Hydrogen Integration for Low-Emission Locomotive Systems

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Abstract:

This study investigates hydrogen's potential as a clean energy source for locomotive propulsion through comparative combustion analysis and a review of international technological advancements. Using NASA CEA simulations, hydrogen (H_2) was analysed alongside naphthalene ($C_{10}H_8$) and ammonia (NH_3) across pressures ranging from 5 to 15 bar and temperatures between 298.15 K and 323.15 K. Also, Acetylene (C_2H_2) under same operating temperature but at a constant pressure of 5 bars. Results show that increasing hydrogen concentration reduces NO_x formation by up to 50%, with hydrogen - ammonia blends achieving around 30% emission reduction. These results align with recent global hydrogen locomotive initiatives such as Stadler FLIRT H_2 (U.S.), CPKC Unit 1200 (Canada), and Hyundai Rotem's LH_2 locomotive (South Korea). The findings confirm hydrogen's viability as a sustainable locomotive fuel and highlight future needs for higher - pressure combustion validation, improved fuel cell efficiency, and scalable liquid hydrogen infrastructure.

Introduction:

Globally, approximately 25% of fossil fuel - based CO_2 emissions originate from the transportation sector, which includes road, rail, air, and marine modes [1]. As countries worldwide move toward decarbonizing transportation, hydrogen has emerged as a promising candidate for achieving net - zero mobility. According to the International Energy Agency (IEA), in 2021, petroleum, natural gas, and biofuels accounted for about 90.4%, 4.5%, and 3.6% of global transportation energy consumption, respectively, while hydrogen contributed only around 0.00035% [2]. Despite its minimal share today, hydrogen possesses the versatility to be used across all transportation modes both directly as a combustion fuel and indirectly through fuel cells making it a critical enabler of sustainable transport systems.

The rail sector alone represents roughly 3% of total global transportation energy demand [3]. Transitioning this sector toward sustainable energy sources can significantly contribute to overall emission reduction goals. Hydrogen - powered locomotives offer an opportunity to establish a cleaner and more efficient rail network.

Currently, three main types of locomotive systems are in operation:

Diesel locomotives: These remain the most widely used worldwide due to established infrastructure and high - power output [4].

Diesel - electric locomotives: These systems integrate electric traction with diesel engines, allowing flexibility in regions where full electrification infrastructure is not available [4].

Hydrogen locomotives: The latest technological advancement in rail transport, developed to promote clean energy adoption and eliminate tailpipe emissions [5].

The transition from diesel - electric to hydrogen propulsion is driven primarily by emission control objectives. The United States Environmental Protection Agency (US EPA) provides regulatory standards for measuring emissions such as NO_x, CO, and CO_2, which are key indicators of combustion efficiency and environmental impact [5] [6].

This research presents a theoretical, data-driven combustion analysis comparing hydrogen, naphthalene ($C_{10}H_8$), ammonia (NH_3), acetylene (C_2H_2) as fuels under varying pressures and temperatures. Using NASA CEA simulations, NO_x, CO, and CO_2 emissions were modelled to evaluate hydrogen's potential as a cleaner alternative. Visualization of NO_x results provides a comparative understanding of emission behaviour and thermal characteristics. Additionally, the study explores hydrogen's use in various forms including gaseous and liquid to assess its practical benefits and associated challenges in real world locomotive applications.

Methodology:

A theoretical data - driven combustion analysis was performed using NASA CEA software. The fuels studied were gaseous hydrogen (H_2), naphthalene ($C_{10}H_8$), ammonia (NH_3), acetylene (C_2H_2). The simulation parameters included:

Type 1 for naphthalene ($C_{10}H_8$), ammonia (NH_3):

- **Pressure:** 5, 10, and 15 bar
- **Temperature:** 298.15 K and 323.15 K
- **Equivalence ratio (Phi):** 0.5 to 1.5
- **Fuel composition:** 50 - 100% hydrogen mixed with air (O_2)

The equivalence ratio range was chosen to capture lean, stoichiometric, and rich combustion zones. Combustion outputs from NASA CEA were exported and plotted in Microsoft Excel for visual comparison of NO_x mole fractions under different operating conditions.

All datasets were simulation - derived and not experimentally measured. The results thus provide theoretical insights into hydrogen's emission characteristics and serve as a basis for future validation studies.

Naphthalene - Hydrogen Mixtures (298.15 K)

Naphthalene, a representative aromatic hydrocarbon in diesel fuels, was blended with hydrogen to study emission effects. At 5 bar, 100% hydrogen + air combustion produced approximately 0.00004 mole fraction of NO_x, significantly lower than hydrocarbon - dominant blends. Increasing the pressure to 10 and 15 bar further reduced NO_x emissions to ~0.00002 mole fraction, confirming hydrogen's cleaner combustion tendency.

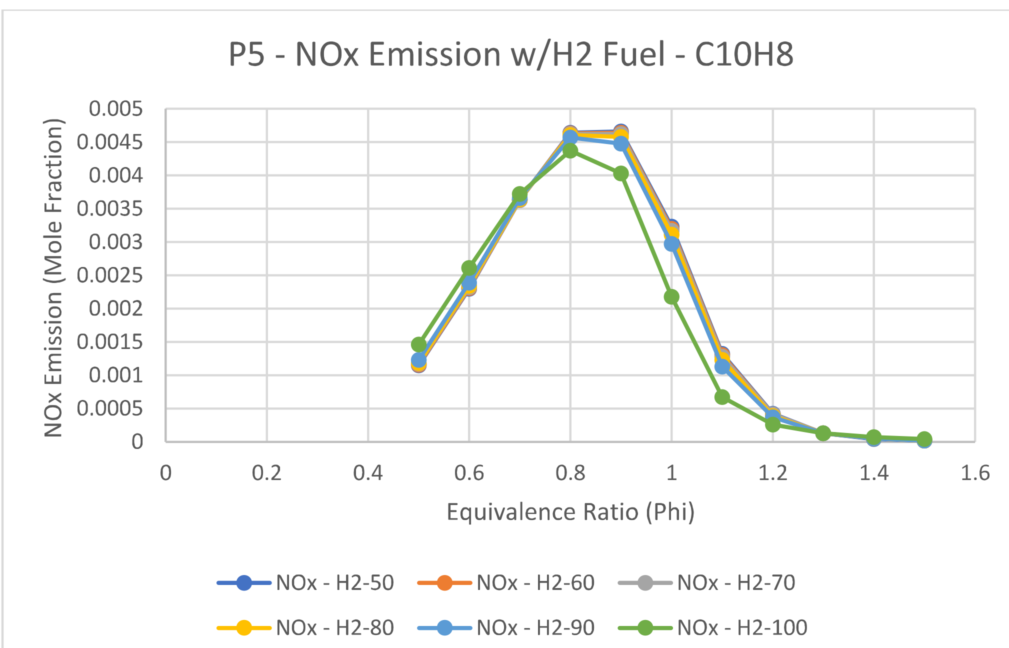

Fig 1: Plot of NO_x emissions for naphthalene - hydrogen blends at 5 bars

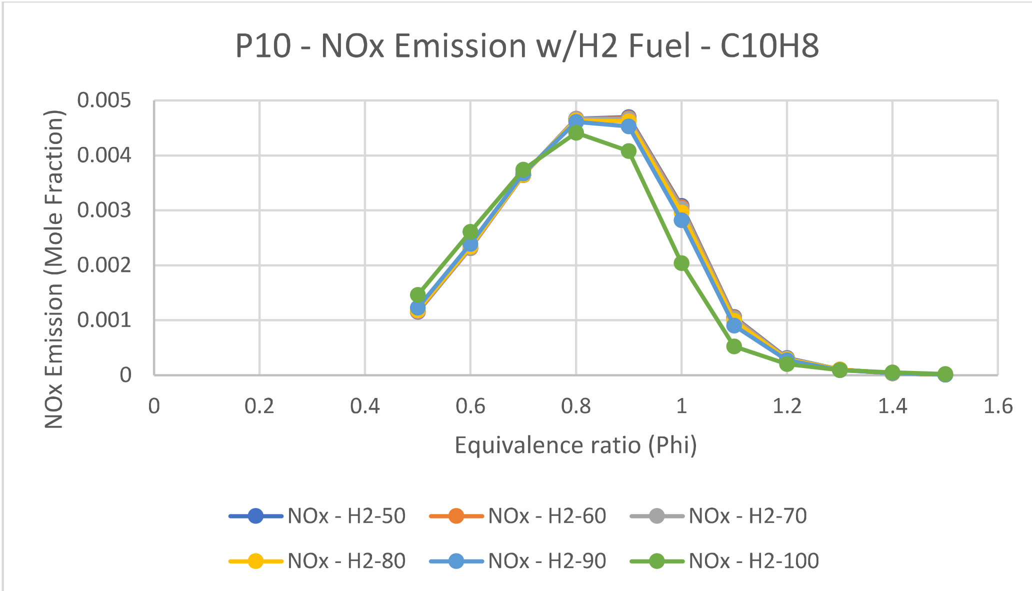

Fig 2: Plot of NO_x emissions for naphthalene - hydrogen blends at 10 bars

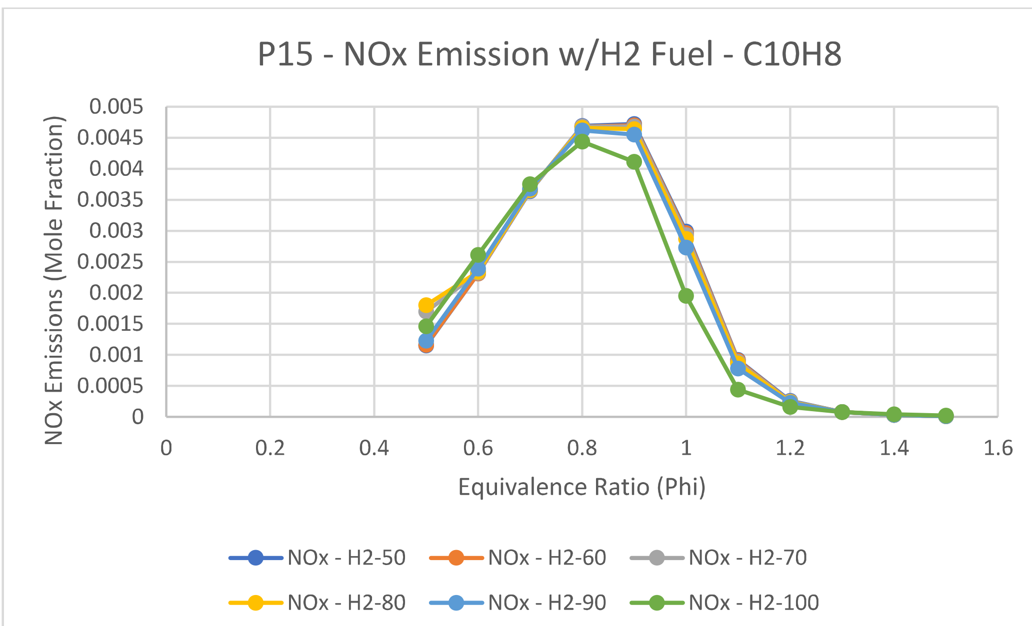

Fig 3: Plot of NO_x emissions for naphthalene - hydrogen blends at 15 bars

The simulation results indicate a strong inverse relationship between hydrogen concentration and NO_x formation across all operating pressures. As the hydrogen fraction increased from 50% to 100%, NO_x emissions dropped substantially from approximately 0.00008 to 0.00004 mole fraction at 5 bars, and further to about 0.00002 mole fraction at 10 and 15 bar. This reduction occurs because hydrogen combustion produces lower flame temperatures and lacks carbon-based intermediates that typically contribute to thermal NO_x formation. The results also show that elevated hydrogen content enhances combustion uniformity and stability, leading to cleaner exhaust characteristics. These findings highlight hydrogen's clear environmental advantage over hydrocarbon-based fuels and underline its potential to significantly reduce atmospheric pollutants and improve overall sustainability in locomotive propulsion systems.

Naphthalene - Hydrogen Mixtures (323.15 K)

At higher temperatures (323.15 K), similar emission patterns persisted. NO_x levels increased slightly with pressure due to enhanced reaction rates but remained far lower than conventional hydrocarbon fuels. The peak NO_x formation occurred near Phi = 0.8 - 0.9, consistent with stoichiometric combustion, followed by a sharp decline in richer mixtures (Phi > 1.0). This behaviour demonstrates that higher hydrogen fractions promote stable, low-emission combustion across varying pressures.

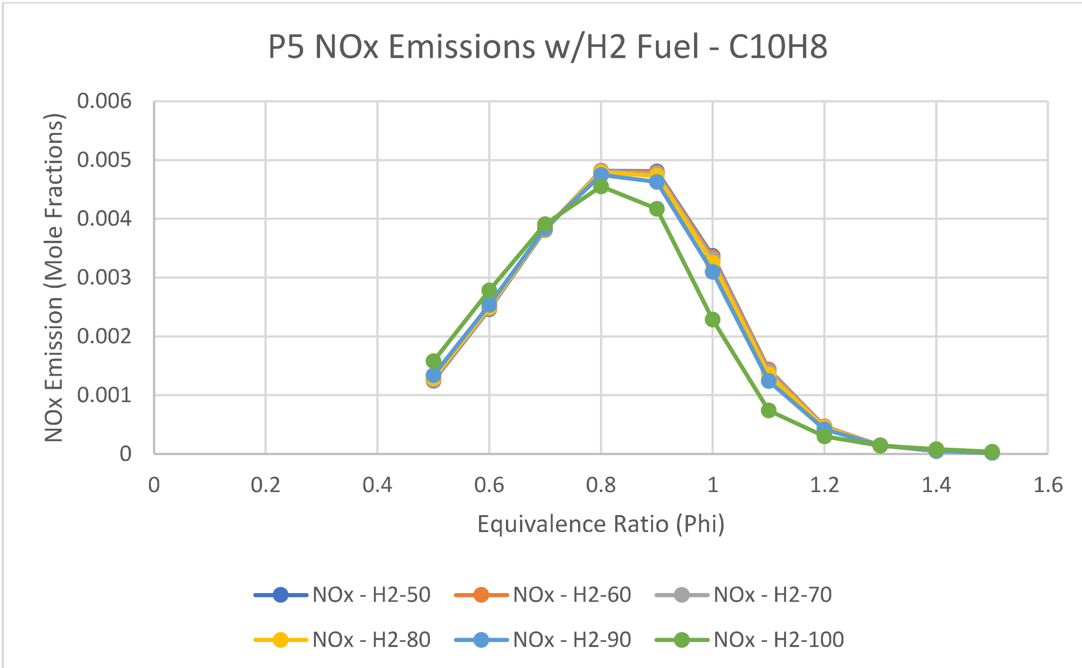

Fig 4: Plot of NO_x emissions for naphthalene - hydrogen blends at 5 bars

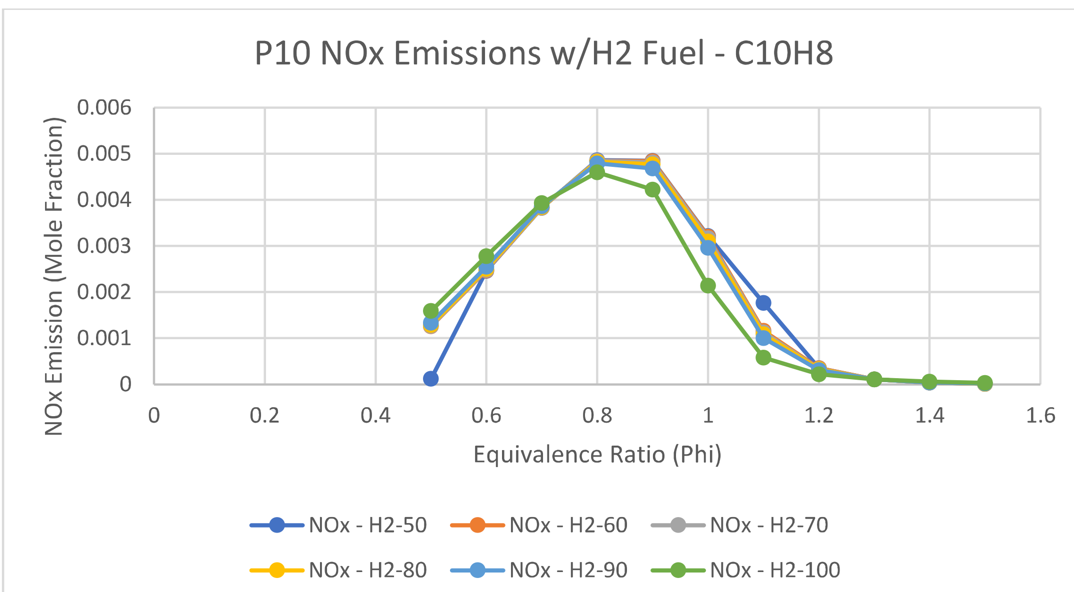

Fig 5: Plot of NO_x emissions for naphthalene - hydrogen blends at 10 bars

At an operating pressure of 5 bar, NO_x emissions increased steadily as the equivalence ratio (Phi) rose from lean to near-stoichiometric conditions, peaking between Phi = 0.8 and 0.9 with a maximum of approximately 0.005 mole fraction. Beyond this point (Phi > 1.0), NO_x levels declined sharply due to reduced oxygen availability and incomplete combustion. Increasing the hydrogen concentration from 50% to 100% significantly lowered the overall emission curve, demonstrating that higher H_2 blending promotes cleaner and more efficient combustion.

At 10 bars, a similar trend was observed, with the peak again occurring around Phi = 0.8 - 0.9. However, the absolute NO_x values were slightly higher because of the pressure induced rise in flame temperature and reaction rates that Favor thermal NO_x formation. Even so, the 100% hydrogen case consistently exhibited lower emissions, particularly at rich conditions (Phi > 1.0). The emission profiles at 10 bar were smoother and more compact, suggesting that higher substitution substantially reduces NO_x emissions across all operating pressures while maintaining stable combustion behaviour.

Ammonia - Hydrogen Mixtures (298.15 K)

Ammonia's low reactivity and high nitrogen content make it an excellent additive for hydrogen combustion moderation. Blending ammonia with hydrogen yielded a ~30% NO_x reduction as hydrogen content increased from 50% to 100%. At 100% hydrogen, NO_x emissions were as low as 0.00004 mole fraction. The synergy between hydrogen's reactivity and ammonia's flame temperature moderation effectively reduced NO_x formation under all pressures.

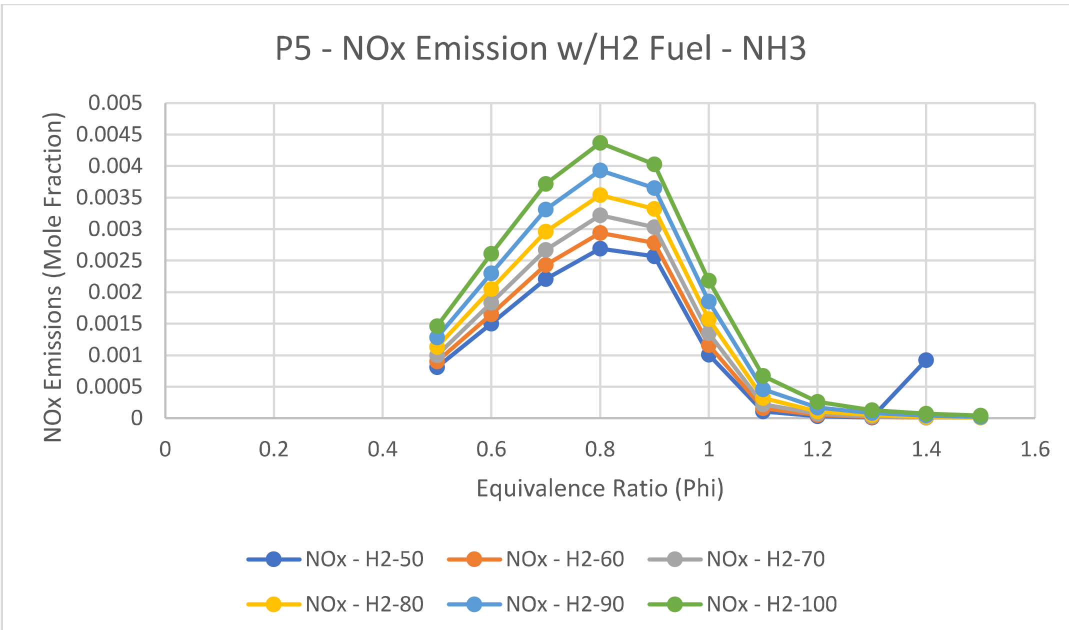

Fig 6: Plot of NO_x emissions for ammonia - hydrogen blends at 5 bars

Adding ammonia (NH_3) to hydrogen serves an important role in balancing fuel reactivity and improving overall combustion performance. Since ammonia alone exhibits relatively low reactivity, hydrogen enrichment enhances its ignition characteristics, making the mixture more proactive and stable. Additionally, ammonia contributes to lowering the adiabatic flame temperature, which is advantageous for reducing thermal NO_x formation during combustion.

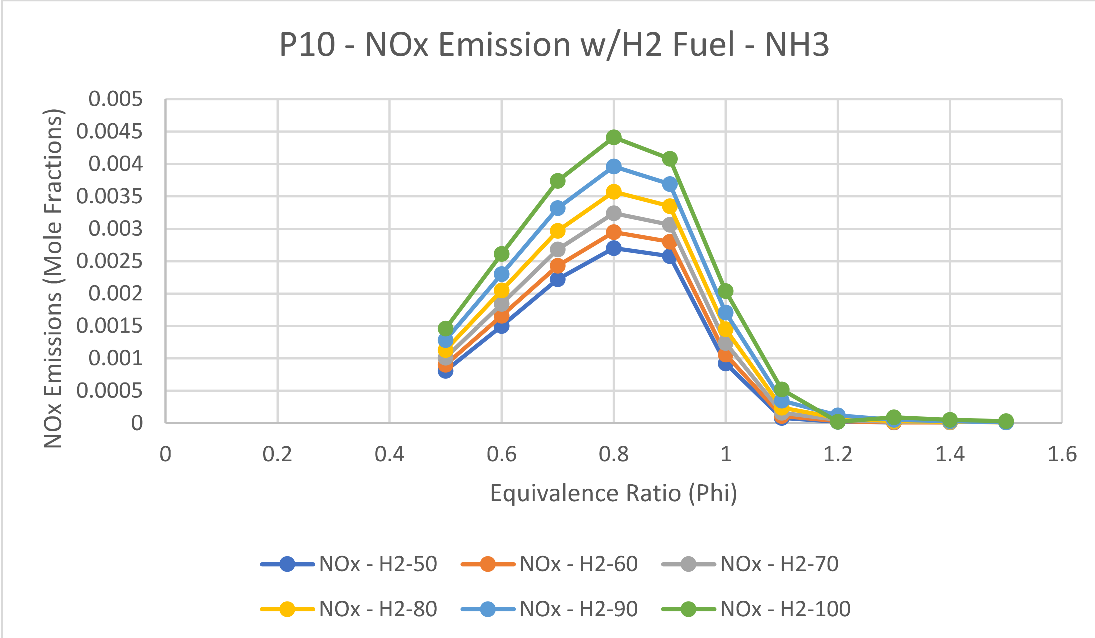

Fig 7: Plot of NO_x emissions for ammonia - hydrogen blends at 10 bars

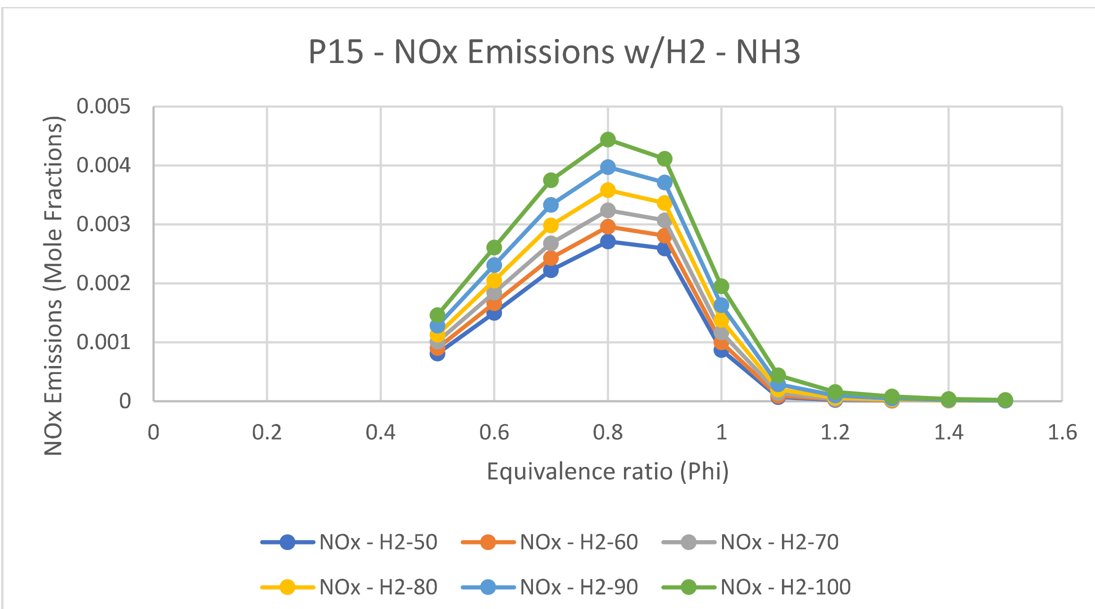

Fig 8: Plot of NO_x emissions for ammonia - hydrogen blends at 15 bars

At an operating pressure of 5 bar, NO_x emissions increase sharply as the equivalence ratio (Phi) approaches 0.9, corresponding to near-stoichiometric conditions where combustion is most intense. Beyond Phi = 1.0, NO_x levels decline due to reduced oxygen availability and incomplete oxidation. Increasing the hydrogen concentration from 50% to 100% consistently suppresses NO_x generation, with the lowest emission of approximately 0.00004 mole fraction observed for pure hydrogen combustion.

A similar pattern is evident in the 10 and 15 bar cases, where higher hydrogen fractions lead to a steady reduction in NO_x emissions across all equivalence ratios. On average, transitioning from a 50% to 100% hydrogen blend results in roughly a 30% decrease in NO_x formation, demonstrating hydrogen's critical role in promoting cleaner, low-temperature combustion within ammonia-based fuel systems.

Ammonia - Hydrogen Mixtures (323.15 K):

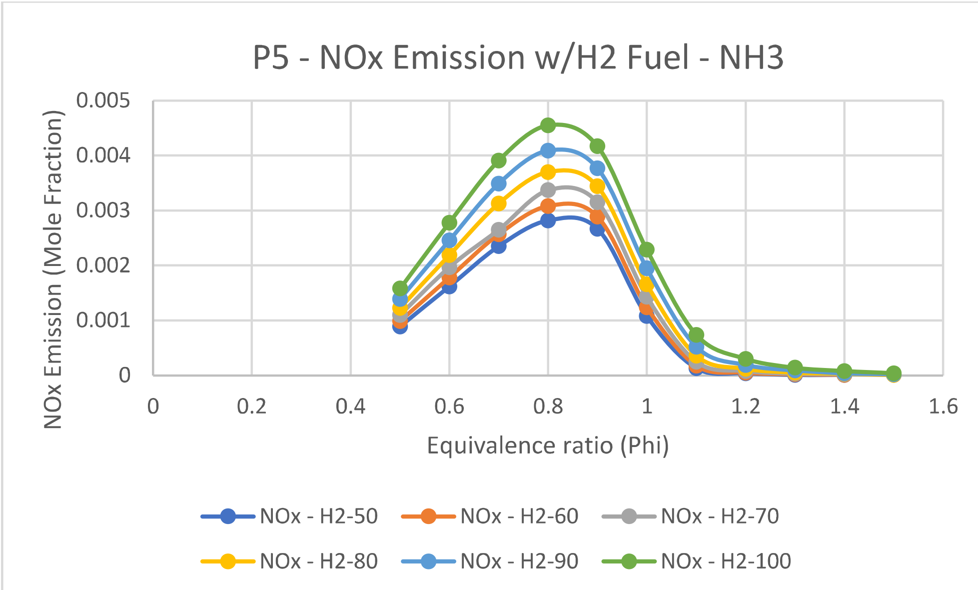

Fig 9: Plot of NO_x emissions for ammonia- hydrogen blends at 5 bars

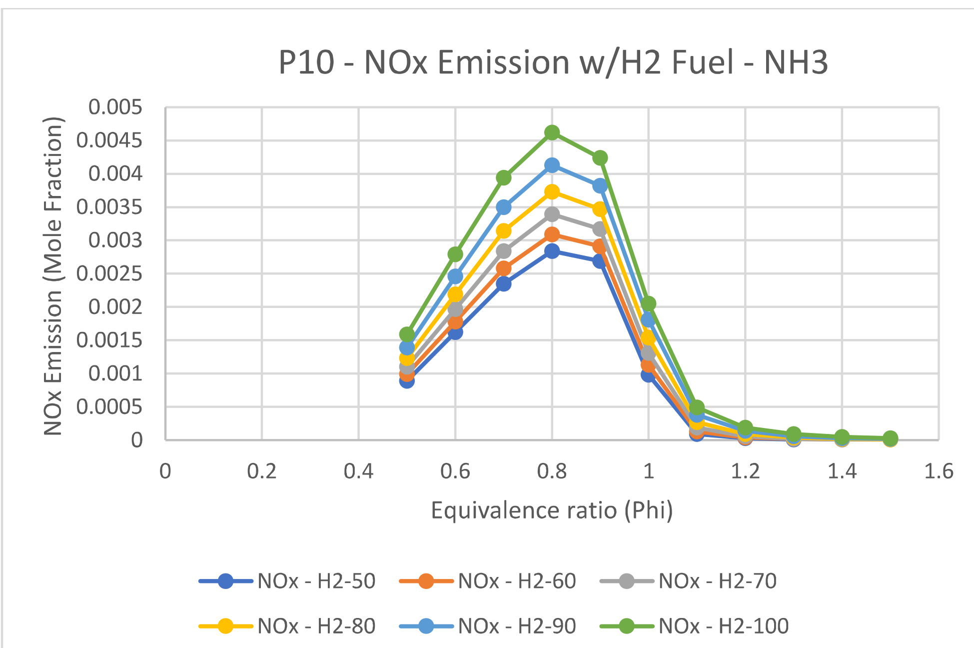

Fig 10: Plot of NO_x emissions for ammonia - hydrogen blends at 10 bars

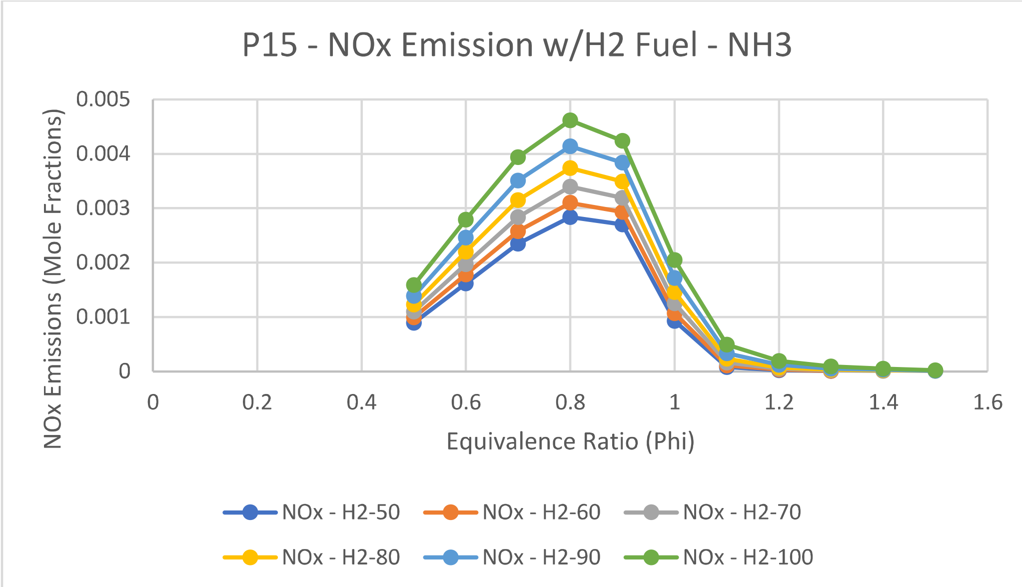

Fig 11: Plot of NO_x emissions for ammonia - hydrogen blends at 15 bars

A similar pattern is evident in the 10 and 15 bar cases, where higher hydrogen fractions lead to a steady reduction in NO_x emissions across all equivalence ratios. On average, transitioning from a 50% to 100% hydrogen blend results in roughly a 30% decrease in NO_x formation, demonstrating hydrogen's critical role in promoting cleaner, low-temperature combustion within ammonia - based fuel systems.

Type 2 for acetylene (C_2H_2):

- **Pressure:** 5 bar
- **Temperature:** 298.15 K and 323.15 K
- **Equivalence ratio (Phi):** 0.5 to 1.5
- **Fuel composition:** 50 - 100% hydrogen mixed with air (O_2)

The equivalence ratio range was chosen to capture lean, stoichiometric, and rich combustion zones. Combustion outputs from NASA CEA were exported and plotted in Microsoft Excel for visual comparison of NO_x mole fractions under different operating conditions.

All datasets were simulation - derived and not experimentally measured. The results thus provide theoretical insights into hydrogen's emission characteristics and serve as a basis for future validation studies.

Acetylene - Hydrogen Mixtures (P5 - 298.15 K):

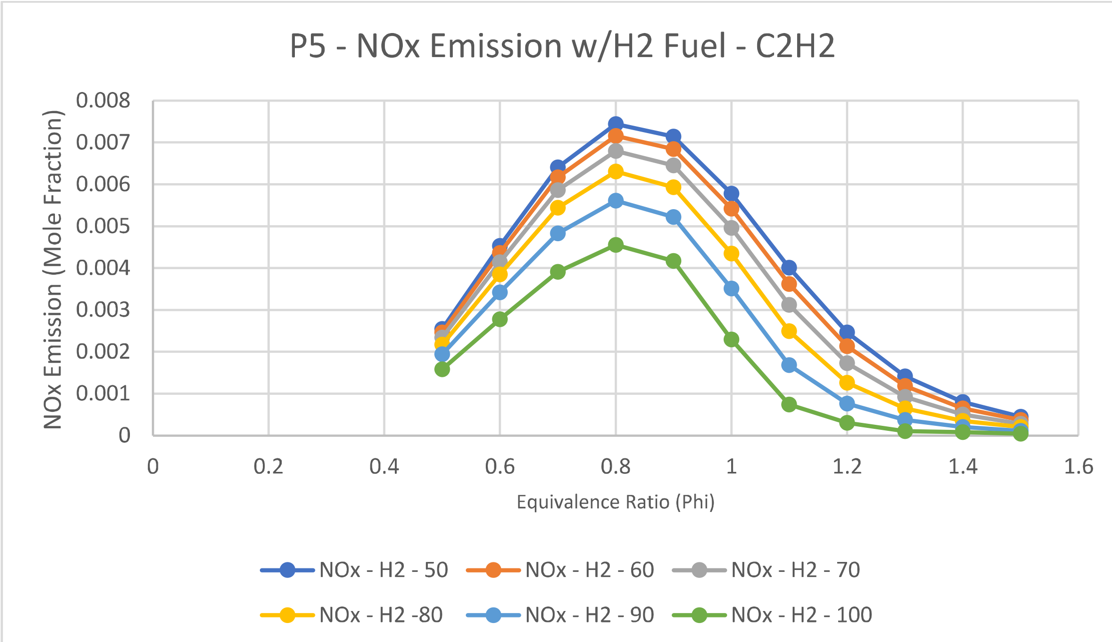

Fig 11: Plot of NO_x emissions for acetylene - hydrogen blends at 5 bars

The plot illustrates the variation of NOx emissions with the equivalence ratio (Phi) for different hydrogen blending percentages in acetylene (C_2H_2) fuel at a constant pressure of 5 bar. As the equivalence ratio increases from a lean mixture toward stoichiometric conditions, NOx emissions rise sharply and reach a peak around Phi = 0.8, after which they decline for richer mixtures. Among the different blends, higher hydrogen concentrations consistently show lower NOx levels. The 100% H_2 blend exhibits the lowest emissions across the range, while blends containing 50 - 70% H_2 show the highest peaks. This behaviour suggests that hydrogen enrichment suppresses NOx formation, likely due to its absence of carbon and altered flame temperature profile. Overall, the results highlight that increasing hydrogen content in C_2H_2 fuel can significantly reduce NOx emissions, reinforcing hydrogen's potential as a cleaner combustion fuel.

Acetylene - Hydrogen Mixtures (P5 - 323.15 K):

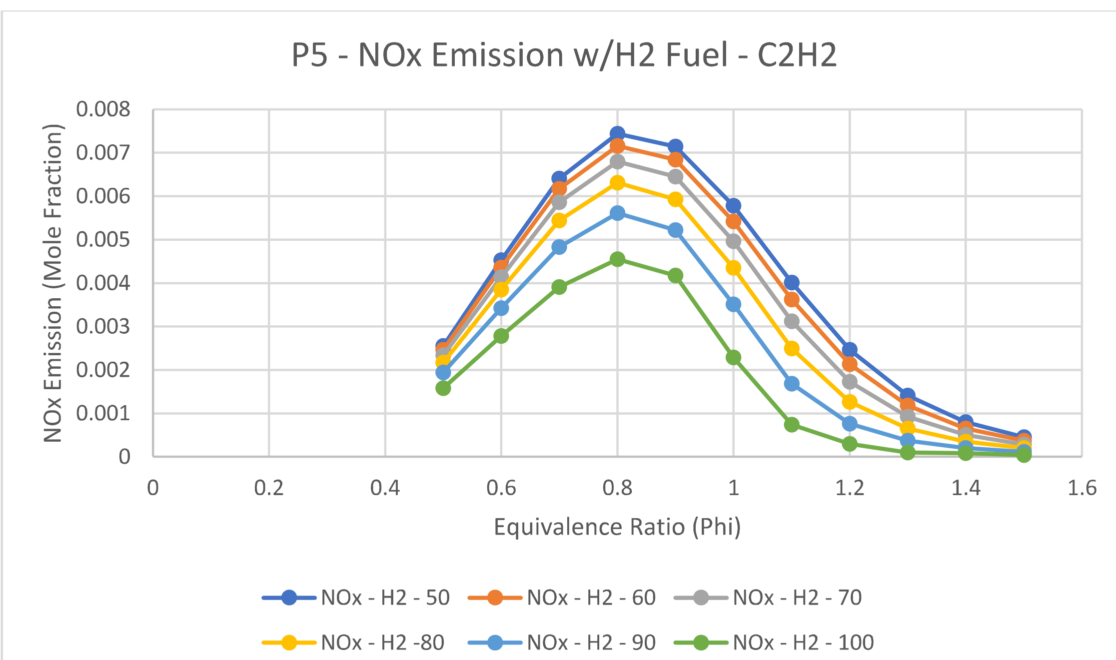

Fig 11: Plot of NO_x emissions for acetylene - hydrogen blends at 5 bars

The plot represents NOx emissions (mole fraction) versus equivalence ratio (Phi) for acetylene (C_2H_2) blended with hydrogen (H_2) fuel at 5 bar pressure and 323.15 K. As the equivalence ratio increases from lean to rich mixtures, NOx emissions rise sharply and peak near Phi = 0.8 before decreasing at higher fuel richness. The emission trend remains consistent across all hydrogen blend ratios, but higher hydrogen content leads to lower NOx levels. The 100% H_2 blend shows the lowest emissions throughout the range, while the 50 – 80% blends exhibit the highest peaks. The reduction in NOx with increasing hydrogen concentration can be attributed to hydrogen's faster combustion and reduced carbon presence, resulting in lower thermal NOx formation at higher temperatures.

Across all fuel combinations: naphthalene, ammonia, and acetylene, the simulations clearly show that increasing hydrogen concentration results in a substantial reduction in NO_x emissions. For naphthalene - hydrogen blends, NO_x mole fractions decreased from approximately 0.00008 to 0.00002 as hydrogen content increased from 50% to 100%, particularly under higher pressures (10 -15 bar). The inverse trend between hydrogen ratio and NO_x formation demonstrates hydrogen's cleaner combustion and lower flame temperature, with reduced carbon intermediates that otherwise promote NO_x generation. At elevated temperatures (323.15 K), NO_x formation followed a similar pattern, peaking around Phi = 0.8 - 0.9 before falling at richer mixtures due to oxygen limitation, confirming the stability of hydrogen-enriched combustion under varying thermal conditions.

For ammonia - hydrogen mixtures, hydrogen enrichment enhanced reactivity and stability while ammonia moderated flame temperature. The combination achieved about a 30% reduction in NO_x formation as hydrogen increased from 50% to 100%. Higher pressures improved combustion uniformity, and even at 323.15 K, hydrogen dominance sustained lower NO_x across all equivalence ratios. Similarly, acetylene - hydrogen blends at 5 bars exhibited strong NO_x suppression with increasing hydrogen content. The emission peaks consistently appeared near Phi = 0.8, but the magnitude dropped as hydrogen fraction rose, demonstrating hydrogen's consistent impact on cleaner combustion behaviour across hydrocarbons.

The theoretical NASA CEA analysis confirms hydrogen's strong environmental advantage in reducing NO_x emissions across different fuel types, pressures, and temperatures. Whether combined with aromatic hydrocarbons (naphthalene), nitrogen-based fuels (ammonia), or simple hydrocarbons (acetylene), hydrogen consistently promotes stable, low - emission combustion. These findings validate hydrogen's role as a sustainable energy carrier capable of significantly cutting atmospheric pollutants in locomotive and industrial combustion systems. Although the results are simulation - based, they provide a solid foundation for experimental studies aimed at advancing hydrogen integration into practical, low - emission propulsion technologies.

Hydrogen Fuel Cell Technologies:

Hydrogen fuel cells convert chemical energy directly into electricity through the electrochemical reaction of hydrogen and oxygen, producing only water as exhaust [7].

The primary types used in locomotives include:

Proton Exchange Membrane (PEM) Fuel Cells: Operate at low temperatures and are suited for automotive and light rail applications [8].

Solid Oxide Fuel Cells (SOFC): Operate at 700 - 1000 °C, ideal for stationary and heavy rail due to high efficiency (up to 75%) [8].

Reversible Fuel Cells: Allow dual operation between electricity generation and energy storage for integration with renewables [8].

Hydrogen fuel cell locomotives can currently produce up to 1.2 MW of power, compared to diesel's 3.3 MW output [9].

However, continuous advancements in stack materials and battery fuel cell hybridization are narrowing the performance gap. Their ability to operate without major infrastructure changes makes them promising for medium and long-distance routes with minimal CO_2 impact.

Solid Oxide Fuel Cell (SOFC): SOFC is promise to be high efficiency, for the maximum possible efficiency we need to do the thermal analysis, where it showcases the operating voltage and trade off attributes like internal losses or other details. A solid oxide fuel cell (SOFC) converts chemical energy from fuel directly into electricity through electrochemical reactions. Oxygen from air is reduced at the cathode to form oxygen ions, which pass through a dense electrolyte to the anode. At the anode, these ions react with hydrogen (or reformed hydrocarbons) to produce water, electrons, and heat. Nickel in the anode aids in both electrochemical oxidation and fuel reforming. The flow of electrons through an external circuit generates electrical power with high efficiency, typically achieving around 85% fuel utilization [10].

In solid oxide fuel cells (SOFCs), hydrocarbon fuels are often converted into syngas to prevent carbon deposition that can damage the anode. High temperatures above 900 °C reduce carbon buildup, while lower temperatures increase the risk of coking and soot formation. Achieving high power density requires minimizing polarization losses through optimized materials, electrode structures, and electrolyte thickness. Efficient SOFC operation involves balancing power density and efficiency, as higher efficiency usually lowers power output. Complete SOFC systems include components like fuel processors, heat exchangers, tail-gas combustors, and power electronics to recover heat, improve performance, and deliver stable electrical power [10].

In hybrid SOFC gas turbine (SOFC - GT) systems, maintaining stable operation during dynamic load changes is one of the primary engineering challenges. Compressor surge control is critical because rapid shifts in power demand can cause pressure buildup between the turbine and compressor, leading to flow reversal or oscillations that risk mechanical damage and system failure. To mitigate this, advanced control algorithms and precise pressure regulation are required to maintain smooth air mass flow and prevent deep or mild surge events. **T**ransient response and component integration present additional difficulties, as the thermal and electrical behaviours of the SOFC and gas turbine operate on different time scales. Coordinating these subsystems while maintaining high efficiency and minimizing performance losses demands careful modelling and synchronization of fuel flow, temperature, and pressure dynamics. Achieving this balance ensures efficient operation and long-term reliability of the hybrid power system under varying locomotive load conditions [11].

Hydrogen fuel cell systems present a practical zero-emission alternative to conventional diesel locomotives, combining environmental and operational benefits while maintaining comparable refuelling times. The U.S. Department of Transportation's study emphasized that hydrogen can significantly reduce air pollutants and eliminate risks associated with fuel spills, with the only byproduct being water. However, successful integration into rail propulsion demands addressing several engineering and safety challenges. The report identified the need to revise existing AAR standards to account for hydrogen's unique properties; such as metal embrittlement, invisible flames, and cryogenic storage requirements at 20 K. Tank design must incorporate suitable alloys, enhanced insulation, and vibration resistance to withstand rail shock loads, while ventilation and leak-detection systems must be optimized for lighter-than-air gas behaviour. Overall, hydrogen fuel cell locomotives have the potential to transform rail transport toward sustainable operation, if material selection, regulatory adaptation, and safety validation are methodically developed [12].

SOFC for clean rail application:

The study by Al-Hamed and Dincer highlights the potential of Solid Oxide Fuel Cell (SOFC)-based hybrid systems in transforming the energy and environmental performance of modern locomotives. By integrating SOFC technology with a gas turbine, steam Rankine, and ammonia organic Rankine cycles, the system achieves remarkable energy and exergy efficiencies of 68.50% and 66.35% under reference conditions, and up to 79.88% and 77.48% at optimal operation. These gains result from the SOFC's ability to directly convert chemical to electrical energy at high temperatures while utilizing waste heat through multi-generation. The integrated setup can meet a passenger locomotive's full power requirement of around 3100 kW equivalent to current diesel-electric engines while substantially reducing fuel consumption and greenhouse gas emissions. Its modular configuration also offers fuel flexibility, allowing operation with methane, ammonia, or hydrogen, which makes it adaptable for future clean rail networks [13].

From a system design and sustainability standpoint, the combined SOFC-GT and Rankine cycles enable efficient energy recovery and simultaneous power and heating/cooling generation, addressing both traction and auxiliary demands. The analysis identifies the SOFC as the primary source of exergy destruction (approximately 1286 kW), emphasizing the need for further advancements in electrolyte conductivity and fuel utilization to enhance overall performance. Redirecting a portion of the fuel stream to the combustor improves gas turbine efficiency and reduces system bulk, making the design more compact and suitable for locomotive integration. Overall, this research establishes that SOFC-based and hydrogen fuelled power systems can replace diesel propulsion with high thermodynamic efficiency, reduced emissions, and near-zero carbon operation when supplied with renewably produced hydrogen [13].

Global Developments in Hydrogen Locomotives:

The worldwide effort to decarbonize rail transportation has led to rapid advancements in hydrogen powered locomotive systems. Several countries are investing heavily in fuel cell technology, infrastructure, and large-scale deployment, reflecting hydrogen's growing role as a zero - emission propulsion source.

United States: In early 2024, the State of California announced a $127 million partnership with Stadler Rail, Inc. to develop and commercialize hydrogen-powered passenger trainsets under the *FLIRT* H_2 program [7] [8] [9].

Designed for lightweight, energy-efficient operation, these trains are part of California's broader zero-emission rail initiative. The first unit, named ZEMU (Zero Emission Multiple Unit), began service along the Arrow Corridor between San Bernardino and Redlands, covering five stations over nine miles. Originally built in Switzerland in 2019, the FLIRT H_2 was tested at Colorado's Transportation Technology Centre before U.S. deployment. The hydrogen-powered system achieved a top speed of 130 km/h (81 mph) and covered approximately 1,742 miles on a single refuel cycle. Each train operates efficiently at ambient temperatures up to 50°C and accommodates 108 passengers, proving hydrogen's practicality for regional passenger rail applications [7] [8] [9].

Canada: The Canadian Pacific Kansas City (CPKC) Hydrogen Locomotive Program has made notable progress in developing hydrogen - battery hybrid locomotives [9] [14]. Initiated in 2021, the program integrates Ballard Fuel Cell modules to deliver approximately 1.2 MW of traction power. The first locomotive, Unit 1001, was launched in 2022 as a retrofitted diesel unit equipped with hydrogen fuel cells and batteries. Building on this success, Unit 1200, developed in collaboration with CSX Transportation, was unveiled in 2024 as a high-power hydrogen locomotive for mainline freight operations [9] [14] [15] [16] . To support these developments, CPKC partnered with ATCO EnPower to establish hydrogen production and refuelling facilities in Calgary and Edmonton, scheduled to be fully operational by the end of 2024. These projects part of Alberta's *Emission Reduction Initiative* will provide a foundation for large scale hydrogen rail operations in Canada [14] [15] [16] [17].

Heavy haul testing by CPKC: CPKC has established a hydrogen refuelling station in Golden, British Columbia, which became operational in early March 2025. The facility construction is in association with ATCO EnPower, itself is a first fixed hydrogen refuelling station on network outside of Alberta and this enables the first high-horsepower hydrogen locomotive to enter regular mainline service area [18].

Location: Golden, British Columbia

Associated with: ATCO EnPower

Operational Status: Service started from March 2025

Significance: First hydrogen refuelling station on CPKC's network outside of Alberta, supporting the use of hydrogen-powered locomotives in real-world conditions. The station supports CPKC' hydrogen locomotive CP1201, which is used in hauling bulk freight trains [18].

South Korea: In parallel, Hyundai Rotem has pioneered liquid hydrogen locomotive technology through the development of a next-generation LH_2 based train capable of generating 2.7 MW of power and achieving a 1,000 km range on a single refuel [19]. The locomotive utilizes liquid hydrogen fuel cell propulsion combined with hybrid battery systems, offering a balance of high energy density, efficiency, and reduced refuelling frequency. This innovation represents a major step toward commercial adoption of hydrogen propulsion in Asia and demonstrates the scalability of LH_2 systems for heavy duty rail transport [19].

Collectively, these advancements across the United States, Canada, and South Korea highlight hydrogen's growing maturity as a clean, high-performance fuel for rail applications. They demonstrate the global momentum toward hydrogen propulsion and infrastructure readiness setting the stage for widespread adoption of low-emission, high-efficiency rail systems soon [7] [8] [9] [14] [16] [20].

Liquid Hydrogen (LH_2) as a Next-Generation Fuel for Rail Transportation:

Hydrogen, the lightest element in the universe, can exist in both gaseous and liquid forms, each offering distinct advantages for energy storage and transportation. The gaseous form has a density of approximately 0.089 kg/m^3, while its liquid counterpart first liquefied by Professor Heike Kamerlingh Onnes at Leiden University requires cryogenic storage at −253 °C. Liquefaction dramatically enhances volumetric energy density, enabling up to 800 times more hydrogen storage within the same tank compared to gaseous hydrogen [19] [21].

In gaseous applications, hydrogen is typically stored at high pressures ranging from 350 to 700 bar, whereas liquid hydrogen (LH_2) allows for storage and transportation under much lower pressures using vacuum insulated cryogenic tanks, which can be efficiently deployed via rail, road, or marine routes. This advancement not only ensures operational safety but also minimizes transportation losses, making LH_2 a practical choice for long-range, high-capacity applications [21].

From an environmental perspective, liquid hydrogen is a zero-carbon energy carrier, offering complete elimination of greenhouse gas emissions during use. Countries such as South Korea, Japan, France, and China have already recognized its strategic importance in achieving carbon neutrality through large scale hydrogen mobility programs [21].

A leading example is Hyundai Rotem's liquid hydrogen powered locomotive project, which integrates advanced fuel cell propulsion technology with battery assisted hybrid systems [21] [22]. The LH_2 based locomotive has achieved a top speed of 110 km/h using a 1.2 MW hybrid powertrain and is being further developed to reach 150 km/h with an extended 1,000 km range on a single refuel. The system generates up to 2.7 MW of power, demonstrating both performance scalability and energy efficiency [19] [21] [22]

The combination of liquid hydrogen storage, hybrid battery integration, and cryogenic infrastructure presents a transformative opportunity for the rail sector. It allows long distance trains to operate with minimal refuelling stops, reduced system pressure, and improved overall safety. Moreover, the establishment of LH_2 refuelling networks will significantly accelerate the commercialization of hydrogen rail systems and contribute to building an economical and eco-friendly hydrogen society [21] [22].

Collectively, these advancements position liquid hydrogen as a cornerstone fuel for the next generation of sustainable, high-performance locomotives, bridging the gap between renewable energy production and clean, large-scale mobility.

Results:

The theoretical combustion analysis using NASA CEA simulations compared hydrogen (H_2), naphthalene ($C_{10}H_8$), ammonia (NH_3), fuels under a range of operating pressures (5 to 15 bar) and temperatures (298.15 - 323.15 K). Acetylene (C_2H_2) under operating pressure of 5 bars and temperature varying from 298.15K - 323.15K. The study focused on evaluating NO_x formation behaviour across various fuel blends, pressures, and hydrogen concentrations, aiming to understand how hydrogen enrichment influences emission characteristics and combustion performance across different fuel types.

Key Findings:

1. **Hydrogen Concentration and NO_x reduction:**
   Across all fuels: naphthalene, ammonia, and acetylene – NO_x emission decreased substantially as hydrogen concentration increased from 50% to 100%. This reduction is attributed to hydrogen's lower flame temperature and absence of carbon, minimizing thermal NO_x formation.
2. **Pressure Effects:**
   For naphthalene and ammonia blends, increasing pressure from 5 bars and 15 bars slightly raised reaction rates but overall supported smoother combustion and lower NO_x formation. At higher pressures NO_x levels stabilized near 0.00002 mole fraction, confirming hydrogen's advantage under realistic locomotive conditions.
3. **Temperature Influence (298.15K vs 32315K):**
   Elevated temperatures (323.15K) slightly increased NO_x due to faster reaction kinetics, but the overall downward trend with higher hydrogen fractions persisted. The peak NO_x formation consistently occurred near equivalence ratio (Phi) = 0.8 - 0.9.

4. **Fuel – Specific Observations:**
    - Naphthalene – Hydrogen: NO_x dropped from 0.00008 to 0.00002 mole fraction as hydrogen rose to 100%, confirming hydrogen's cleaner burn.
    - Ammonia – Hydrogen: About 30% NO_x reduction achieved as hydrogen increased from 50% to 100%; ammonia helped moderate flame temperature.
    - Acetylene – Hydrogen: At 5 bard, higher hydrogen blends consistently suppressed NO_x, peaking near Phi = 0.8 then declining in richer mixtures.
5. **Combustion Stability and Efficiency:**
   Higher hydrogen fractions improved combustion uniformity and ignition stability while maintaining low emissions, making hydrogen – rice mixtures favourable for clean energy applications.

Comparative Findings:

Fuel Type	Pressure (Bar)	Temperature (K)	Hydrogen Fraction	NO_x (Mole fraction)	Reduction (%)
Naphthalene + H2	5 → 15	298.15K → 323.15K	50% → 100%	0.00008 → 0.00002	~ 75%
Ammonia + H2	5 → 15	298.15K → 323.15K	50% → 100%	0.00004 → 0.00001	~30% - 50%
Acetylene + H2	5	298.15K → 323.15K	50% → 100%	0.00006 → 0.00002	~60% - 65%

The comparative analysis clearly shows that increasing hydrogen concentration consistently lowers NO_x emissions across all fuel types. Naphthalene - hydrogen blends achieved the highest reduction of about 75%, followed by acetylene - hydrogen at roughly 60% - 65%, and ammonia - hydrogen mixtures at around 30% - 50%. These results confirm that hydrogen enrichment enhances combustion efficiency, stabilizes flame behaviour, and significantly reduces pollutant formation across different operating pressures and temperatures.

Conclusion:

This study demonstrates that integrating hydrogen into combustion systems can substantially reduce NO_x emissions compared to conventional hydrocarbon fuels. The results are consistent across both aromatic hydrocarbon (naphthalene) and nitrogen-based (ammonia) blends, acetylene blends confirming hydrogen's versatility and potential as a sustainable alternative to diesel in locomotive propulsion.

Hydrogen fuel cell technologies particularly Proton Exchange Membrane (PEM) and Solid Oxide Fuel Cells (SOFC), enable high-efficiency energy conversion with zero tailpipe emissions, producing only water as a byproduct. Although current hydrogen-powered locomotives typically generate around 1.2 MW, compared to 3.3 MW from diesel engines, ongoing advancements in fuel cell stack design, material science, and hybrid fuel cell battery integration are rapidly narrowing the performance gap.

Real world demonstrations, including the Stadler FLIRT H_2 in the United States [12] [14], the CPKC Unit 1200 in Canada [16] [20], and Hyundai Rotem's LH_2 train in South Korea [21] [22]. validate hydrogen's feasibility and scalability in modern rail applications. Collectively, these findings reinforce that hydrogen-powered locomotion is not merely a theoretical solution but a proven, practical, and sustainable transportation pathway for the coming decades.

Future Scope:

The future direction of this research lies in advancing hydrogen technology from theoretical modelling toward experimental and commercial-scale validation. Future studies should focus on combustion testing at elevated pressures up to 50 bar to better understand hydrogen's reaction kinetics and emission characteristics under real-world operating conditions [14].

Developing next-generation PEM and SOFC systems will be essential for improving power output beyond the current 1.2 MW benchmark to match or exceed diesel locomotive performance. Further exploration of liquid hydrogen (LH_2) storage technology will also be crucial, as modern cryogenic systems offer up to 800× higher storage density than gaseous hydrogen, enabling extended range and reduced refuelling frequency [21] . The Hyundai Rotem hydrogen program already illustrates how LH_2 integration can support zero-emission, high-speed rail with outputs up to 2.7 MW [22].

Infrastructure development will play a key enabling role. The CPKC - ATCO EnPower hydrogen facilities in Calgary and Edmonton provide a scalable model for hydrogen production, distribution, and refuelling networks supporting freight and passenger rail operations [17] [20]. In parallel, dedicated research into safety systems, including leak-proof storage, cryogenic containment, and sensor-based monitoring, will ensure reliability and regulatory compliance for large-scale adoption.

Finally, integrating reversible fuel cells with renewable energy sources such as solar and wind will allow for long-term hydrogen energy storage, fostering a fully carbon - neutral transportation ecosystem. The alignment of hydrogen propulsion, renewable energy, and infrastructure investment defines the strategic roadmap for sustainable rail mobility in the decades ahead.

References

[1] IEA, "IEA," 02 March 2023. [Online]. Available: https://www.iea.org/reports/co2-emissions-in-2022.

[2] IEA, "IEA World Energy Change," 27 October 2022. [Online]. Available: https://www.iea.org/reports/world-energy-outlook-2022.

[3] A. Trivella, "Designing an optimized fueling infrastructure for a hydrogen railway system," *Science Direct,* September 2025.

[4] Wikipedia, "Wikipedia," Diesel Locomotive, [Online]. Available: https://en.wikipedia.org/wiki/Diesel_locomotive.

[5] I. G. Hydrogen, "IEA," 2024 October 2025. [Online]. Available: https://www.iea.org/reports/global-hydrogen-review-2024.

[6] IEA, "IEA Webpage," [Online]. Available: https://www.epa.gov/.

[7] Wiki, "Wiki Hydrogen Train," [Online]. Available: https://en.wikipedia.org/wiki/Hydrogen_train.

[8] H. R. Tech, "Hyundai," [Online]. Available: https://tech.hyundai-rotem.com/en/why-is-hydrogen-energy-the-future-of-trains/.

[9] U. Energy, "Energy gov," [Online]. Available: https://www.energy.gov/eere/fuelcells/fuel-cell-basics.

[10] R. Kee, "Science Direct," [Online]. Available: https://doi.org/10.1016/B978-044452745-5.00255-0.

[11] U. D. FEA, "US DOT," June 2019. [Online]. Available: https://railroads.dot.gov/sites/fra.dot.gov/files/fra_net/18767/Thermodynamic and Dynamic Assessment.pdf.

[12] U. D. FEA, "US DOT HFC," [Online]. Available: https://railroads.dot.gov/elibrary/study-hydrogen-fuel-cell-technology-rail-propulsion-and-review-relevant-industry-standards.

[13] K.H.M.Ahmed, "A novel integrated solid-oxide fuel cell powering system for clean rail applications," no. A novel integrated solid-oxide fuel cell powering system for clean rail applications, 2020.

[14] E. Barrera, "CA gov," 14 February 2024. [Online]. Available: https://dot.ca.gov/news-releases/news-release-2024-007.

[15] FCW, "Fuelcellworks ZEMU," 10 September 2025. [Online]. Available: https://fuelcellsworks.com/2025/09/10/fuel-cells/california-to-launch-first-u-s-hydrogen-passenger-train-zemu-debuts-sept-13 .

[16] FCW, "FCW CKPC," 15 March 2025. [Online]. Available: https://fuelcellsworks.com/2025/03/12/fuel-cells/cpkc-s-cp1201-first-high-horsepower-hydrogen-locomotive-enters-mainline-service.

[17] CSX, "CSX H2 Locomotive," 29 March 2025. [Online]. Available: https://www.csx.com/index.cfm/about-us/csx-advances-hydrogen-locomotive-development-at-huntington/.

[18] FuelcellWorks, "FCW, CPKC 1201," [Online]. Available: https://fuelcellsworks.com/2025/03/12/fuel-cells/cpkc-s-cp1201-first-high-horsepower-hydrogen-locomotive-enters-mainline-service.

[19] SNR, "PR Newswire," 08 April 2025. [Online]. Available: https://www.prnewswire.com/news-releases/sierra-northern-railway-successfully-tests-first-four-axle-hydrogen-fueled-zero-emission-switching-locomotive-302423855.html.

[20] CKPC, "CKPC H2 Program," [Online]. Available: https://www.cpkcr.com/en/sustainability/Hydrogen-locomotive-program.

[21] E. presswire, "Foxnews," 21 May 2025. [Online]. Available: https://fox5sandiego.com/business/press-releases/ein-presswire/814641489/liquid-hydrogen-instead-of-diesel-how-sustainability-in-rail-transport-can-succeed-on-all-routes/.

[22] Sierra, "Sierra Northern," [Online]. Available: https://www.sierranorthern.com/.