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IGNITION EXPERIMENTS AND SIMULATIONS OF AQUEOUS AMMONIA AND HYDROGEN PEROXIDE MIXTURES IN A DIESEL ENGINE

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Abstract: This work provides first experimental results of the use of ternary fuel blend consisting of ammonia (NH_3), water (H_2O) and hydrogen peroxide (H_2O_2) being used as carbonless diesel fuel blends in a conventional small-bore diesel engine. The work is aimed at identifying safe mixtures of fuels that contain zero carbon and that could replace current fossil fuels without requiring major engine replacements. Another important aspect of this work is that the fuels should be liquid at typical atmospheric conditions, so as to provide a safer alternative to gaseous ammonia and hydrogen for smaller marine applications. The results showed small but clearly visible heat release from the fuel decomposition in the engine following fuel injection. This could be replicated by simulations combining thermodynamic and chemical kinetic modelling. The simulation results showed promise that the results may be extended to different engine loads and different fuel injection timings, whilst achieving reliable fuel ignition. A life-cycle assessment (LCA) was conducted to analyse the potential benefits of using these carbonless fuel mixtures as a single fuel, compared to dual-fuel injection strategies using fossil diesel fuel as pilot injection and anhydrous ammonia as the main fuel. The LCA results showed that the mixture of NH_3 and H_2O_2 can reduce GWP100 by about 73.5% compared with conventional diesel, showing strong potential for reducing the climate impact of marine engines. However, further improvements in H_2O_2 production and fuel use are needed to reduce impacts in other environmental categories.

Keywords: Ammonia, Ammonium nitrate, Diesel Engine, Fuel, Water.

1. INTRODUCTION

The World Meteorological Organisation reported that the year 2025 was 1.44± 0.13 °C above the 1850-1900 average (WMO, 2026 [[1.]]), which is just short of the 1.5°C aim set out in the Paris Agreement (UNFCCC, 2016 [[2.]]). Shipping contributes around 3% of global greenhouse gas emissions (IMO, 2020 [[3.]]), which is expected to increase if not regulated appropriately. The final energy demand for shipping is expected to remain at around 10 EJ per annum for the foreseeable future, according to predictions up to 2050 (IMO, 2024 [[4.]]).

International shipping is a global industry and its emissions are regulated by the International Maritime Organization (IMO), which has set out its aim for net-zero greenhouse gas emissions by 2050 (IMO, 2023 [[5.]]), and is currently in the difficult process of trying to agree on a framework of globally binding regulations for meeting this aim (IMO, 2025 [[6.]]). Worldwide consensus on regulations is likely a key element for decarbonisation of international shipping, and such global consensus will be aided by the existence of accessible and cost-effective decarbonisation solutions. Many of the older vessels may not be easily retrofitted if a high capital expenditure is needed upfront to upgrade the engine and fuel system, which is why drop-in fuel solutions may be key to accelerating greenhouse gas reduction from shipping, by offering an accessible solution to older ships, and to those less-able to invest larger amounts of capital up-front.

Bio-fuels are currently the only drop-in fuels that can be used without any change in engine or fuel system. In practice these often end-up becoming the preferred option for older ships trying to reduce emissions, for which expensive technical upgrades may not be economically feasible. Biofuels are as of now amongst

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the cheaper options for reducing greenhouse gas emissions [[4.]], due to the low capital expense. At the same time, it is apparent that the supply of sustainable biomass is physically limited, and some LCA in the literature have shown that the consequences of increased biofuel production can in some cases lead to higher climate impacts than those from fossil fuels [[7.], [8.]].

The production of e-fuels such as hydrogen and ammonia, is one possible way of decoupling renewable fuel production from biomass resources. In the case of methanol, the production is still linked to the requirement for limited resources of biogenic CO_2, in order for the methanol to be sustainable. The use of CO_2 from direct air capture would be sustainable, but predictions for future costs of direct air capture of CO_2 estimates a cost range of 226-885 $/tCO2 [[9.]]. Even assuming the lowest cost scenario of 226 $/t$CO_2$ and assuming a calorific value of 21 MJ/kg of methanol, that would add a cost of 14.73 $/GJ, just for the captured CO_2 in future sustainable methanol. Aviation is also a competing sector, that arguably is in more dire need for carbon-based liquid fuels than shipping.

The trivial solution to avoiding the need for CO_2 as a feedstock for fuel productions is to use carbonless e-fuels. The challenge with the most prominent carbonless e-fuels hydrogen and ammonia is that both are gaseous at atmospheric pressure and common atmospheric temperatures, and are therefore more difficult to store. Hydrogen has the additional challenge of having a significant greenhouse gas impact itself (hydrogen GWP_{100} = 11±5 [[10.]]) and requiring very low temperature to be stored in liquid form (-253°C). Ammonia, although not having any climate impact itself, is toxic and gaseous at a pressure of 1 atmosphere and 20°C, and either requires cooling to -33.33°C at atmospheric pressure, or pressurising to around 1 MPa (at 25°C) to become liquid [[11.]]. If used as fuels in pure form, both hydrogen and ammonia require entirely different fuel systems and engine operational settings to work as fuels in marine diesel engines. Hydrogen and ammonia usually require an additional pilot fuel injection to ignite reliably in a diesel engine [[12.], [13.]].

Ammonia is a promising carbonless fuel, but for a broader success of its application, effective solutions for mitigating its toxicity risk and its difficulty to ignite in a diesel engine need to be found.

A potential solution is to use ammonia in a form that is liquid at room temperature. This can be achieved by using aqueous ammonia [[14.]], but also by blending ammonia with ammonium nitrate, to reduce the water content and improve its ignitability [[15.], [16.]]. To achieve the reliable ignition of ammonia, whilst at the same time ensuring that the physical mixture remains liquid at atmospheric pressure and typical atmospheric temperatures, it is necessary to study and measure the physical properties of ternary mixtures of ammonium nitrate, ammonia and water [[17.], [18.]]. Another chemical composition that is receiving interest by recent research, are the mixtures of ammonia with hydrogen peroxide (H_2O_2). The first study to examine the autoignition dynamics of hydrogen peroxide and ammonia mixtures diluted with water, was that of Khalil et al. (2020) [[19.]]. The first study to apply this mixture to engine applications was that of Frost et al. (2021) [[20.]]. Frost et al. (2021) found through simulation that it may be possible to remove the need for a pilot fuel injection in a diesel engine, if hydrogen peroxide was used as ignition improver in aqueous mixture with ammonia. Shafiq and Tingas (2022) [[21.]] carried out a systematic analysis of the performance of using ammonia and hydrogen peroxide (H_2O_2) with water dilution as fuel for Homogeneous Charge Compression Ignition (HCCI) engine applications, and reported significant influence of H_2O_2 as ignition improver and higher indicated mean effective pressure (IMEP) resulting from its use, compared with inlet air heating. Singh et al. (2022)[[22.]] investigated the effects of hydrogen peroxide on ignition delays and laminar flame speeds for premixed blends of ammonia, methane and air using chemical kinetic simulations. Single-fuel diesel-type engine combustion simulations for ammonia, hydrogen peroxide and water fuel mixtures in air where reported by Schönborn & Lee (2022)[[23.]]. Paterson et al. (2024)[[24.]] reported chemical kinetic engine simulations in which a pilot injection of 10% (vol.) hydrogen peroxide in water was used to help ignite fumigated fuel mixtures of ammonia and hydrogen (0.8 and 0.2 mole fraction respectively).

The literature thus provides quite a few studies of the use of hydrogen peroxide as ignition improver for ammonia as fuel, but apart from the studies by Frost et al. (2021)[[20.]], Schönborn & Lee (2022)[[23.]] the simulations used premixed combustion approaches. In the case of Paterson et al. (2024)[[24.]] this consisted of a hybrid approach using premixed ammonia and hydrogen in air as the main fuel, with a pilot fuel injection of hydrogen peroxide. A gap in the current literature is the lack of experimental studies, especially for non-premixed combustion, i.e. diffusion-controlled diesel combustion, which is the most reliable combustion mode for large marine engines.

The first works to provide experimental evidence for the use of hydrogen peroxide as ignition improver for ammonia, are the works of Han et al. (2024)[[25.]], followed by Hassan Ali & Ali (2024)[[26.]] and Han et al. (2025)[[27.]]. These investigations of Han et al. used a pilot injection of diesel fuel to provide a source of ignition, whilst the investigations of Hassan Ali & Ali (2024) analysed the ignition of homogeneously premixed blends of fuel in air, in HCCI engine operating mode.

The aim of this current work is to provide the first experimentally measured evidence of ignition for direct injection diffusion-controlled combustion, using liquid

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hydrogen peroxide, ammonia and water mixtures for a single-fuel approach. The direct injection diffusion-controlled combustion approach is the safest and most reliable way of operating large marine diesel engines, and is significantly different from other approaches such as HCCI, which have only practically been applied to small bore high-speed engines. The ultimate aim for the use of hydrogen peroxide as ignition improver would be to make a pilot fuel injection of conventional diesel fuel entirely redundant, and to thereby facilitate the transition from accepted high-pressure dual-fuel approaches, which typically still use conventional fossil fuels for a pilot injection, to high-pressure single-fuel approaches, using a liquid carbonless fuel. So far, no investigations with this aim have been reported in the literature.

2. MATERIALS AND METHDOS

Experiments were conducted using a direct injection generator engine with mechanical fuel pump and injector on a small-bore diesel engine (Lutian 5GF-LDE). The engine was turned-over electrically using the electrical starter motor of the generator, ensuring a constant engine speed of 165 ± 0.0 rpm during the tests used for this analysis. The engine cylinder pressure was measured at 10 000 Hz sampling frequency using a piezoresistive thin-film-on-steel pressure sensor (Trafag 8253) with a pressure range of 0...250 bar gauge and a pressure accuracy of ±0.3 % or 0.75 bar.

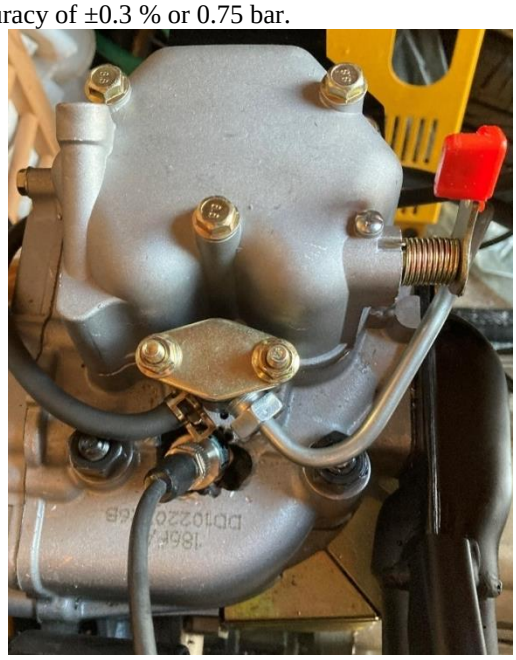


Figure 1. Test engine

The injection timing was set at 173° crank angle, i.e. 7° crank angle before top-dead-centre. The pressure sensor was fed using an 18V voltage supply and the 4-20 mA signal was acquired by measuring the voltage over a 470 Ohm resistor using a Labjack U3-LV time-triggered data acquisition system.

The fuel composition consisted of water, ammonia and hydrogen peroxide, in the molar fractions shown in Table 1.

Table 1. Fuel composition in mass fraction

Fuel blend number	NH_3	H_2O	H_2O_2
0	0.26	0.74	0.00
1	0.2314	0.74825	0.0204
2	0.2028	0.7565	0.0407
3	0.17	0.76	0.06

The fuel was prepared through volumetric blending of aqueous hydrogen peroxide (30% m/m) to the aqueous ammonia (25% m/m) using an open glass beaker. The mixture was delivered directly through a clean pipe to the fuel pump inlet using a gravity feed from a funnel from a 0.35 m height. The engine was operated either with the fuel injection switched on or with the fuel injection switched off, which was controlled using a mechanical switch. The experiments were repeated several times in various orders in order to verify the repeatability of the results.

2.1. Engine simulations

The experimental operation of the engine was compared with a thermodynamic and chemical kinetic model of the engine, which simulated the evolution of the molar composition, temperature and pressure of the air aspirated into the engine, as well as the fuel injected into the engine and the ensuing chemical reactions. This model assumed air being aspirated into the engine at a composition of 21% O_2, and 79% N_2, at atmospheric pressure and a temperature of 443 K, which was the temperature that could be reached in steady-state operation of the engine. The air was then compressed to around 3.3 MPa, assuming near-adiabatic compression, and at 179 degrees crank angle (i.e. 1 crank angle degree before top-dead-centre (TDC)) the fuel was injected into the engine. The fuel consisted of a ternary mixture of water, ammonia, and hydrogen peroxide, in the mole fractions given in

Table 1. The chemical reactions were simulated using the gas-phase chemical kinetic combustion model developed by Song et al. (2016) [[28.]].

A comparison of this chemical kinetic model with experimental results has been reported in an earlier work [[20.]].

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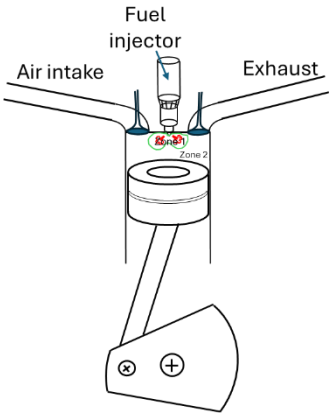


Figure 2. Schematic of engine simulation approach [20]

In order to reflect the different fuel-air stoichiometries present in a diesel engine, the engine was simulated using two reactor zones, which were spatially separated to have different stoichiometries of fuel and air, but the same pressure. These two zones were defined as Zone 1 (ignition zone) which had a fuel air stoichiometry close to unity, to represent the reactions taking place in the region around the fuel spray, and Zone 2 that represented the bulk gases within the engine, consisting of air.

2.2. LCA methods

The Life Cycle assessment (LCA) was carried out following the guidance and framework described in ISO14040 (ISO, 2006)[[34.]]. Assessing the life-cycle climate impact of the fuel is important in taking into account not only emissions during the The modelling was performed using LCA for Experts (version 10.9.3.0) software with data from the Eco invent database (version 3.8).

A simplified attributional LCA was carried out to compare the well to wake (WTW) environmental performance of three fuel scenarios:

(i) Diesel - using 100% conventional diesel fuel,

(ii) (ii) NH_3 & Diesel - using green ammonia and diesel as pilot fuel,

(iii) NH_3 & H_2O_2, using ammonia blending with hydrogen peroxide (**Error! Reference source not found.**).

Table 2. Fuel consumption in three scenarios

Scenarios	Items	Unit	Diesel	Ammonia	Hydrogen peroxide
	LHV	MJ/kg	43.10	18.60	1.5887
	Efficiency	%	51.00%	51.00%	51.00%
Diesel	% Energy share	%	100.00%	0.00%	0.00%
	Fuel consumption	g	163.78	0.00	0.00
NH_3 & Diesel	% Energy share	%	5.00%	95.00%	0.00%
	Fuel consumption	g	8.19	360.53	0.00
NH_3 & H_2O_2	% Energy share	%	0.00%	93.52%	6.48%
	Fuel consumption	g	0.00	354.93	247.49

The functional unit was defined as "**1 kWh shaft power output**". An engine efficiency of 51% was assumed for all three scenarios. In the NH_3 & Diesel scenario, 95% of the fuel energy was supplied by ammonia and the remaining 5% by diesel as pilot fuel, following the assumptions in (Dong et al., 2023)[[29.]].

The system boundary included fuel production (well to tank, WTT) and fuel combustion in the engine (tank to wake, TTW). Fuel transportation and waste treatment are excluded from the calculation.

Diesel fuel was assumed to be fossil-based. Green ammonia was modelled using life cycle inventory data adapted from [[29.]], with European wind electricity. Green hydrogen peroxide production was based on Eco invent inventory data, where conventional electricity inputs were replaced by renewable wind electricity in hydrogen peroxide production. presents the inputs and outputs for the hydrogen peroxide production from Eco invent database.

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Table 2. Data used for 1 kg of in 50% hydrogen peroxide solution state production (source: Eco invent version 3.8)

Items	Amount	Unit
Input		
GLO: anthraquinone [allocatable product]	0.000952	kg
GLO: benzene [allocatable product]	0.00193	kg
GLO: chemical, inorganic [allocatable product]	0.00068	kg
GLO: sodium hydroxide, without water, in 50% solution state [allocatable product]	0.00064	kg
GLO: solvent, organic [allocatable product]	0.00145	kg
IAI Area, EU27 & EFTA: aluminium oxide, non-metallurgical [41432: Alumina (aluminium oxide), except artificial corundum]	0.00961	kg
RER: chemical factory, organics [allocatable product]	4.00E-10	pcs.
RER: electricity, medium voltage [allocatable product]	4.37	MJ
RER: hydrogen, liquid [allocatable product]	0.0656	kg
RER: nitrogen, liquid [allocatable product]	0.0508	kg
RER: oxygen, liquid [allocatable product]	0.0293	kg
RER: steam, in chemical industry [allocatable product]	1.58	kg
Water, cooling, unspecified natural origin [Water]	0.17	m^3
Water, unspecified natural origin [Water]	0.00192	m^3
Outputs		
Water [Inorganic emissions to air]	0.066269	m^3
Solids (suspended) [Particles to fresh water]	0.000151	kg
NMVOC (unspecified) [Group NMVOC to air]	0.00053	kg
Total organic bound carbon (TOC) [Analytical measures to fresh water]	0.0003	kg
Hydrogen [Inorganic emissions to air]	3.83E-05	kg
Hydrogen peroxide, without water, in 50% solution state [allocatable product]	1	kg
Aromatic hydrocarbons (unspecified) [Hydrocarbons to fresh water]	3.75E-07	kg
Hydrocarbons, aromatic [Group NMVOC to air]	0.000128	kg
Chemical oxygen demand (COD) [Analytical measures to fresh water]	0.00094	kg
Phosphate [Inorganic emissions to fresh water]	1.25E-05	kg
Nitrate [Inorganic emissions to fresh water]	0.000203	kg
Water [Other emissions to fresh water]	0.105651	m^3
Chloride [Inorganic emissions to fresh water]	0.00038	kg
Biological oxygen demand (BOD) [Analytical measures to fresh water]	0.00026	kg
Hydrogen peroxide [Inorganic emissions to fresh water]	0.0006	kg
Dissolved Organic Carbon [Analytical measures to fresh water]	0.0003	kg

Table 4 and

Table 4 present the WTT and the emission factors of fuels (energy carriers) in this LCA study. It is assumed that the combustion of hydrogen peroxide does not generate any polluting emissions.

Table 3. WTT carbon factors of fuels (GWP100 - kg CO_2 eq./kg of fuel)

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Fuels	Value (kg CO_2 eq./kg of fuel)
Diesel	7.31E-01
Ammonia	1.45E-01
Hydrogen peroxide (2kg of 50% hydrogen peroxide solution state), equivalent to 1kg of pure hydrogen peroxide	3.60E-01

Table 4. TTW emission factors (kg of emission per kg of fuels)

Emissions	Diesel	NH_3	H_2O_2 (pure)
CO_2	3.19	0	0
CO	0.0109	0	0
PM2.5	0.00412	0	0
CH4	0.00005	0	0
NO_X	0.0425	0.02033	0
NMVOC	0.00472	0	0
SO_X	0.0001	0	0
N_2O	0.00018	0.00033	0
NH_3	0	0.0095	0

Note: Emission factors for ammonia combustions are collected from [[30.]][[31.]]. TTW emission factors for diesel are taken from [[32.]] and [[33.]].

The main environmental indicator considered in this study was the GWP100 (expressed as gCO_2 eq. per kWh). In addition, other environmental indicators from the CML2001 method were also evaluated. The results were presented into WTT and TTW contributions to identify the relative importance of fuel production and fuel use phases.

3. RESULTS

The results of this work comprise of a combination of engine experiments, thermodynamic and chemical kinetic engine simulations, and environmental LCA, focusing on the climate impact of the use of aqueous ammonia hydrogen peroxide as fuel.

3.1. Engine Experiments

The experimentally measured pressure traces were recorded for the fuel mixture with the highest fraction of hydrogen peroxide previously referred to as Fuel Blend Number 3 in
Table 1. The mixture showed small but significant differences as the fuel injection was turned on. The pressure traces with fuel injection off and on are shown in Figure 3.

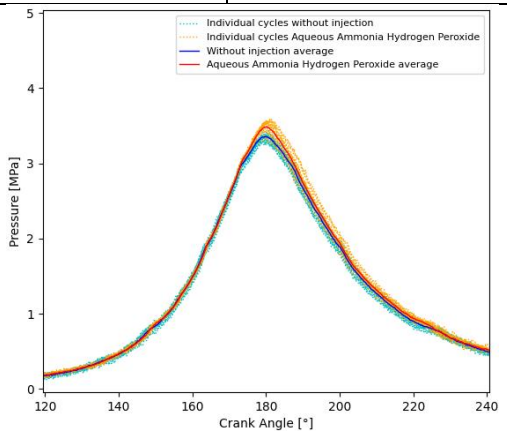


Figure 3. Pressure traces for generator engine without fuel injection and fuel injection of aqueous ammonia hydrogen peroxide blend.

The results show that when the engine was operated with a direct injection of aqueous ammonia hydrogen peroxide fuel blend, a clear increase in pressure is visible after the start of injection at around 173 degrees crank angle. This is shown by the individual pressure traces shown in orange colour in Figure 3, and by their ensemble averaged pressure trace shown in red colour. For the cycles with the fuel injection deactivated, as shown by the plots in cyan colour, and their ensemble averaged trace shown in blue colour, the peak pressures achieved during the cycle were lower, and the slope of pressure versus crank angle just before top-dead-centre (180 degrees crank angle) was lower than when the injection was switched on. This indicates that the aqueous ammonia hydrogen peroxide mixture was subject to some chemical decomposition taking place,

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with the result of gas formation or heat release being present ensuing the fuel injection. The gravimetric heating value of the fuel (aqueous ammonia, hydrogen peroxide and water blend) was much lower (1.58 MJ/kg) than for conventional diesel fuel (42.7 MJ/kg).

3.2. Engine Simulations

The first set of simulations tried to replicate the conditions under which the experimental measurements were carried out in the small generator engine, shown in section 3.1, in order to validate the simulation model. The simulations show similar results to what the experiments showed, in that a small but visible difference exists by chemical composition of the mixture following fuel injection at around 173 degrees crank angle.

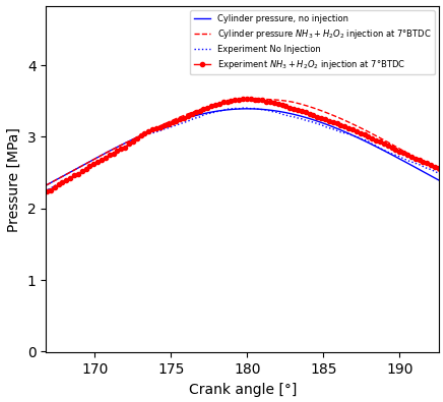


Figure 4. Simulated and comparison with corresponding measured pressure traces.

Figure 44 shows that the increase in pressure was relatively low with respect to the compression pressure of the engine, even when no fuel was injected. This can be at least partly explained by the low heating value of the fuel. The aqueous ammonia, hydrogen peroxide and water mixture had a gravimetric heating value of 1.58 MJ/kg, which is only about 3.7% of the gravimetric heating value of diesel fuel (around 43 MJ/kg).

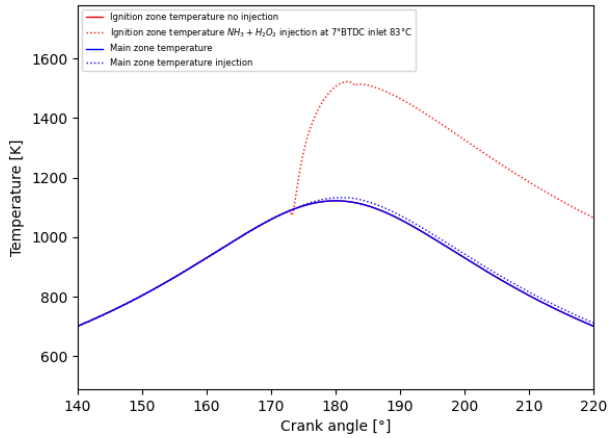


Figure 5. Temperature within the two zones in the simulation, with and without hydrogen peroxide.

In order to better understand the effect of adding hydrogen peroxide to reactivity of the fuel mixture, the temperature within the two engine zones is visualized in Figure 5 above. It is visible that for the case of no fuel injection taking place, the temperature in Zone 1 and Zone 2 was identical, and followed the expected curve of a motored engine, with temperature increasing due to compression of the air up until 180 degrees crank angle (i.e. top-dead-center, TDC), and the temperature decreasing again during the ensuing expansion. For the case in which fuel injection took place, a strong increase in temperature is notable in Zone 1, the zone into which the fuel was injected. The temperature increased following the injection of the fuel from around 1050 K, to just below 1600 K around TDC.

In order to investigate the effect of systematically varying the amount of hydrogen peroxide in the fuel mixture, a series of simulations were carried out to model this effect. The simulations were carried out for four fuel mixtures, namely Fuel Blend Numbers 0-4, which varied the mole fraction of hydrogen peroxide from 0 to 6 %. The results of these simulations are shown in Figure 6 below.

Figure 6 shows how increasing the amount of hydrogen peroxide in the fuel mixture progressively increased the peak cylinder pressure achieved in the cycle for mass fractions of H2O2 changing from 0.00 to 0.02, and 0.04.

For a mass fraction of 0.06 H_2O_2 the peak cylinder pressure reduced again slightly from that for a mass fraction of 0.04 H_2O_2, indicating that the amount of ignition improver was sufficient to achieve reliable and that no further increase in ignition improver may be necessary beyond 0.06 for these engine operating conditions.

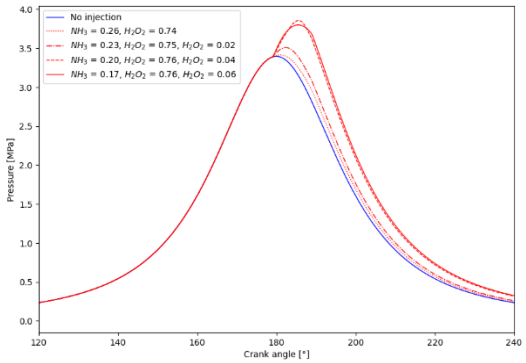


Figure 6. Influence of varying H2O2 fraction in the fuel mixture.

The influence of adding varying the amount of engine load by adjusting the amount of fuel mass

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injected for fuel blend 3 was investigated in a series of simulations shown in Figure 7. The results show that for all the indicated mean effective pressures (IMEPs) describing various engine loads that were investigated (0.0, 1.0, 1.5 bar IMEP) Fuel blend number 3 consisting of molar fractions of 0.17 NH_3, 0.76 H_2O, and 0.06 H_2O_2 were simulated to reliably ignite under the simulated conditions. This provides some indication of the fuel concept being applicable to varying engine loads, as long as ignition can be reliably achieved.

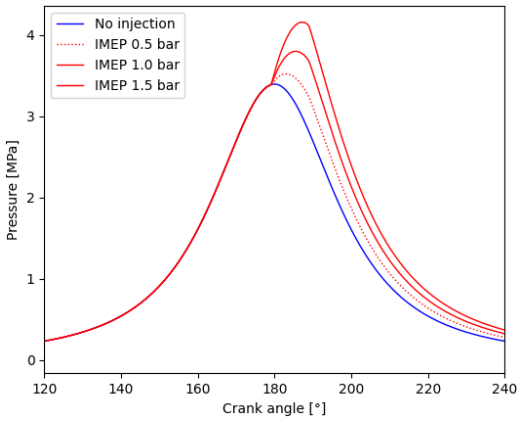


Figure 7. Engine load changes simulated for Fuel blend 3 consisting of mole fractions of molar fractions of 0.17 NH_3, 0.76 H_2O, and 0.06 H_2O_2

In order to investigate the ignition stability for various injection timing, a series of simulations were performed to investigate different injection timings. Figure 78 shows the pressure traces simulated for injection timings of 173, 179 and 185 degrees crank angle for the engine developing a load of 1.0 bar IMEP.

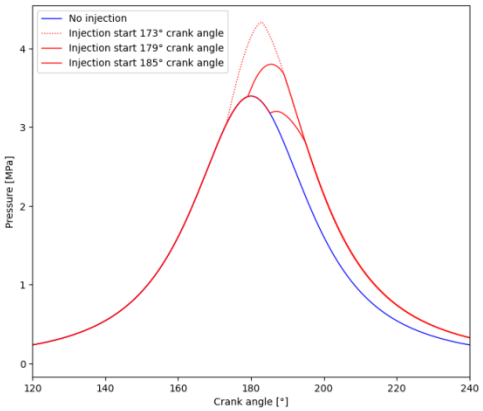


Figure 8. Injection sweep for 1.0 bar IMEP for fuel blend 3 consisting of molar fractions of 0.17 NH3, 0.76 H2O, and 0.06 H2O2

The simulations show that for all injection timings ignition was reliable, and that there were no visible reductions in the final amount of cumulative heat release achieved by the fuel, since all simulated pressure traces aligned to a single curve after about 195 degrees crank angle.

3.3. LCA results

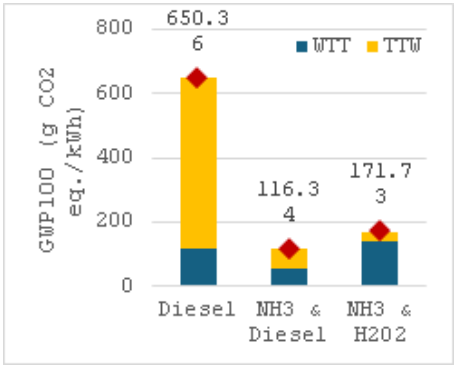


Figure 9. GWP100 results of three investigated scenarios

9 presents the GWP100 results for the three investigated fuel scenarios, with consideration of WTT and TTW contributions. The conventional fossil diesel scenario showed the highest climate impact, with a total WTW impact of approximately 650.36 g CO_2 eq./kWh. Most of the emissions originated from the TTW phase due to CO_2 emissions during combustion.

The NH_3 & Diesel scenario shows the lowest overall climate impact, with a WTW value of 116.34 g CO_2 eq./kWh, equivalent to a reduction of around 82% compared to the first scenario. In this scenario, the majority of impacts originated from the WTT phase associated with renewable ammonia production, while TTW emissions were reduced due to the low contribution of fossil pilot fuel.

Table 5. Environmental indicators of three scenarios

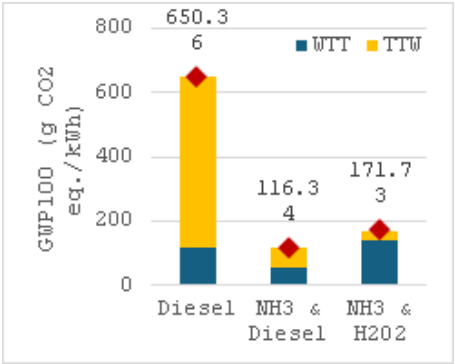


Figure 9. GWP100 results of three investigated scenarios

The NH_3 & H_2O_2 scenario also shows a significantly lower climate impact than conventional

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fossil diesel, with a total WTW impact of 171.73 g CO_2eq./kWh. Although TTW emissions remained relatively low, the WTT contribution increases compared with the second scenario due to the production of and the considerable consumption of green hydrogen peroxide (**Error! Reference source not found.**6). Overall, both ammonia-based scenarios demonstrated significant reductions in GWP100 compared with fossil diesel operation.

Table 5 shows the additional environmental indicators for the three scenarios in this study. Compared with conventional diesel, both ammonia-based scenarios showed much lower fossil resource use and lower GWP100 values. The NH_3 & Diesel scenario generally gives the lowest impacts on Abiotic Depletion (fossil), Freshwater Aquatic Ecotoxicity, Photochemical Ozone Creation Potential, and Terrestic Eco toxicity Potential.

Environmental indicators	Diesel	NH3 & Diesel	NH3 & H2O2
Abiotic Depletion (ADP elements) (g Sb eq./kWh)	1.83E-05	6.75E-04	7.56E-03
Abiotic Depletion (ADP fossil) (J/kWh)	8.47E+03	1.04E+03	1.81E+03
Acidification Potential (AP) (g SO_2 eq. /kWh)	3.86E+00	9.57E+00	9.80E+00
Eutrophication Potential (EP) (g Phosphate eq. /kWh)	9.61E-01	2.25E+00	2.38E+00
Freshwater Aquatic Ecotoxicity Potential (FAETP inf.) (g DCB eq. /kWh)	3.04E+00	3.40E-01	1.63E+02
Global Warming Potential (GWP 100 years) (g CO2 eq. /kWh)	6.50E+02	1.16E+02	1.72E+02
Human Toxicity Potential (HTP inf.) (g DCB eq. /kWh)	1.95E+01	8.08E+01	4.87E+02
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) (g DCB eq. /kWh)	1.02E+04	1.03E+04	2.36E+05
Ozone Layer Depletion Potential (ODP, steady state) (g R11 eq. /kWh)	9.40E-11	1.96E-10	1.34E-05
Photochem. Ozone Creation Potential (POCP) (g Ethene eq. /kWh)	4.51E-01	2.45E-01	2.97E-01
Terrestric Ecotoxicity Potential (TETP inf.) (g DCB eq. /kWh)	5.60E-01	4.07E-01	3.63E+00

However, the ammonia-based scenarios show higher impacts in several other categories, including Abiotic Depletion of Elements, Acidification, Eutrophication, Human Toxicity, Marine Aquatic Ecotoxicity, and Ozone Layer Depletion. These increases are particularly substantial for the NH_3–H_2O_2 scenario, mainly due to the upstream production of ammonia and hydrogen peroxide. In addition, the low energy content of H_2O_2 results in higher H_2O_2 consumption per unit of energy output, increasing the associated upstream environmental impacts. The results remind ammonia-based fuels can strongly reduce climate impacts, but some trade-offs exist in other environmental impact categories.

4. DISCUSSION

The small engine experiments showed that aqueous ammonia hydrogen peroxide mixtures showed sensible reactivity following their injection into a diesel engine. The experiments provided initial validation for earlier studies in which these fuel mixtures were predicted to show reactivity at engine-relevant conditions, based purely on simulations.

The LCA showed that on a life-cycle basis, ammonia hydrogen peroxide mixtures could provide significant

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reductions of climate impact. When ammonia and hydrogen peroxide were produced using wind electricity, the total GWP100 was about 171.73 g CO_2 eq./kWh, around 73.5% lower than conventional diesel. However, its environmental performance is limited by the upstream production and high consumption of hydrogen peroxide due to its low heating value. Improvements in hydrogen peroxide production and fuel formulation are therefore needed to reduce these trade-offs.

5. CONCLUSIONS

This work investigated the possibility of igniting mixtures of carbonless, safe carbonless fuel mixtures consisting of ammonia, water and hydrogen peroxide in a conventional direct injected diesel engine. The work used simple cylinder pressure measurements to verify the first experimentally determined heat released from the fuel in a diesel engine. The engine experiments were supplemented by a series of thermodynamic and chemical kinetic simulations, evaluating the engine operating at different fuel compositions in terms of varying amounts of 30% mass/mass hydrogen peroxide in water. Further to this different engine loads in terms of indicated mean effective pressure and different injection timings were simulated for the fuel blend which worked best. This work also analysed the potential WTW emissions from the use of such a fuel.

This investigation provides some evidence that the fuel mixtures discussed in this work are promising as carbonless fuel mixtures for future maritime applications, where safety is of utmost importance, and replacing existing diesel engines is difficult.

The LCA found that the mixture of NH_3 and H_2O_2 fuel could substantially reduce life-cycle climate impacts compared with conventional diesel. However, the upstream production and high consumption of H_2O_2 increased several other environmental impacts. Further improvements in H_2O_2 production and fuel formulation are therefore needed.

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