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Design and demonstration of a NH₃-fueled two-stroke uniflow engine for greenhouse gas reduction

Emission Reduction Technologies - Engine Measures & Combustion Development

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ABSTRACT

The maritime shipping industry is increasingly interested in both low- and non-carbon-containing fuels to meet future greenhouse gas emission targets. Specifically of interest is ammonia, as it has a relatively high volumetric energy density compared with other future fuels, such as hydrogen, making it more economical to transport. The robust engine architecture of low-speed two-stroke marine engines makes them an ideal candidate for ammonia fuel, overcoming many of the issues surrounding its poor ignitability and low flame speed. If emissions and fueling system challenges can be addressed, retrofits of current low-speed two-stroke dual-fuel engines represent a viable pathway for bringing ammonia engines to market.

This study explores these technical hurdles by describing the design, analysis, and experimental validation of a single cylinder research engine converted to operate on ammonia fuel. The engine is a reduced-scale uniflow two-stroke marine engine with two previous hardware configurations available – diesel and high-pressure CNG dual-fuel. A concept study was used to evaluate possible ammonia-fueled engine architectures and the associated tradeoffs and design considerations. With the chosen architecture, low-pressure dual-fuel, 1D and 3D analysis tools were used to inform hardware selection and to determine hardware configurations which minimized ammonia-slip while maximizing ammonia substitution. In addition to these considerations, the hardware and engine configuration were designed to provide a versatile and robust testing platform. This includes options to test both gaseous and liquid ammonia injection, as well as a wide range of performance parameters such as AFR, swirl, valve timing, SOI, and many others. Design constraints imposed by the existing engine hardware necessitated an iterative loop between design and analysis toolsets, ultimately converging on a final design for the ammonia-conversion hardware.

The engine was rebuilt with the new hardware and evaluated in an engine test cell. A new control strategy developed and implemented onto a prototype electronic control unit allowed for full control over all engine parameters. An initial calibration was developed, providing test data for validation of the engine 1D and 3D models. Optimization of the calibration has demonstrated the ability to achieve high substitution levels of ammonia (>85%) to substantially reduce CO₂ emissions. The impact of the design choices on engine operability and the ability to meet program targets is discussed as well as opportunities for further optimization of the ammonia-conversion hardware, informed by the validated models.

1 INTRODUCTION

In order to meet international emissions reduction goals, such as the International Maritime Organization (IMO) targets for future transportation goals of reductions in greenhouse gases (GHG) [1], key sectors will require the use of low life-cycle carbon emissions technologies. The marine sector is one of the key target markets for low or non-carbon-based fuels, as it is a significant contributor to overall global GHG emissions [2]. For cargo ship transportation, it is difficult or impractical to apply electrification and so the use of low life-cycle carbon fuels represents a promising, effective near-term de-carbonization strategy [3]

There are several different fuels that are being considered for marine applications, including ammonia, hydrogen, and methanol [4]. There are several notable differences among these fuels including availability, cost, energy density and storage and handling complexity. Each of these needs to be taken into consideration when evaluating the viability of the use of each fuel in the target application, as does the relative change in these parameters (and hence the ease to implement) versus the incumbent fuels.

As the maritime shipping industry continues to investigate the optimum way to reduce GHG emissions by moving towards low and non-carbon-containing fuels, the critical design parameters, and techniques to evaluate fuel system architectures and optimum engine features become increasingly important.

The use of fuels such as natural gas and methanol has facilitated reductions in criteria pollutant emissions in the marine industry over the past decade [5], but in order to achieve the significant decarbonization goals of the future, fuels without carbon must be investigated.

Hydrogen has been investigated as a viable non-carbon fuel for use in several automotive markets, however for marine applications, especially cargo ship transportation, it carries significant disadvantages including its low volumetric energy density [6] and significant mass losses due to liquid

boil-off for fuel storage as described in Yan, *et al.* (Figure 1) [7].

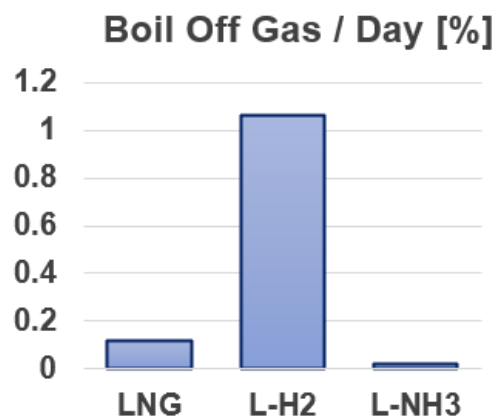


Figure 1 Percentage of stored liquid fuel lost through boil-off per day [7]

Another carbon-free fuel that is generating interest in this market is ammonia, due to its advantages in energy density versus hydrogen, wide global availability, and the ability to leverage existing high capacity marine-based storage infrastructure [8]. Additionally, ammonia fuel can be produced as a E-fuel which makes it a very attractive renewable fuel source for achieving global targets for emissions reduction.

Ammonia fuel has a relatively low flame speed and high activation energy compared to other fuel types, which is not a significant challenge in the large slow-speed engines typical of heavy cargo ships. This is a benefit over smaller applications that tend to use higher speed, higher power density engines such as in the automotive industry. Ignition and combustion enhancement of the ammonia and air mixture can be achieved by using a quantity of diesel or similar fuel injected into the combustion chamber with the ammonia and air mixture. This is often referred to as a “Dual Fuel” combustion system and has been investigated for use with ammonia for a long time with varying degrees of success [9]. With the advent of new and improved injection and control technology, and renewed interest in ammonia as a fuel, many of the challenges encountered previously can be overcome.

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One key challenge of using ammonia as a fuel is its toxicity. The following of strict safety protocols and guidelines is critical to protect the personnel working around and with this fuel. Limits for exposure [10], proper personal protective equipment, and safety procedures are critical to the successful implementation of this fuel in future applications. Because of the safety challenges of storing, handling, burning, and post-treatment of ammonia, it is beneficial to limit the design space of engine components and subsystems and subsequent engine calibration to ensure engine operation with a high likelihood of acceptable combustion completeness during ammonia engine development. Overly broad design spaces for these parameters may result in engine operation that inadvertently produces excessive ammonia emissions that could pose a threat to the safety of the engine operators, laboratory staff, and surrounding community. A more limited design space, guided by analysis-led design and calibration optimization, minimizes the risk of excessive tailpipe ammonia emissions or other leakage pathways during engine development.

This study focused on addressing the challenges of ammonia combustion and the means by which to optimize the overall system design to demonstrate the large GHG reduction potential. Large marine engines pose additional challenges because of the cost, complexity, component lead-times, and safety challenges due to the magnitude of the systems of these full-scale engines. The utilization of an analysis-led design approach, namely utilizing analysis techniques and a limited engine calibration parameter space to optimize the initial performance of an engine converted to ammonia, helped to ensure rapid and safe initial combustion system development. This design approach can be beneficial in the development of these large marine engines going forward.

2 MOTIVATION

The emissions from shipping are a significant contributor to global greenhouse gas emissions [11], primarily due to the reliance on heavy fuel oils for powering ships. These emissions include carbon dioxide (CO_2), particulate matter (PM), oxides of nitrogen (NO_x), and sulfur oxides (SO_x). The GHG emissions from shipping are difficult to abate due to the complexity and scale of the global shipping industry. Ships operate over vast distances, mostly on the open seas requiring large amounts of on-board stored energy. The long lifespan of ships also means that replacing vessels with new technologies is expensive and logistically complex. Being able to safely, rapidly, and cost-effectively develop and deploy an ammonia conversion approach for large marine engines is seen as one of the most promising approaches to

achieving the large GHG reductions required in this industry. Successful implementation of ammonia combustion provides a pathway for the rapid decarbonization of the marine sector.

Ammonia as a fuel is inherently difficult to burn in engines, so utilizing 0D/1D and 3D analysis tools in an empirically based predictive fashion can significantly improve the likelihood of achieving acceptable combustion and emissions results during engine development activities. Analysis tools can be used to determine component and subsystem design direction and calibration parameters with a high likelihood of success. This, coupled with small scale engine testing, can significantly reduce risk, cost, and time needed to develop these advanced fuel systems and control logic compared with full scale large engine investigations and parametric testing.

In this study, a combination of simulation and engine testing results are presented to demonstrate the potential of ammonia to provide a significant reduction to GHG emissions in the shipping industry. The use of extensive simulation tools to inform the design to minimize the amount of hardware iteration, coupled with a low-pressure ammonia injection system that reduces the complexity and level of change can enable near-term adoption of this approach.

3 EXPERIMENTAL SETUP

3.1 Platform

The engine used as the basis for the experimental and analysis activities for this study is a variant of the Enterprise reduced-scale, single-cylinder crosshead marine research engine [12]. This engine has been redesigned to operate with a low-pressure gaseous fuel injection system for ammonia dual-fuel combustion. The key engine parameters are listed below in Table 1. The engine is shown in Figure 2 and Figure 3. A previously developed empirically based computational fluid dynamics (CFD) simulation model corresponding to the baseline engine was modified for the purposes of this study.

Table 1 Engine Parameters

Key Engine Parameters	
Cylinder Bore	Ø 107.95mm
Piston Stroke	432mm
Stroke/Bore Ratio	4:1
Displacement	3.95 liters
Mean Piston Speed	8m/s @ 556rpm
	9m/s @ 625rpm
Max Overspeed	656rpm
Max Engine Load	18-20 bar BMEP
Engine PMAX	150 Bar (Nominal)

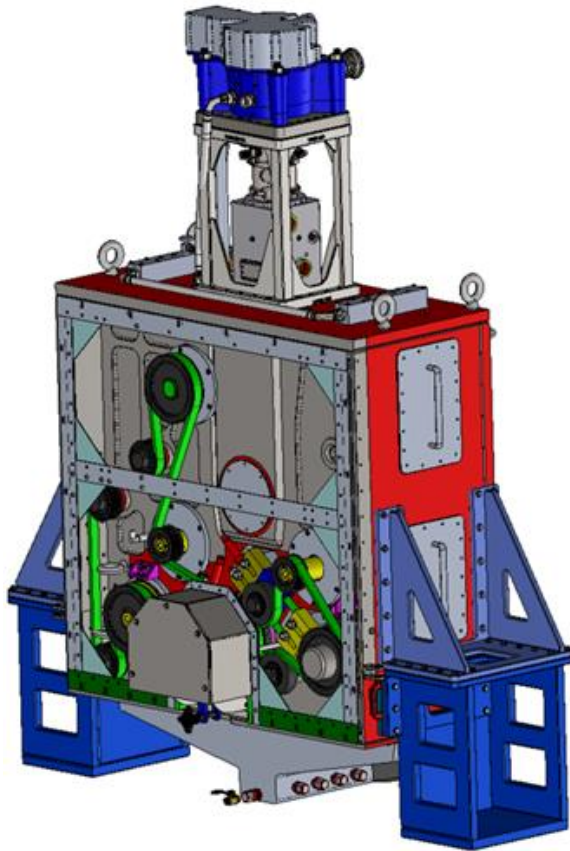


Figure 2 Detailed CAD image of baseline Enterprise engine variant.



Figure 3 Image of baseline Enterprise engine.

3.2 Conversion to Ammonia Fuel

A dual-fuel combustion configuration, utilizing a diesel pilot injection event as the ignition trigger for ammonia, was selected due to the incumbency of this configuration for natural gas engine variants in the marine sector. The primary design goal of the engine conversion to ammonia was to maximize the ammonia substitution rates, with a target of 95% ammonia usage by energy content at the full load rated condition of the engine. Liquid and gaseous injection of ammonia into the engine were considered.

Tradeoffs in using liquid versus gaseous fuel were evaluated using CFD simulations. The CFD model result was analyzed to understand the relative difference in mixing dynamics in the pre-charge stage, with a goal of relative homogeneity prior to the start of injection (SOI) of the diesel pilot.

In this design, the fuel injectors were incorporated into the liner system midway between the intake ports and the cylinder lubricant oil (CLO) injectors. The location of the fuel injectors had several main considerations. First, the allowable fuel injection duration is a function of engine geometry and the fuel injector locations in the liner. This is illustrated in Figure 4 below.

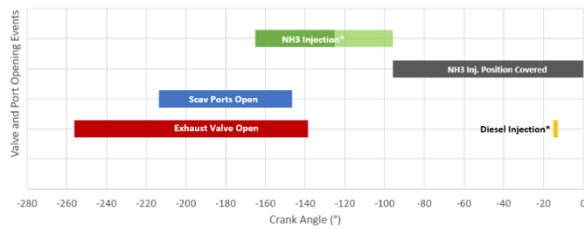


Figure 4 Fuel injection operation window.

Secondly, the combination of required system fuel flow and time between the ammonia SOI and end of injection (EOI) events dictates the required fuel injector flow rates. This can then be used to select the type, size, and number of injectors.

The design of the engine incorporates several features that provide a degree of testing flexibility in the testing environment. This includes the ability to adjust the engine swirl by changing the intake port lengths and changes to air flow with control of the air to fuel ratio (AFR) via a variable inlet manifold air supply pressure. The fuel injection system is also designed to have fully independently controlled injection events allowing for independent tuning of the diesel and ammonia injector solenoids for combustion optimization.

The engine utilizes a low-pressure fuel injection system that is incorporated into the liner system design. The design integration of the injectors into the liner system requires the system to be designed so that it can both seal combustion pressure and isolate engine coolant from the cylinder and external engine environment. An image of the liner is displayed in Figure 5.

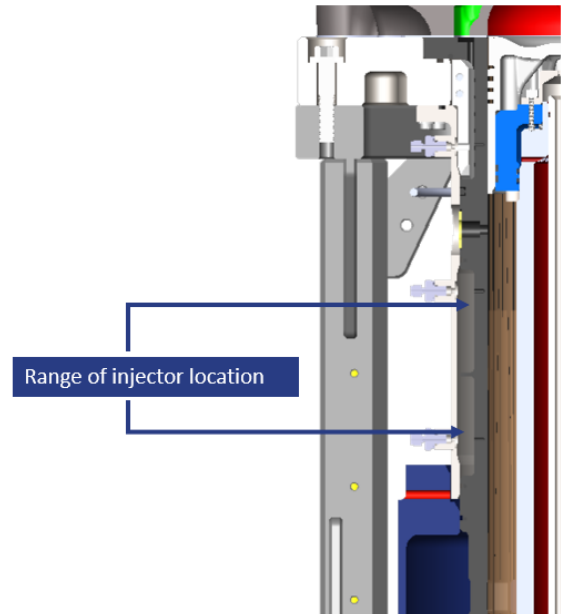


Figure 5 Fuel injection location range

The upstream fuel system is comprised of an on-engine fuel rail that includes instrumentation for temperature and pressure, inlet and outlet connections for system purging, and the inclusion of shutoff valves for each injector. These valves are incorporated as a safety mechanism to contain and stop ammonia fuel flow to the engine in an emergency.

The fuel rail and engine mounting are specific to this prototype engine. The upstream fuel system is designed to be backwards and forwards compatible with different fuel types for the engine operation. Figure 6 shows an overview of the system design.

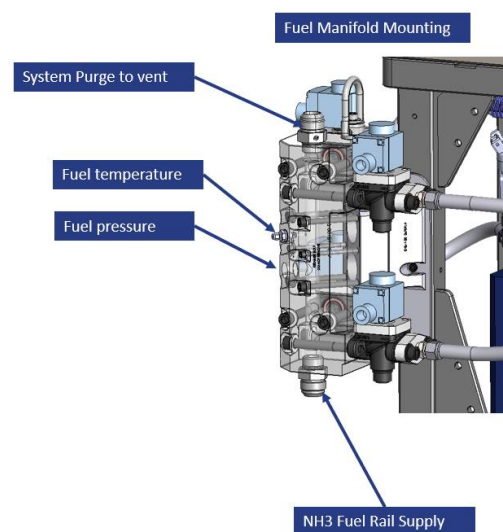


Figure 6 Fuel rail & manifold overview

4 SIMULATIONS

4.1 Methodology

An analysis-led design approach was utilized to evaluate engine performance and emissions trends with changes to component and subsystem design and to calibration parameters. Performance metrics of interest include ammonia slip, and ammonia substitution rate, i.e., minimizing required diesel pilot quantity in a dual-fuel combustion system. These metrics were used to evaluate the benefit of changes in ammonia fuel injector location and quantity, ammonia SOI angle, fuel injection pressure, and air-fuel ratio. Other parameters such as charge motion and pilot fuel injector parameters were also evaluated as part of this study but are not presented here. Due to the sensitivity of ammonia ignition and flame propagation to local air-fuel ratio, directional parameter changes that reduced the standard deviation of air-fuel ratio were deemed beneficial, and this was used as an intermediate metric.

4.2 Simulations Toolset

The analysis conducted to inform the design activity consisted of two main types. 0D and 1D analysis were used to confirm fuel system parameters such as flow rates, injector pressure differential, fuel system pressure drop, and 3D CFD boundary conditions. 3D CFD analysis was used for evaluating mixing dynamics and combustion performance.

The 0D calculations determined the required injector flow needed for the system to achieve the target 95% ammonia substitution. Data from 0D was used for injector specification development, and this specification was harmonized with available prototype components from suppliers. An example of the input to the 0D analysis is shown in Figure 7

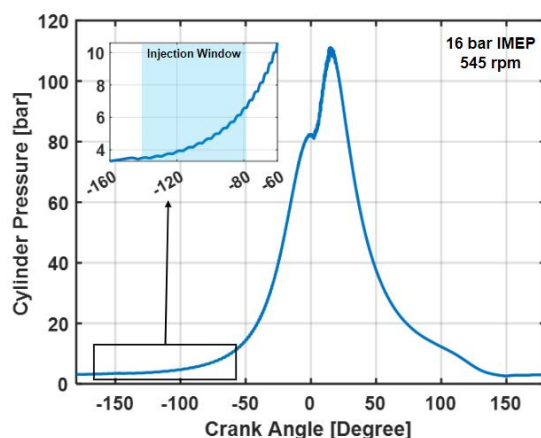


Figure 7 Baseline engine fuel injection background pressure.

The 1D analysis was completed in GT-SUITE. The engine was modeled in 1D to develop the input parameters needed for 3D CFD analysis. This includes high-speed pressure data for both the intake and exhaust as well as in-cylinder residuals remaining from the air scavenging process.

Additionally, 1D analysis of the upstream fuel system was performed to determine the pressure drop in the fuel rail, and supply lines to the ammonia fuel injectors at peak flow. This result informed specifications of the rail cross sectional area and the fuel line inner diameter sizing.

Design elements within the system were analyzed with 3D FEA to assess the natural frequency of the fuel rail and fuel lines. This was necessary to confirm that the design would not operate in one of the key engine resonance zones.

The CFD analysis was used to investigate several key parameters and their impact on fuel stratification and distribution in the combustion chamber. The location of the fuel injector(s), spray targeting, injector nozzle orifice diameters, number of injector orifices, injector umbrella angle, and SOI were evaluated.

4.3 Simulation Results

The ammonia fuel injection location and targeting were evaluated by 3D CFD analysis, aimed at maximising homogeneity of the ammonia/air mixture prior to SOI for the diesel pilot injection event, while minimising the fuel slip of ammonia to the exhaust. The different conditions were evaluated against the target fuel/air equivalence ratio (ϕ) using a probability distribution function (PDF) and standard deviation of the in-cylinder ϕ distribution. The parameters evaluated in depth using for the ammonia fuel injector targeting are illustrated in Figure 8. Simulation results for several different injector targeting cases are shown in Figure 9.

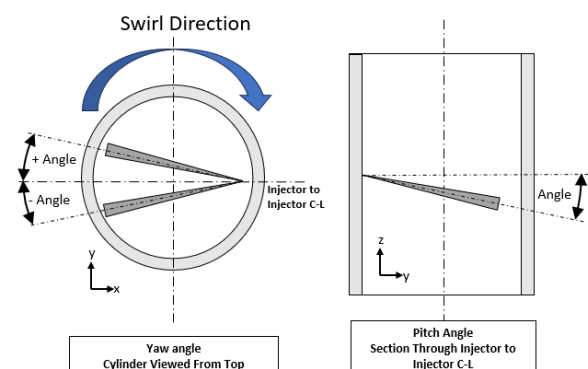


Figure 8 Ammonia Fuel injector targeting parameters diagram.

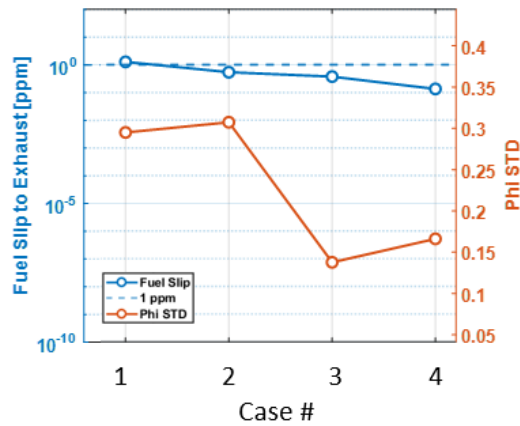


Figure 9 Ammonia fuel distribution and slip to exhaust vs. injector targeting

In Figure 9, Case 3 displays superior mixing characteristics, with the lowest ϕ standard deviation. This case represents a downward pitch angle combined with a positive yaw angle for the injector targeting.

Other parameters that contribute to improved mixing included the number of injectors and injector vapor fraction. The sensitivity of different fuel phases and the number of injection points are shown below in Figure 10 and Figure 11. The results show improvement in homogeneity for gaseous injection compared to liquid injection, and by increasing the number of discrete injection sites. These results are reflected in the improved ϕ standard deviation and increases in the mass values of the PDF of ϕ bins.

The intake manifold pressure and ammonia SOI timing were also evaluated (see Figure 12 to Figure 14).

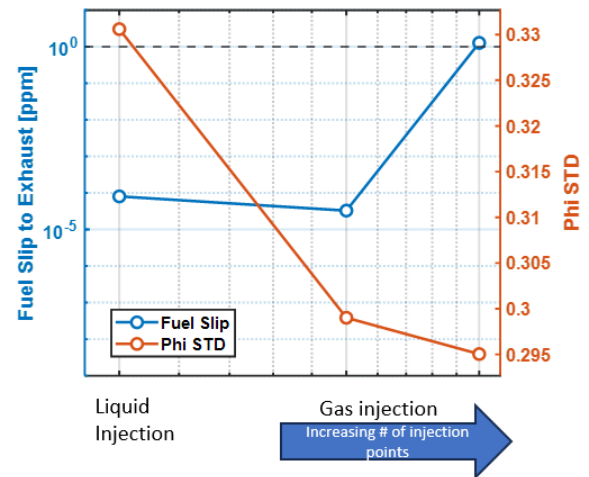


Figure 10 Ammonia fuel distribution and slip to exhaust vs injection phase and # of injection locations

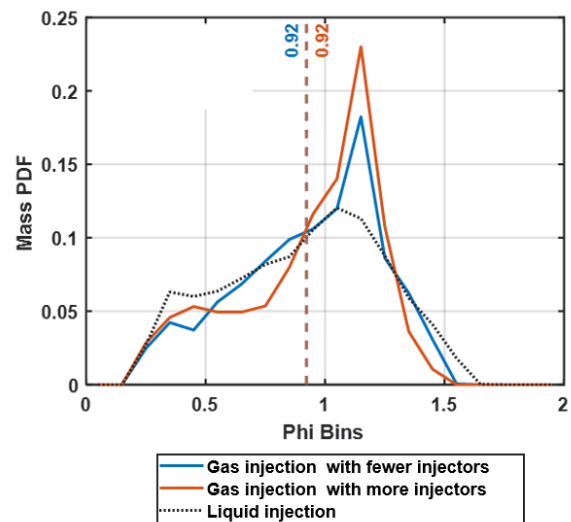


Figure 11 Ammonia fuel distribution vs injection phase and # of injection locations.

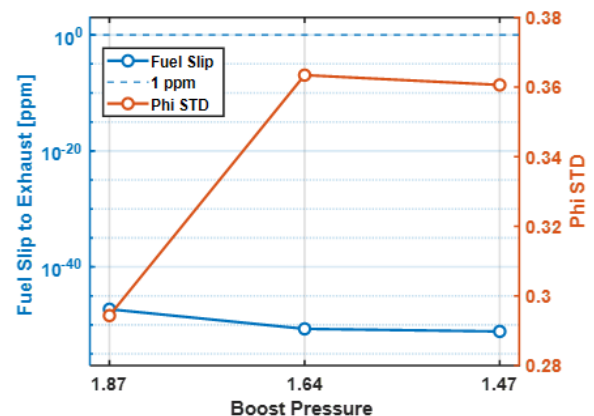


Figure 12 Ammonia fuel distribution and slip to exhaust vs boost pressure.

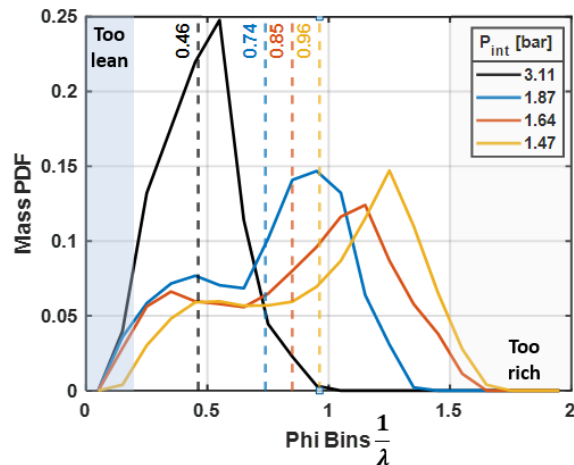


Figure 13 Ammonia fuel distribution vs engine boost level.

Increased boost pressure improved the fuel mixture standard deviation, with little effect on ammonia fuel slip to the exhaust prior to exhaust valve closing (EVC). The manifold pressure directly effects the in-cylinder charge motion leading to improved mixing with increased pressure and thereby swirl ratio. The boost pressure and engine operating ϕ will have to be weighed against the tradeoffs for both emissions and combustion stability when operating at increasing enleanment levels.

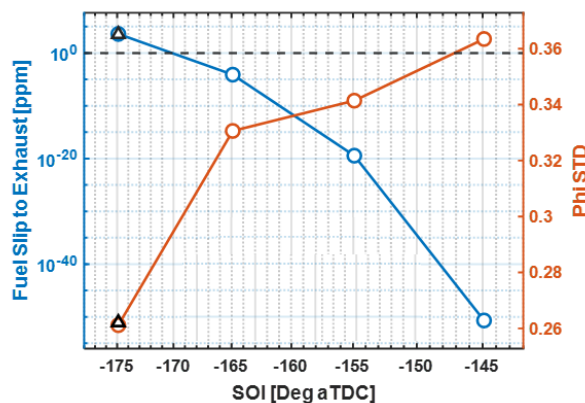


Figure 14 Ammonia Fuel distribution and slip to exhaust SOI of ammonia fuel injection.

The cold flow CFD analysis was completed to guide the design of an optimum set of hardware and other parameters for the engine modifications to enable a solid foundation for initial engine testing and further optimization. Optimum fuel mixing was found to be a combination of a reduced number of injector nozzle holes, early injection timing, low injector position, and proper aiming contributed to the best trade-off between mixing and low fuel slip as shown in Figure 15.

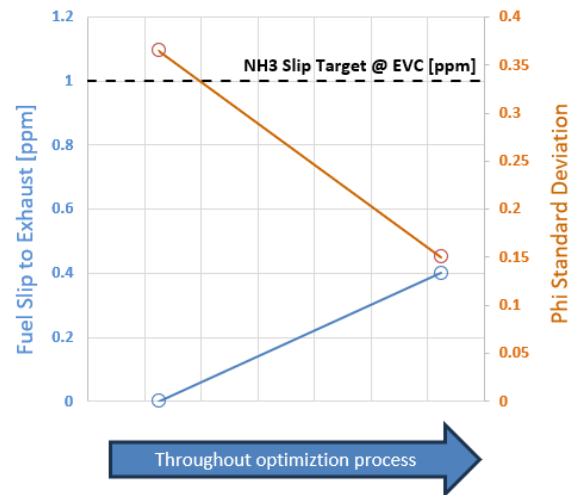


Figure 15 Ammonia fuel distribution and slip to exhaust improvements throughout optimization process.

5 ENGINE TESTING & EMISSIONS RESULTS

5.1 Engine Test Cell & Experimental Setup

The Enterprise research engine used in this study is installed in a test cell on an electric dynamometer. Boost air is provided using an air compressor, and an electronically controlled valve in the exhaust is used to maintain backpressure at an appropriate level to simulate a turbocharger. Diesel fuel is supplied using two hydraulic electronic unit injectors (HEUI), with asymmetric spray patterns injecting into the swirl. Additional details of coolant, oil, and intake air conditioning systems are described in Kaul, *et al.* [12]. An ammonia fuel system was added to the test cell to enable ammonia dual-fuel operation. In order to ensure safe operation with ammonia, a hazard and operability study was conducted [13], and its findings were incorporated into the design of the ammonia fueling system installed in the test cell. Key safety features include multiple ammonia sensors, shutoff valves, and interlocks with test cell ventilation systems to ensure operations can be conducted safely without exposing personnel to hazardous levels of ammonia.

Ammonia was supplied to the test engine via several industrial anhydrous ammonia cylinders with liquid dip tubes plumbed in parallel. At test cell temperatures, the ammonia cylinders were capable of supplying ammonia at between 7 and 8 bar of pressure. The liquid ammonia was routed through the shell side of a shell-and-tube heat exchanger with engine-out coolant flowing through the tube side. A pH meter on the engine coolant return from the vaporizer was used to monitor the heat exchanger for internal leaks. Ammonia fuel flow

was measured using an Emerson Micro Motion Coriolis flow meter. The lines from the heat exchanger to the engine were heat traced and insulated to maintain a temperature of 60°C to avoid condensation and ensure the ammonia was delivered to the engine in a vapor state. A schematic of the system layout is shown in Figure 16.

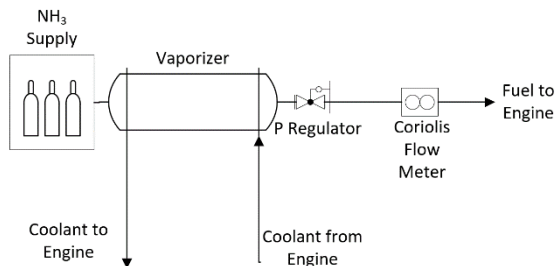


Figure 16 Simplified schematic of ammonia fuel supply system.

Data acquisition and combustion analysis were conducted in real-time using a LabVIEW-based code developed in-house, the Oak Ridge Combustion Analysis System (ORCAS). The engine is instrumented for in-cylinder pressure using a Kistler type 6052C32 transducer, with data collected every 0.2°CA. Exhaust emissions were measured using California Analytical Instruments (CAI) paramagnetic detector for oxygen; a CAI flame ionization detector (FID) for unburned hydrocarbons; an MKS Fourier Transform Infrared (FTIR) analyzer to measure nitrogen oxide (NO), nitrogen dioxide (NO₂), nitrous oxide (N₂O), ammonia (NH₃), carbon monoxide (CO), carbon dioxide (CO₂), water (H₂O), and other species of interest; and an AVL Smoke Meter. Emissions analysis was conducted in real-time in ORCAS using a LabVIEW-based emissions calculator by Dempsey and Ghandhi [14] which was extended by adding ammonia-specific calculations (e.g. ammonia energy substitution ratio, specific N₂O emissions and CO₂-equivalent GHG impact, etc.).

5.2 Optimization Parameters

Stage 1 of the test program was developed to evaluate the impact of various operational parameters on engine efficiency, CO₂ equivalent emissions (CO_{2e}), NH₃ slip, and N₂O emissions. The primary objective was to maximize ammonia energy substitution (AES) while minimising NH₃ slip and N₂O emissions and maintaining a high thermal efficiency. The primary variables identified for testing in stage 1 of the test program were:

- MAP (manifold air pressure)
- Diesel SOI timing

Port timing and exhaust valve timing and duration were held constant during the stage 1 testing as shown in Figure 17. Optimization of exhaust valve timing and duration, pre-injection of diesel fuel, maximising AES and other parameters is planned to be included in stage 2 of the test program.

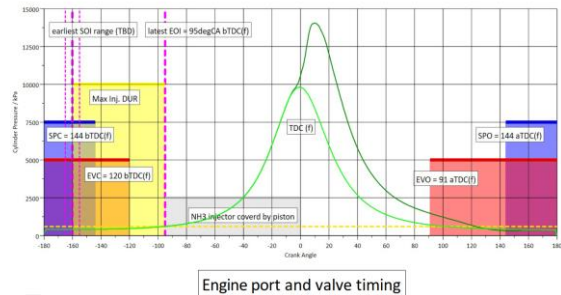


Figure 17 Engine port and valve timing

5.3 Selection of Test Point

The Enterprise research engine used for this study has accumulated a large amount of data, primarily at several discrete steady-state engine speed/load test points as shown graphically in Figure 18. The test points include a “deposit protocol” condition used to conduct lubricant testing and combustion chamber deposits, deliberately chosen to be centralised within the speed/load range of the test points. To take advantage of the historical data, this same point was chosen, operating at 400rpm, 10.9bar IMEP for the majority of the test program.

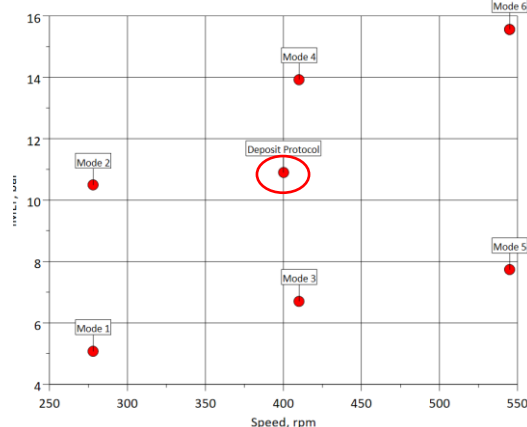


Figure 18 Engine speed and load, selected point

5.4 Emissions & Thermal Efficiency versus Manifold Air Pressure (MAP)

In order to examine the impact of AFR, which has been shown to have a strong impact on emissions of NH₃, NO_x, and N₂O for premixed NH₃ combustion in other engine types [15,16], MAP was varied at the same constant speed and load point defined above. This was performed using a single

diesel pilot injection event. The MAP was adjusted by controlling manifold boost air supply pressure. A diesel SOI scan was conducted at each MAP, with the optimal timing determined to be at the maximum brake torque (MBT) value. During the scan, a constant AES of approximately 60% was maintained to ensure the accuracy and comparability of the results. This comprehensive data collection and analysis provided a detailed understanding of how different MAPs or AFR respectively impact emissions and thermal efficiency, allowing for optimization of engine performance and emissions.

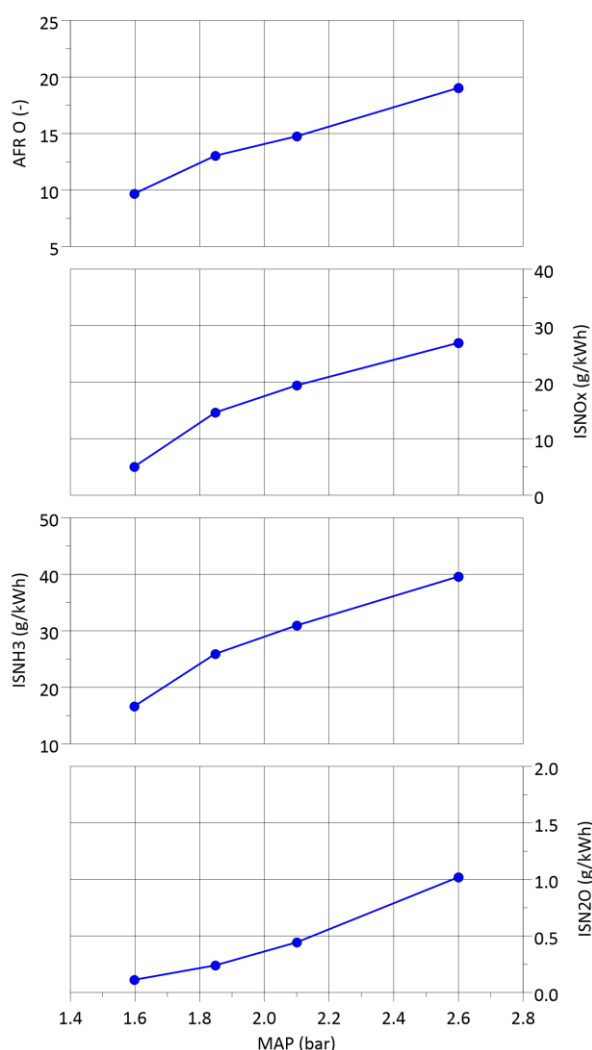


Figure 19 Effect of MAP on Air-Fuel-Ratio and Emissions at 60% AES

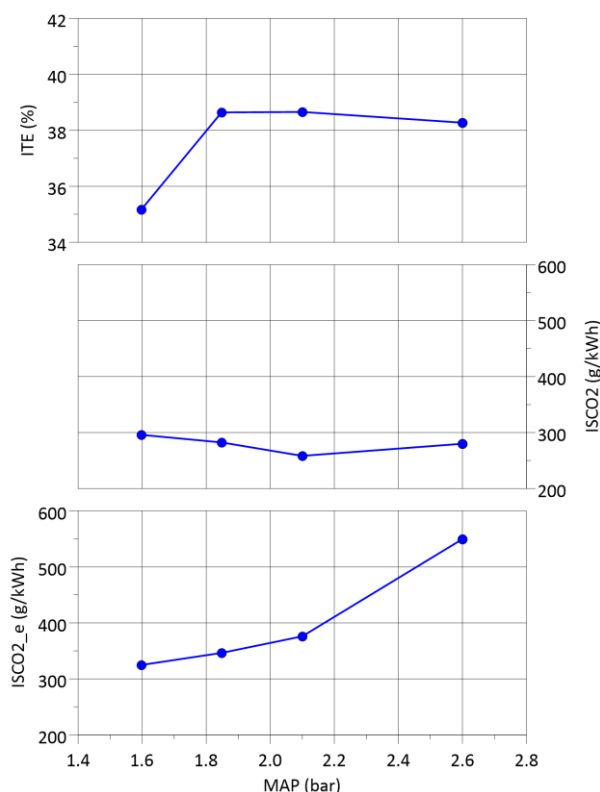


Figure 20 Effect of MAP on Thermal Efficiency & CO₂ Emissions at 60% AES

Figure 19 shows the effect of MAP on AFR, NO_x, NH₃ and N₂O emissions. It was observed that at lower MAP values (richer fuel mixture), emissions of N₂O, NH₃, and NO_x decreased. Westlye et al. [17] reported that N₂O is formed when NH₃ is in the presence of NO and NO₂ at low temperatures during the expansion and exhaust stroke in a reaction known as selective non-catalytic reduction [19]. The creation of N₂O is generally promoted during combustion with lower temperatures as an intermediate product of NO_x formation. By decreasing the MAP, the bulk gas temperature increases, leading to a commensurate reduction in N₂O emissions. A decrease in the effective AFR of the combustion with lower MAP values leads to significant reductions in NH₃ emissions. This effect can be explained by improved flame propagation, less quenching, and higher bulk gas temperature.

Figure 20 shows the effect of MAP on the Indicated Thermal Efficiency (ITE), CO₂, and CO₂ equivalent (CO_{2,e}) emissions. The stoichiometric AFR for an AES of 60% is approximately 8:1. Operation at the lowest MAP value of 1.6bar results in an AFR of less than 10:1, meaning a fuel-air equivalence ratio (ϕ) as high as approximately 0.83. At this low MAP value, the thermal efficiency reduces, resulting in additional fuel (NH₃ and diesel) needed to maintain a constant load (10.9 bar IMEP).

However, even though the thermal efficiency is reduced at the lowest MAP value, the resulting N_2O and NH_3 emissions are at their minimum. Due to the high N_2O emissions global warming potential (GWP) of 273 times that of CO_2 [18], the minimum CO_2e value of 324 g/kWh is achieved at the lowest MAP value. This represents a reduction of 45% in CO_2e compared to the diesel-only baseline of 712 g/kWh.

Figure 21 shows burn data for the MAP scan conducted. Burn duration is seen to increase with increasing MAP. The higher dilution of the fuel (leaner mixture) with increasing MAP reduces flame speed and increases quenching effects as also demonstrated by the increase in NH_3 emissions. The increased burn durations are combined with an earlier combustion phasing as illustrated by the CA10 (location of the cumulative of 10% of the fuel burned) occurring earlier as MAP is increased.

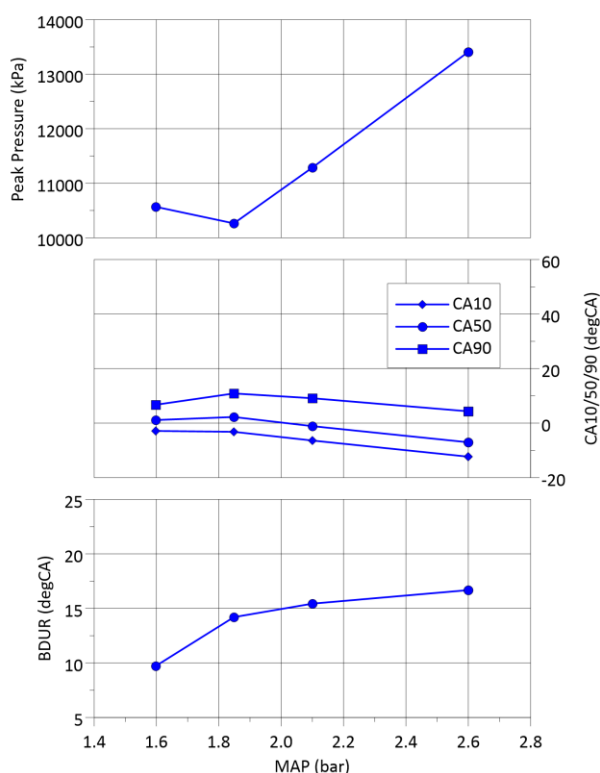


Figure 21 Effect of MAP on Cylinder Pressure and Combustion Burn Metrics at 60% AES

5.5 Emissions & Thermal Efficiency versus Diesel SOI

Varying diesel SOI timing at a constant engine speed and load of 400 rpm, 10.9 bar IMEP and an AES of approximately 80% was performed. The experiments were conducted using a single, fixed

quantity, diesel pilot injection. At each SOI step, all engine data were recorded. The limiting factors considered during the tests included combustion stability, measured by the coefficient of variation (COV) of the indicated mean effective pressure (IMEP), cylinder head temperature, and peak cylinder pressure.

Considering the above limitations, the engine could be operated with diesel SOI values between -24°CA and -6°CA after TDC. Figure 22 shows the effect of diesel SOI on NO_x , NH_3 and N_2O emissions.

At constant AES and mixture strength, NO_x emissions were seen to reduce with later (more retarded) diesel pilot injection timing. The later SOI timings result in more retarded combustion phasing and lower combustion gas temperatures which result in lower NO_x emissions.

NH_3 emissions (or slip) generally increase as the diesel SOI timing is retarded, with a substantial increase at the most retarded SOI timing. Based on the injection timing of the ammonia into the combustion chamber, short-circuiting of ammonia will be limited. Hence, it is hypothesized that most of the NH_3 slip is caused by quenching of the ammonia flame in areas of incomplete combustion. This premature extinguishing of the flame is caused by low flame speed, lowering of combustion temperature near walls, and flame extinguishing in crevices in the combustion chamber.

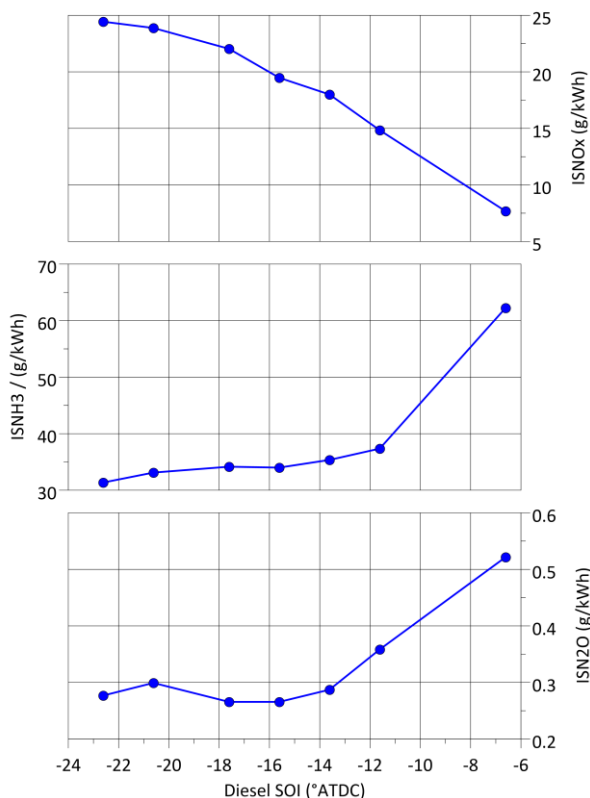


Figure 22 Effect of Diesel SOI on Emissions at 80% AES

Overall, the engine-out NO_x and NH₃ emissions are considerably elevated. The NO_x emissions should be weighed against the levels of NH₃ for potential use in Selective Catalytic Reduction (SCR) systems. The NO_x /NH₃ ratio, often referred to as the alpha ratio, is crucial for the efficiency of SCR systems. The ideal NO_x /NH₃ ratio is typically 1:1, meaning one molecule of ammonia (NH₃) is used to reduce one molecule of nitrogen oxides (NO_x) under optimal conditions. Based on the NH₃ and NO_x emissions shown in Figure 22, the NO_x /NH₃ ratio ranges between 0.1 and 0.8. Reduction of the NH₃ emissions will be a focus area for the next stages of the engine development program including additional diesel injection control, in-cylinder motion, exhaust valve timing and duration as well as combustion chamber design.

N₂O emissions were shown to be relatively insensitive to diesel SOI timing between -23° to -14° ATDC, with a sharp increase for diesel SOI timings later than -14° ATDC. The N₂O emissions generally increase with lower temperatures during combustion, as encountered with retarded combustion phasing with late diesel SOI timing.

Figure 23 shows the effect of diesel SOI timing on the ITE, CO₂, and CO₂e emissions. The indicated CO₂ emissions (ISCO₂) of 132 g/kWh align with the highest ITE of 38.1%. The lowest indicated CO₂e emissions of 203 g/kWh was achieved at a SOI timing of -16°CA ATDC which represents a reduction of approximately 71% in CO₂e compared to the diesel-only baseline of 712 g/kWh. The increase in CO₂e emissions compared to CO₂ only emissions for operation on ammonia is attributed to the N₂O (ISN₂O) emissions. The high GWP of N₂O as detailed in the previous section significantly offsets some of the GHG benefits gained from reduced CO₂ emissions by substituting ammonia for diesel fuel.

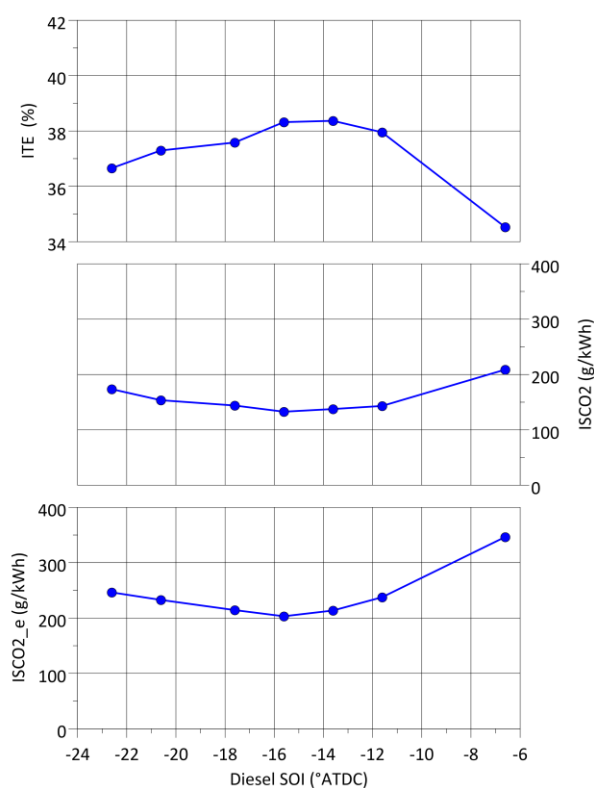


Figure 23 Effect of Diesel SOI on Thermal Efficiency & CO₂ Emissions at 80% AES

Figure 24 demonstrates the impact of diesel SOI on peak cylinder pressure and other key combustion burn metrics. As expected, the diesel SOI timing has a direct relationship with combustion phasing. The trend of increasing N₂O and NH₃ emissions reported with more retarded SOI of the diesel pilot injection can be explained by the more retarded combustion phasing leading to reduced temperature, lower peak cylinder pressures, and resulting increased burn durations (CA₉₀-CA₁₀). A maximum ITE of 38.1% was achieved at a diesel

SOI of -16°CA ATDC corresponding to a CA50 (50% of fuel burned) timing of $\sim 1.2^{\circ}\text{ATDC}$. The burn duration was found to increase with more retarded diesel SOI, leading to lower ITE at injection timings later than -16°ATDC . The slower combustion characteristics of ammonia is shown to reduce the thermal efficiency and results in higher unburned fuel emissions.

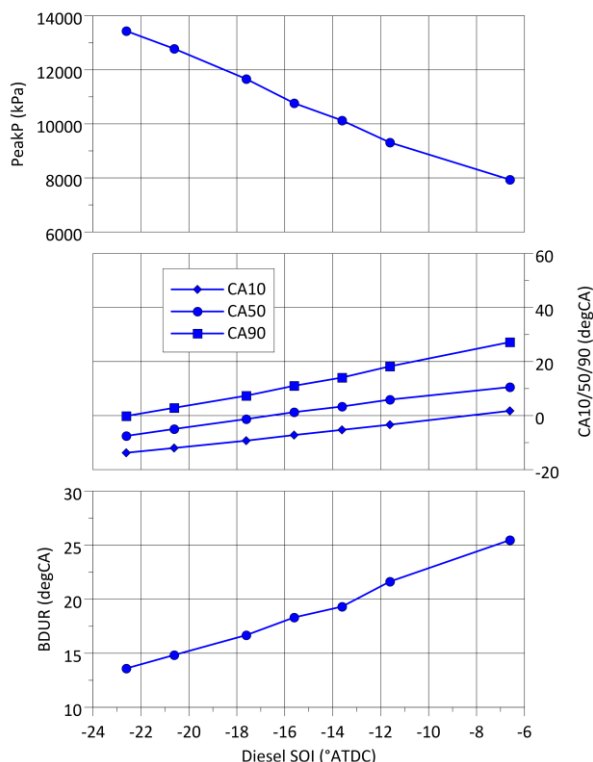


Figure 24 Effect of Diesel SOI on Cylinder Pressure and Combustion Burn Metrics at 80% AES

5.6 Ammonia Dual Fuel to Diesel Baseline Comparison

Figure 25 and Figure 26 show the direct comparison between ammonia dual-fuel operation with 80% AES and diesel operation at the test point of 400 rpm, 10.9 bar IMEP. The baseline diesel calibration was optimized for MBT without regard for emissions control in order to maximise ITE with diesel operation at 0% AES.

Figure 25 shows the comparison in HC, N_2O , NO_x and NH_3 emissions. NO_x emissions are seen to be high in both operational modes. It should be highlighted that due to the baseline diesel calibration targeting maximum efficiency, the typical trade-off between NO_x and soot was not considered. It is expected substantially lower NO_x emissions can be achieved for the diesel mode operation through further calibration optimization.

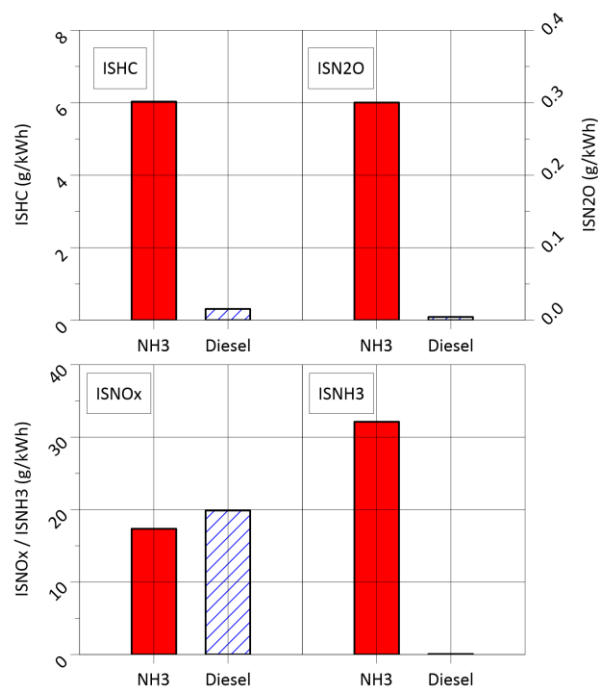


Figure 25 Emissions in Diesel vs NH_3 mode at 80% AES

In dual-fuel mode, a NO_x to NH_3 emissions ratio near one can be desirable when utilizing SCR systems, which use NH_3 as a reduction agent for the NO_x emissions. However, the raw NH_3 slip is high and should be the subject of further optimization.

Diesel diffusion combustion with excess air delivers excellent combustion efficiency, resulting in very low HC emission levels. However, due to the nature of a dual-fuel combustion system, which is a combination of both diffusion and premixed combustion, HC emissions are substantially higher and need to be considered when optimizing for NH_3 dual-fuel operation. The increased HC emissions are caused by similar mechanisms as those leading to the high NH_3 slip levels as explained previously.

Figure 26 shows the comparison between ammonia dual fuel and diesel only operation for CO_2 , CO_2e and ITE at 400 rpm, 10.9 bar IMEP. It was observed that ITE was reduced with higher AES when in dual fuel operation. This compromise in ITE indicates that while ammonia substitution can substantially reduce CO_2 emissions, it may also lead to less efficient fuel conversion due to slower combustion and resulting higher unburned fuel emissions.

The ammonia dual fuel operation achieved a minimum CO_2e value of 217 g/kWh compared to 712 g/kWh achieved for the diesel only mode operation. This represents more than a 70%

reduction in CO₂e including the offset due to the N₂O emissions.

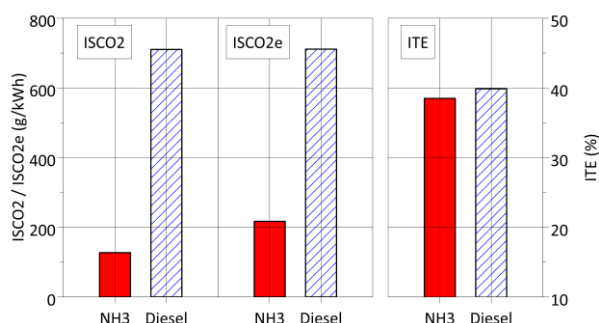


Figure 26 CO₂, CO₂e and ITE in Diesel vs NH₃ mode at 80% AES

The initial results presented reflect the status of early testing in stage 1 of the overall program. More detailed analysis will be performed in the future to optimize the best achievable AES and reduce CO₂e, N₂O, and/or NH₃ emissions respectively, by deploying other optimization parameters such as pre-pilot injection of diesel, increased NH₃ pressure, and enhanced diesel injector control. The current engine and its calibration are still in the process of being further optimized for the specific engine conditions and operating points, to improve the overall engine efficiency.

6 CONCLUSIONS & NEXT STEPS

6.1 Conclusion

Analysis-led design enabled the development of a capable set of engine hardware prior to any experimental testing. This approach has the potential to provide a significant advantage to advanced developments of ammonia fuel for usage in the marine market. This type of technical approach and in-depth investigation allows for decreased development times and cost, safety risk mitigation, and the ability to evaluate a wide range of parameters not likely possible with conventional hardware testing.

The use of a reduced scale, single cylinder research engine for fundamental studies provided a method for rapid development of hardware, control strategies and calibration in comparison to full scale large marine engines. Fuel supply requirements were also significantly reduced compared to a full-scale engine, enabling operation with small quantities of ammonia on site and simplifying the required safety systems for ammonia storage.

Initial results from engine testing show potential for large reduction in GHG emissions using a relatively simple to adopt combustion system using ammonia as the primary energy source. Ammonia substitution of 80% combined with CO₂e emissions reductions of approximately 70% compared to the diesel fuel only baseline have been demonstrated with limited optimization. Several opportunities exist for further optimization to further increase ammonia substitution as well as reduce the noxious and GHG emissions.

6.2 Next steps

Further stages are planned for continued development and optimization of engine hardware, control system, calibration and the simulation toolset. Several limitations are evident in the current hardware set, including limited authority and flexibility of the diesel injection system. Higher turn down, reduced minimum flow rate, faster response and multiple diesel injection events are planned as part of the diesel injection system optimization. This will allow pre, post and main diesel injection events to be instigated, providing significantly improved control.

Additional scope planned includes optimization of in-cylinder airflow and exhaust valve timing and duration, including adoption of a fully variable active valvetrain to allow real-time adjustment in a running engine. Further optimization of engine hardware such as combustion chamber and piston designs to reduce crevice volume within the engine will be investigated. This, in conjunction with an optimized engine calibration including ammonia injection sequencing strategies is expected to significantly reduce NH₃ slip emissions.

A further step includes correlation of the models used in the various analysis toolsets used in this study to the experimental results. After this is complete, model robustness and scaling will be interrogated through correlation to other engines operating with ammonia fuel. With scaling guidelines established and model accuracy verified, a fully integrated co-simulation toolset will be available to promote rapid, safe, cost-effective development of large engines utilizing low life-cycle carbon fuels.

7 DEFINITIONS, ACRONYMS, ABBREVIATIONS

ϕ : fuel-air equivalence ratio

λ : excess air ratio (air-fuel equivalence ratio)

AES: ammonia energy substitution

AFR: air fuel ratio

BMEP: brake mean effective pressure

CFD: computational fluid dynamics

CLO: cylinder lubrication oil

COV: coefficient of variation

DUR: injection duration

EOI: end of injection

EVC: exhaust valve close

EVO: exhaust valve open

FEA: finite element analysis

FID: flame ionization detector

FMEP: friction mean effective pressure

FTIR: Fourier transform infrared spectroscopy

GHG: green house gas

GWP: global warming potential

HC: hydrocarbon

ITE: indicated thermal efficiency

IMEP: indicated mean effective pressure

IMO: International Maritime Organization

IPC: intake port close

IPO: intake port open

MBT: maximum brake torque

MAP: manifold air pressure

ORCAS: Oak Ridge combustion analysis system

ORNL: Oak Ridge National Laboratory

PDF: probability density function

PHI: fuel–air equivalence ratio

SCR: selective catalytic reduction

SOI: start of injection

TDC: top dead centre

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