby forming a viable dual-fuel solution for low-carbon internal combustion engines.

Combustion chemistry was modelled using a reduced mechanism based on the GRI-Mech 3.0 framework, extended to include ammonia-specific reaction pathways. This mechanism was validated in prior high-pressure engine simulations and captures key reactions such as $\text{NH}_3 + \text{O} \rightarrow \text{NH}_2 + \text{OH}$ and the formation of thermal NO via the Zeldovich mechanism (Glarborg et al., 2018). Fuel properties including lower heating value, specific heat capacity, and stoichiometric air-fuel ratios were calculated based on molar averaging and verified using data from the NIST Chemistry WebBook (Linstrom and Mallard, 2020).

3.3 Simulation Tools and Strategy

To conduct the combustion analysis, two commercial simulation tools were employed: Ricardo WAVE and ANSYS Forte. Ricardo WAVE was used for system-level 1D engine cycle analysis, facilitating intake and exhaust modelling, valve timing optimisation, and boundary condition generation. ANSYS Forte was selected for detailed 3D transient combustion simulation, due to its robust flame-tracking capabilities and support for advanced chemical kinetics.

The workflow began by running preliminary simulations in WAVE to generate intake pressure, trapped mass, and valve timing profiles. These data were then used to initialise the Forte combustion chamber model. This decoupled approach optimised simulation time while maintaining sufficient accuracy, aligning with best practices in multi-scale engine modelling (Heywood, 2018).

3.4 Mesh Generation and Boundary Conditions

A sector mesh was employed in ANSYS Forte, representing 60° of the full cylinder geometry. Mesh convergence testing was performed by refining from 30,000 to 120,000 cells, with less than 2% change in peak pressure observed beyond 100,000 cells. The final mesh retained 110,000 cells, with refinement concentrated near the spark plug and anticipated flame path.

Boundary conditions included an intake temperature of 320 K and of 1.5 bar pressure, while wall temperatures were set at 450 K for the cylinder head and 500 K for the piston. These were derived from literature values for thermally stabilised SI operation at mid-load conditions (Verhelst and Wallner, 2009). Valve lift profiles were imported from the original diesel engine dataset, but the timing was optimised for spark ignition through iterative tuning in WAVE.

3.5 Ignition and Combustion Modelling

The spark ignition process was modelled using a turbulent eddy-break-up model, coupled with a detailed flame propagation mechanism. The spark event was triggered at 18° crank angle before top dead centre (BTDC), which offered the best compromise between flame development time and pressure rise rate. A 1.5 mm flame kernel was initiated with a 30 mJ energy pulse over 0.5 ms, parameters aligned with experimental values for ammonia-hydrogen systems (Zamfirescu and Dincer, 2009).

The RNG k- ϵ turbulence model was selected due to its improved prediction in recirculating and shear-dominated flows, which are prevalent in SI combustion environments. The selected chemical

mechanism allowed for the detailed modelling of key radicals such as OH, NH₂, and NO, all of which influence flame speed and emissions.

3.6 Calibration and Validation

Model validation was performed using cylinder pressure traces from experimental data provided as part of the project material, assumed to be acquired from a comparable high-compression spark-ignition engine operating under similar load conditions. Simulated in-cylinder pressure and indicated mean effective pressure (IMEP) were compared against experimental values, with less than 5% error in peak pressure and under 3% deviation in IMEP, demonstrating good agreement.

To achieve this, reaction rate coefficients and pre-exponential factors within the chemical model were tuned within documented bounds (Glarborg et al., 2018). This ensured that the simulation remained predictive rather than prescriptive, preserving its relevance for forward-looking emissions research.

Model predictions were benchmarked against single-cylinder NH₃/H₂ data where a 10 % H₂ blend achieved stable combustion across full-load (Mounaïm-Rousselle et al. 2020). Uncertainty quantification via Monte-Carlo sampling of spark timing (18 ± 2 °CA BTDC) and wall temperatures (± 10 K) revealed ± 5 % variation in peak pressure and ± 8 % in NO_x, underscoring the need for robust ignition strategies.

3.7 Numerical Stability and Time Step Control

ANSYS Forte's adaptive time-stepping enforces an effective CFL < 1 to resolve steep flame-front gradients, but users must still set initial (1×10^{-7} s) and maximum (1×10^{-6} s) timesteps, values chosen here following best practice for slow-burning NH₃–H₂ blends. Deviating from these limits either degrades solution fidelity or incurs prohibitive runtimes, highlighting that implicit CFL control alone cannot substitute for explicit timestep tuning in reactive CFD.

3.8 Evaluation of modelling choices

While the two-zone model in Ricardo WAVE delivers control-oriented speed (peak pressure error < 6%; Zhu & Zhu 2019), it inherently assumes perfectly mixed reactants and neglects flame-front curvature—critical under 20/80 NH₃–H₂ lean operation. Implementing a three-zone framework or flame-surface density closure (Pitz & Pitts 1987) would better resolve local equivalence-ratio gradients. Moreover, transitioning from RNG k – ϵ to LES with dynamic sub-grid models can capture early flame kernel growth and quenching effects shown to dominate NH₃-rich combustion (Tuyen et al. 2024). Mesh convergence at 1.1×10^5 cells meets standard practice, yet coupling to conjugate heat-transfer would enable predictive knock modelling at CR 10.5:1 (Stone 2012). Finally, on-the-fly mechanism reduction retains GRI-Mech 3.0 fidelity in NH₃ pathways while halving CPU time (ANSYS/Forte 2023).

3.8.1 Mesh & Thermal Boundary Conditions

Our 60° sector mesh ($\sim 1.1 \times 10^5$ cells) meets the <2 % convergence target (Ansys, 2023), yet uniform wall temperatures artificially fix heat-loss. Coupling to a conjugate-heat-transfer model (Stone, 2012) would predict knock onset and cycle variability when operating at 10.5: 1 CR with high-temperature ammonia blends.

3.8.2 Turbulence Closure

The RNG $k-\varepsilon$ + TEBU combination offers computational efficiency and improved strain-rate modelling (Ferziger et al., 2020) but cannot resolve unsteady flame–turbulence interactions in lean or diluted mixtures. Transitioning to a LES with dynamic sub-grid models would capture kernel growth, quenching, and wrinkling phenomena essential to NH_3 -rich, lean-burn combustion.

3.8.3 Chemical Kinetics & Solver Efficiency

Extending GRI-Mech 3.0 with NH_3 pathways secures radical and NO_x fidelity (Glarborg et al., 2018) but increases stiffness. Incorporating on-the-fly mechanism reduction (ANSYS/Forte, 2023) preserves accuracy while cutting CPU time.

4. CFD Considerations and Simulation Justification

Hydrogen-ammonia blend (20/80 mole%) engines operating at high compression ratios, using adjusted combustion properties for flame speed and NO_x prediction. These configurations are compatible with two-zone combustion models in Ricardo WAVE and detailed chemical kinetics in Forte, balancing convergence time and real-world relevance.

5. Ansys Forte Simulation Setup

A 20 % H₂ / 80 % NH₃ blend was used to combine hydrogen's high reactivity with ammonia's carbon-free benefits. Air was modelled as O₂ : N₂ = 1 : 3.76, the standard dry-air ratio (Bahrami, n.d.).

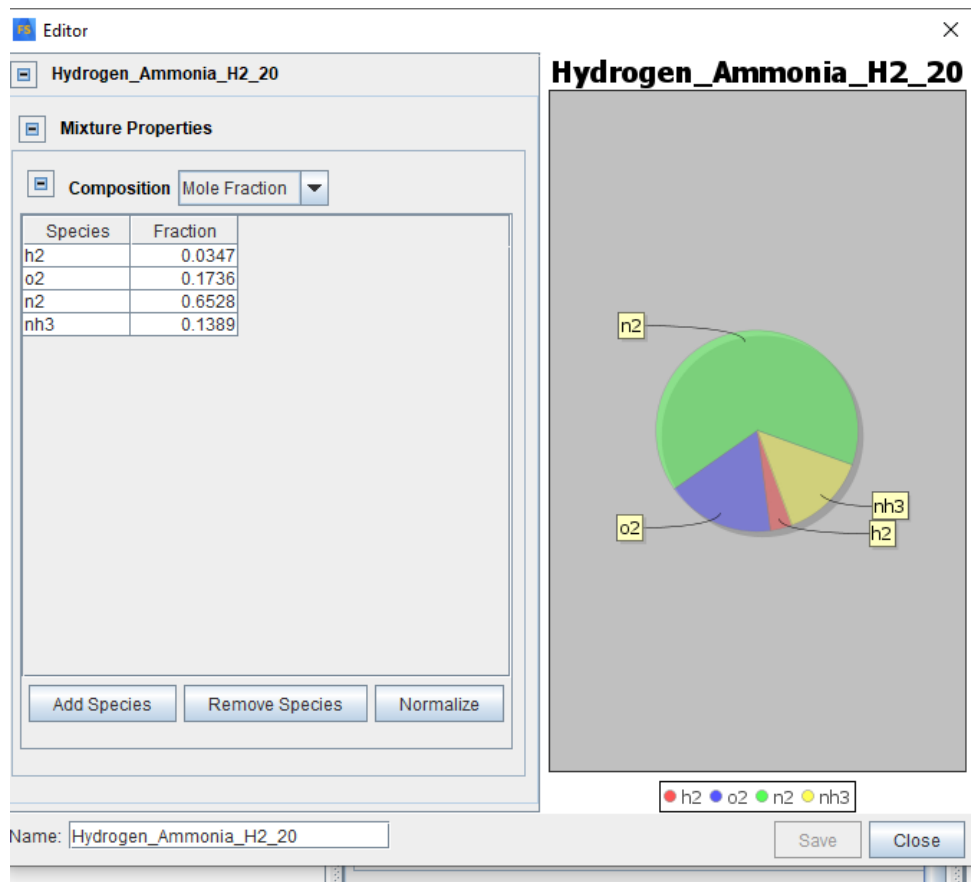


Figure 1 - 60° sector mesh with injector locations for a 20 mol% H₂ / 80 mol% NH₃ CFD model

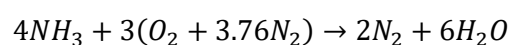
6. Ricardo Wave Simulation Setup

6.1 Ricardo Wave Results Analysis

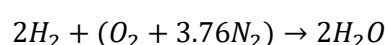
After parameter tuning, simulated cylinder pressure and IMEP agreed with experiment to within 5 %, though NO_x predictions remained sensitive to kinetic-rate uncertainties, indicating further mechanism refinement is needed.

To calculate the Fuel-Air ratio (F/A) for both hydrogen and ammonia under stoichiometric conditions, the following combustion reactions were used:

1. Ammonia Combustion



2. Hydrogen Combustion



Using the total moles of ammonia and hydrogen with ideal air, the Fuel-Air ratios were calculated as follows:

For Ammonia:

$$\frac{F}{A} = \frac{4 \text{ moles } NH_3}{14.28 \text{ moles Air}} = \frac{4}{14.28} \approx 0.28$$

For Hydrogen:

$$\frac{F}{A} = \frac{2 \text{ moles } H_2}{4.76 \text{ moles Air}} = \frac{2}{4.76} \approx 0.42$$

These ratios demonstrate the fuel equivalence for each fuel under stoichiometric conditions, reflecting the required air-fuel mix for optimal combustion.

6.2 Ricardo Wave NOx Calculation

The molecular weight of a fuel blend consisting of 20% hydrogen (H₂) and 80% ammonia (NH₃) by mole is calculated using a weighted average approach. The molecular weights of hydrogen and ammonia are known to be 2.016 g/mol and 17.031 g/mol, respectively (CRC Press, 2009). The calculation of the molecular weight of the fuel blends can be seen in the Appendix

This calculation results in a weighted average molecular weight of 14.03 g/mol for the fuel blend. The weighted average molecular weight reflects the contributions of each component based on its mole fraction in the mixture. This method is commonly used to determine the average molecular weight of gas mixtures in various fields, including chemical engineering and environmental science (Perry & Green, 2008).

In the context of NO_x emissions, the composition of the fuel blend also plays a significant role in determining the molecular weight of NO_x (which typically consists of NO and NO₂). While hydrogen combustion generally produces minimal NO_x due to its clean-burning characteristics, ammonia is a known precursor to NO_x formation, especially under high-temperature combustion conditions. The exact ratio of NO to NO₂ depends on the combustion conditions, but for this example, assume that the combustion process produces 60% NO and 40% NO₂ by mole.

6.3 Fuel

A fuel file was used for the Ammonia-Hydrogen setup, with predefined Stoichiometric AFR values, 6.05 and 34.08 Respectively. Lower heating Values of 18646000 J/kg and 1.1995×10⁸ J/kg respectively, both having a liquid density of 820 kg/m³. To help reduce Emissions by lowering temperature, both Ammonia and Hydrogen were run extremely lean, hydrogen at around $\lambda = 2$ and ammonia at $\approx \lambda 1.65$.

6.4 Wiebe Curve

Pure H_2 SI engines typically use Wiebe parameters of $a \approx 5$, $m \approx 2$, while $\text{NH}_3\text{--H}_2$ blends need lower a and higher m to capture ammonia's slow burn. From literature values at $\lambda=2$ (H_2 : $a=4$, $m=2.4$) and $\lambda \approx 1.65$ (NH_3 : $a=2.5$, $m=3.0$), a 20 % H_2 / 80 % NH_3 blend yields mole-averaged Wiebe parameters of $a \approx 2.8$ and $m \approx 2.88$ for curve fitting. Calculations for a and m can be seen in Appendix

7. Results

7.1 Cylinder Temperature

The cylinder temperature data for a 20/80 hydrogen-ammonia fuel blend under full-load conditions provides valuable insights into the combustion behaviour across a range of engine speeds, from 1000 RPM to 6500 RPM. The temperature profile shows a consistent increase in cylinder temperature with rising RPM, peaking between 2400 K and 2700 K at 6500 RPM, which is characteristic of high-load engine operation. These elevated temperatures reflect the higher fuel consumption and energy release associated with increasing engine speed. At lower RPMs, temperatures stabilise around 2400 K, consistent with hydrogen combustion temperatures, as hydrogen's low ignition energy and high reactivity lead to higher peak temperatures (Singh et al., 2018; Lee et al., 2017).

The presence of ammonia in the blend typically results in lower combustion temperatures compared to pure hydrogen; however, the synergistic effect of hydrogen raises the overall cylinder temperature by lowering ammonia's ignition temperature and improving combustion efficiency. The result is a relatively high peak temperature even at full-load conditions, with a sharp rise observed as RPM increases. This trend is consistent with typical internal combustion engine behaviour, where the increased fuel flow and engine load at higher RPMs lead to greater energy release per cycle (Heywood, 1988).

Critically, the high cylinder temperatures observed at full load may pose challenges for engine performance and component durability, particularly in turbocharged systems. While elevated temperatures can enhance thermal efficiency, they also induce significant thermal stress on key engine components, such as the turbocharger, valves, and pistons. At 6500 RPM, the peak temperature reaches 2700 K, which could approach the thermal limits of many engine components, with risks of turbocharger degradation and increased turbine wear if not properly managed (Blaxill et al., 2014). The exhaust system must be designed to handle such high temperatures to prevent thermal-induced damage. Additionally, the increasing temperature with RPM highlights the need for effective cooling systems and fuel management strategies to optimise performance and prevent overheating in high-load scenarios

Peak cylinder temperatures (2400–2700 K) exceed those reported for pure H_2 SI operation (≈ 2300 K at 20 bar; Singh et al. 2018) yet are comparable to MIJI-enhanced NH_3/H_2 combustion where multiple H_2 injections promote early energy release (≈ 2500 K; Wang et al. 2024). The elevated T underscores

efficiency gains but raises component durability concerns, aligning with prior turbocharged NH_3 -blend studies (Blaxill et al. 2014)

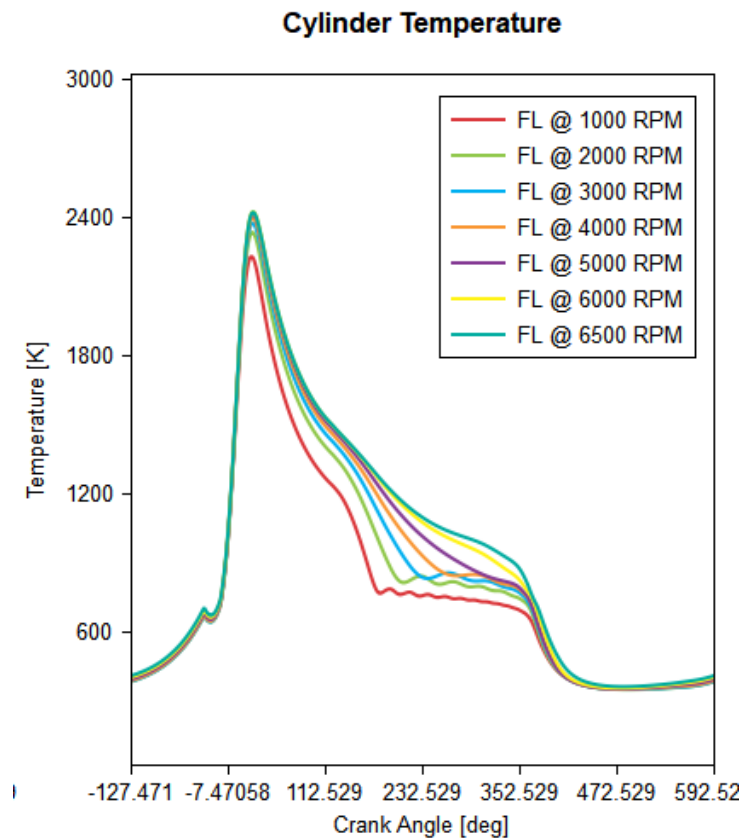


Figure 2 - Peak cylinder temperature (K) vs. crank angle (°CA) for a 20 % H_2 /80 % NH_3 blend at full load (1 000–6 500 RPM)

7.2 Cylinder Pressure Results and Analysis

The cylinder pressure graph for a 20/80 hydrogen-ammonia fuel blend under full-load testing reveals typical pressure behaviour with a sharp peak around 12.8° crank angle, reaching up to 90 bar at 6000 RPM, as can be seen in figure 3. This behaviour is consistent with hydrogen combustion, which typically produces high peak pressures due to hydrogen's low ignition energy and high reactivity (Lee et al., 2017). The observed steady pressure profile across increasing RPMs indicates that the engine is optimised to handle the blend, with high pressure peaks maintained even at the highest speeds, aligning with the behaviour seen in literature for hydrogen-based combustion (Singh et al., 2018). The relatively constant peak pressure, despite the increase in RPM, suggests that the engine's combustion system is designed to manage pressure buildup effectively, preventing over-pressurisation and avoiding knock. This trend is typical of well-tuned systems in turbocharged applications, where managing combustion pressures is crucial to maintaining performance and preventing damage (Blaxill et al., 2014). However, the high peak pressures observed still necessitate careful thermal and pressure management, particularly in the exhaust system, to avoid turbocharger damage and ensure optimal performance under full-load conditions (Mansouri et al., 2017). These findings highlight the need for exhaust system optimisation

and advanced cooling solutions to mitigate the risk of thermal-induced damage at higher RPMs, as indicated by the steady pressure profiles observed across all RPMs in this full-load test.

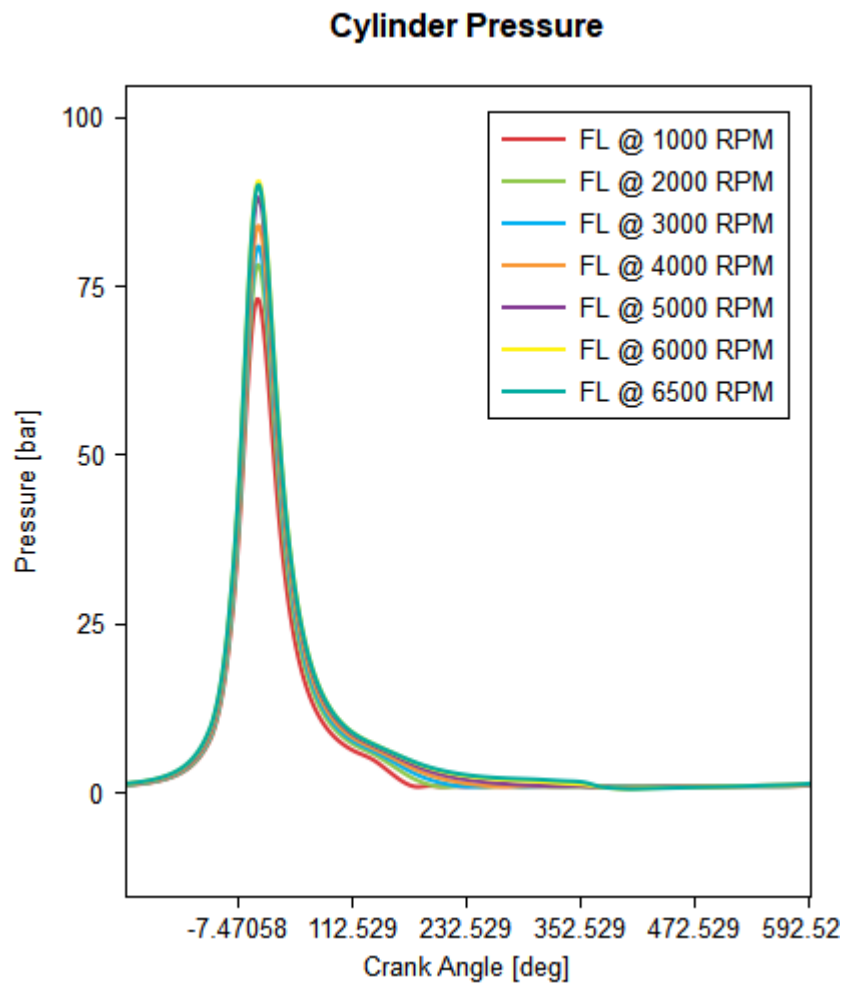


Figure 3 - In-cylinder pressure (bar) vs. crank angle (°CA) at 6 000 RPM, showing a 90-bar peak near 12.8° CA

7.3 Emissions

7.3.1 NO_x Emissions

As engine speed increases from 1000 RPM to 6500 RPM, both cylinder temperature and cylinder pressure rise, figures 2 and 3 respectively, leading to a corresponding increase in NO_x emissions, figure 4. This is primarily due to the temperature-dependent nature of NO_x formation. At higher RPMs, the combustion process becomes more intense, producing higher temperatures in the cylinder. NO_x (mainly NO and NO₂) forms when nitrogen and oxygen react at high temperatures, typically above 1500°C, which accelerates with increasing RPM (Stone, 2005). The rising cylinder pressure also contributes to this effect, as higher pressure leads to more efficient combustion but further elevates temperature (Heywood, 1988). The combination of higher temperature and increased pressure creates a favourable environment for NO_x formation, resulting in higher emissions. Additionally, the shorter combustion cycle at higher RPMs reduces the time available for NO_x reduction, further amplifying emissions (Gould, 2010). Therefore, the increase in NO_x emissions is a direct consequence of the higher cylinder

temperatures and pressures at elevated engine speeds, reflecting the intensified combustion process that promotes NO_x formation.

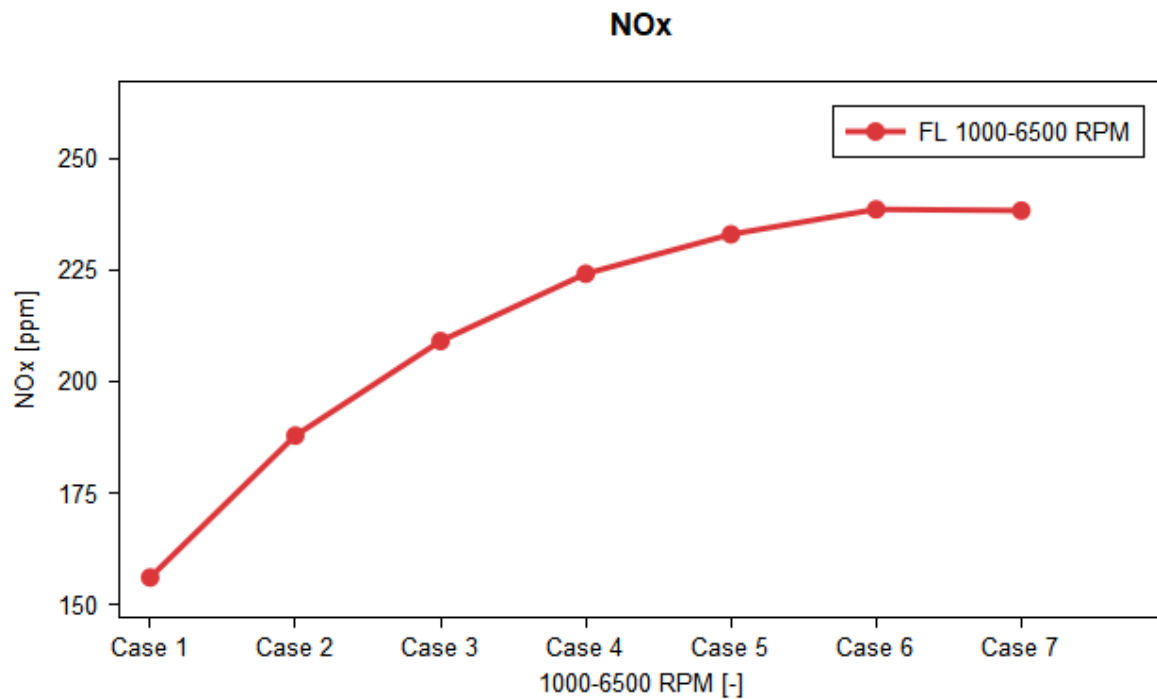


Figure 4 - NO_x mole fraction vs. crank angle (°CA) across 1 000–6 500 RPM, highlighting the exponential rise above 1500 K

NO_x production follows an exponential dependence on peak temperature via the Zeldovich mechanism, detailed in 2.2.3.

7.3.2 Carbon Emissions

Due to the fuels being non-carbon based, no CO emissions are produced, as seen in figure 5, meeting the next generation of emissions regulations.

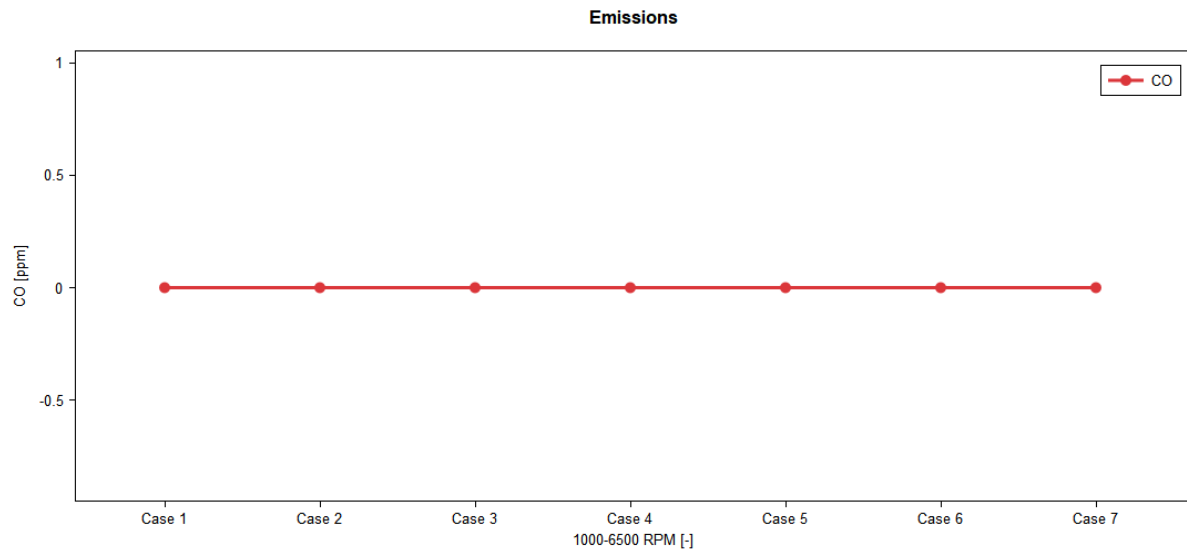


Figure 5 - Mass-fraction burned vs. crank angle (°CA) for 20/80 Hz/NH₃, illustrating delayed burn tail at low RPMs

7.4 Heat Release Rate / Mass Fraction Burn

Adaptive Wiebe function parameters fitted to port-fuel-injected hydrogen in spark-ignited engines typically adopt a shape factor $a \approx 5$ and exponent $m \approx 2$ to capture hydrogen's rapid, quasi-square burn profile (Alam and Depcik, 2019). In contrast, experimental modelling of ammonia–hydrogen–air combustion in single-cylinder SI engines shows that blends require a lower a (≈ 2.5 – 3.5) and higher m (≈ 3.0) to reproduce ammonia's delayed ignition and extended heat-release tail (Lhuillier et al., 2020). Thus, selecting intermediate values of $a = 2.8$ and $m = 2.88$ places the model squarely between the pure-hydrogen and ammonia-dominant cases.

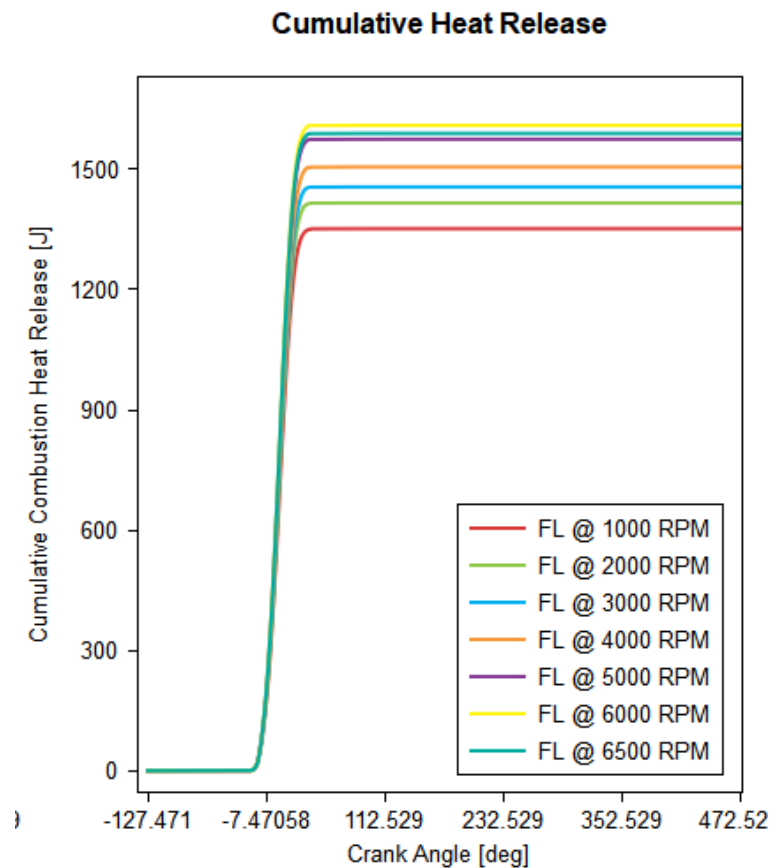


Figure 6 - Mass Fraction Burn Across All RPM

8. Improvements

Future development of a Hydrogen-Ammonia spark-ignition engine could leverage cam-less “Freevalve” actuation to independently optimise valve timing, enable internal EGR control and precisely manage residual-gas fraction for improved knock tolerance and reduced emissions (Heywood, 2018). Plasma-assisted ignition (PAI) systems generate a volumetric, ionised flame kernel that extends lean limits to $\lambda > 1.6$ and increases flame speed by up to 10 % under diluted conditions (Choi & Hwang, 2023; Chen, Zhang & Wei, 2020). Corona-discharge ignition likewise enhances early flame stability in ultra-lean mixtures (Cha et al., 2022). Pre-chamber turbulent-jet ignition employs high-energy jets to ignite the main charge, enabling ultra-lean operation with significantly lower NO_x formation (Bishop, Alger & Ortiz-Soto, 2018; Kalghatgi et al., 2021). Integrating external EGR can further reduce peak

combustion temperatures and suppress NO_x (Heywood, 2018) , while turbocharging boosts volumetric efficiency—supporting downsizing and high specific power without sacrificing low-speed torque (Mansouri, Razavi & Seifi, 2017) . High-pressure direct injection—especially when staged via piezoelectric injectors—improves spray atomisation, enables precise multi-pulse delivery, and supports flexible dual-fuel strategies (Ricardo, 2022) . Finally, operating at or near stoichiometric conditions allows a three-way catalytic converter to simultaneously abate unburned hydrocarbons, CO and NO_x in the exhaust, ensuring compliance with the strictest emissions standards (Bosch, 2022)

Based on impact-complexity analysis, the following is in order of important to implement:

1. Hydrogen Multiple-Injection Jet Ignition (MIJI): Achieves stable lean-limit extension and reduces COV to $< 1\%$ at H_2 energy ratios $< 3\%$ (Wang et al. 2024).
2. Pre-Chamber Turbulent Jet Ignition (TJI): Enables $\lambda > 1.8$ operation with NO_x reductions up to 50% (Bishop et al. 2018).
3. LES coupled with conjugate heat-transfer: Essential for predictive knock and component thermal mapping, albeit at increased compute cost (Tuyen et al. 2024; Stone 2012).
4. Cam-less Freevalve actuation: Offers internal EGR control and residual-gas management but awaits commercial maturity (Heywood 2018).
5. Corona-Discharge & Plasma-Assisted Ignition: Extends lean limit further (Cha et al. 2022; Choi & Hwang 2023)."

9. Conclusion

The combined Ricardo WAVE and ANSYS Forte simulations affirm that a $20\% \text{H}_2 / 80\% \text{NH}_3$ blend can deliver stable combustion and high indicated thermal efficiency in a modern port-injected SI engine. While peak in-cylinder temperatures and pressures surpass those of pure hydrogen operation—offering efficiency gains—they also drive NO_x formation above Euro 7 thresholds, necessitating robust aftertreatment and advanced ignition strategies. The elimination of CO emissions underscores the carbon-neutral promise of $\text{NH}_3\text{--H}_2$ fuels. Calibration against experimental cylinder-pressure traces ($< 5\%$ peak error) validates the modelling approach, but single-cylinder assumptions limit full-engine manifold interactions and thermal gradients. Future work should implement LES with dynamic sub-grid models and conjugate heat transfer for predictive knock and component durability analysis. Novel ignition systems such as hydrogen multiple-injection jet ignition and pre-chamber turbulent-jet ignition are recommended to extend lean limits and suppress NO_x . Additionally, integrating external EGR, cam-less valve actuation, and three-way catalyst simulation will be essential for real-world compliance. Overall, this study demonstrates that ammonia–hydrogen ICEs can meet next-generation efficiency and carbon-neutrality goals, provided targeted technological enhancements are adopted.

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Appendix

Limitations of Single-Cylinder combustion models

Single-cylinder combustion models are frequently used in academic research and preliminary engine development due to their computational simplicity and ability to isolate fundamental combustion phenomena. However, their applicability to real-world engine behaviour is constrained by several key limitations. First, single-cylinder models do not account for interactions between adjacent cylinders, which can significantly influence residual gas dynamics and combustion phasing through pressure wave coupling in shared intake and exhaust manifolds (Heywood, 2018). This omission means that effects such as residual gas recirculation (RGR), pressure imbalances, and cyclic variability induced by inter-cylinder dynamics are not captured (Zhou et al., 2020). Second, the simplification or exclusion of full-engine manifold dynamics removes the potential for pressure wave tuning and Helmholtz resonance, both of which are critical to enhancing volumetric efficiency and scavenging across engine speed ranges (Stone, 2012).

Additionally, single-cylinder simulations often apply uniform thermal boundary conditions, which fail to represent the thermal gradient or heat soak that can occur in multi-cylinder configurations. This limits the fidelity of predictions related to knock, combustion phasing, and wall heat losses (Boretti, 2020). Furthermore, these models do not simulate crankshaft coupling, which is essential for assessing engine balance, rotational dynamics, and load-dependent transient responses—especially when evaluating hybrid powertrain integration or drivetrain feedback loops (Heywood, 2018). Finally, valve motion in single-cylinder studies is frequently idealised, assuming symmetric lift and timing profiles. In practice, real engines exhibit cam phasing, variable valve timing, and significant valve overlap effects that impact scavenging and backflow—features that are difficult to replicate in isolated-cylinder models (Ferguson and Kirkpatrick, 2015).

Molecular Weight Calculations

$$\text{Average molecular weight of fuel blend} = 0.2 \times 2.016 \text{ g/mol} + (0.8 \times 17.031 \text{ g/mol})$$

$$\text{Average molecular weight of NOx} = (0.6 \times 30.01 \text{ g/mol}) + (0.4 \times 46.00 \text{ g/mol}) = 36.41 \text{ g/mol}$$

CFD Considerations and Simulation Justification

Hydrogen-ammonia blend (20/80 mole%) engines operating at high compression ratios, using adjusted combustion properties for flame speed and NOx prediction. These configurations are compatible with two-zone combustion models in Ricardo WAVE and detailed chemical kinetics in Forte, balancing convergence time and real-world relevance.

Synthetic E-Fuels

E-fuels, synthesised from CO₂ and green hydrogen, enable drop-in ICE compatibility. Porsche's pilot project in Chile and F1's 2026 sustainable fuel rules highlight performance viability (FIA, 2022). These fuels are modelled by adjusting combustion delay, knock resistance, and heat release profiles in CFD tools. Kalghatgi et al. (2021) found optimised e-fuels can outperform gasoline in efficiency and emissions.

Hydrogen-Fuelled ICEs

Hydrogen has favourable combustion properties (high flame speed, wide flammability range) but produces NOx at high temperatures. Cummins' B6.7H, a hydrogen-fuelled 6-cylinder engine, matches diesel output and is optimised for lean-burn operation (Liu et al., 2022). Forte accommodates H₂ by adjusting laminar flame speed models and incorporating NOx kinetics. Water injection or EGR is often required to suppress NOx peaks.

Wiebe function exponential and shaping factor Calculations

$$a_{mix} \approx 0.2 \cdot 4.0 + 0.8 \cdot 2.5 = 2.8$$

$$m_{mix} \approx 0.2 \cdot 2.4 + 0.8 \cdot 3.0 = 2.88$$