CIMAC CONGRESS 25
ZURICH, MAY 19 – 23, 2025

2025 | 291

Assessment of ammonia combustion in large engines

Basic research & advanced engineering - new concepts

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ABSTRACT

To reduce greenhouse gas emissions, zero-carbon and (net) zero-carbon fuel alternatives such as hydrogen, ammonia, and methanol will play a crucial role for shipping, power generation and specific off-road applications.

One of the fuels in focus is ammonia, with its potential to significantly reduce carbon intensity, at least from the combustion perspective.

This paper describes different engine concepts, mixture formation and combustion technologies for ammonia, covering high- and medium-speed four-stroke large engines.

The comparison and assessment are based on test data collected on single-cylinder test engines and selected CFD simulation results (HPDI).

Single-cylinder engine test results covering premixed and diffusive combustion of ammonia will be discussed. Results for diesel- and spark-ignited ammonia combustion will be shown.

The prechamber concept uses hydrogen enrichment to generate strong flame torches that ensure appropriate ignition and fast combustion.

The diesel -ignited concepts cover port gas admission and direct injection of ammonia.

The results include load limitations, the requirement to reduce excess air ratio, combustion phenomena and achieved engine performance characteristics. Heat release rates will be compared for further explanation.

Specific emission results like unburned NH3 and nitrous oxide N2O are included in the analysis.

The CO2 equivalents of unburnt NH3 resulting from engine and aftertreatment are considered to assess the remaining greenhouse gas reduction potential.

The trade-offs for the relevant engine out emission species NOx/N2O/NH3 will be described as depending on the engine concept and layout.

Finally, the conceptual requirements for the exhaust gas aftertreatment system will be described.

The paper will conclude with an assessment of the engine concepts covering the perspective of an easy retrofit and quick time-to-market approach and the perspective of a dedicated ammonia solution.

Lastly, an outlook to next development steps will be given.

1 INTRODUCTION

Ships powered by large internal combustion engines are responsible for about 2% of the global energy-related CO_2 emissions [1], per some sources, even 3%. Therefore, the IMO's Marine Environment Protection Committee (MEPC 80) in July 2023 adopted a revised Greenhouse Gas (GHG) strategy with ambitious emissions reduction targets. These targets include, compared to the 2008 levels, a 20% reduction by 2030, a 70% reduction by 2040 , and ultimately, achieving net-zero emissions by 2050, as shown in Figure 1.

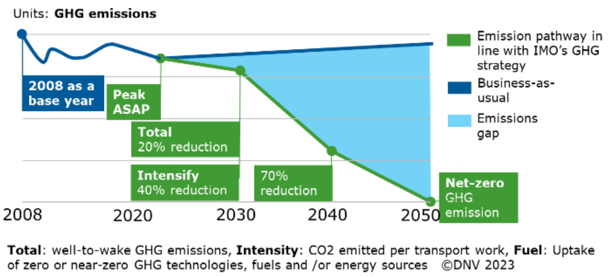


Figure 1: Revised IMO GHG strategy, Source DNV

One way to achieve the set goals is seen in the widespread use of so-called alternative fuels, especially those that are carbon-free. Ammonia is one of the options being intensively looked at these days. Ammonia is a carbon free fuel which can be processed on board of vessels without directly producing GHG emissions. If produced by electrolysis with renewable power sources, the well to wake emissions over the whole supply chain are on the same low level (100gCO_2/kWh-GWP100) as e-Methane, e-Methanol and e-H_2 [3]. Ammonia is attractive for the maritime industry not only because of its zero direct GHG emissions. Its physical properties appear more favourable compared to hydrogen if it is about the storage of the fuel, and, since ammonia is already a commonly sea-traded good, it can be provided in many seaports via an already existing infrastructure. This is, however, in most cases, ammonia produced from fossil resources. The status quo is therefore seen as a well-suited basis for the exploration of the potential of ammonia as fuel for combustion engines and the provision of the fuel to the ports and ships. But to some extent it also needs to be considered as an intermediate solution, until a green ammonia infrastructure is available.

This paper explores three different ammonia combustion concepts for high-speed internal combustion engines.

- First, premixed ammonia with a diesel pilot ignition available for retrofitting
- Second, a zero-carbon emission solution utilizing a mixture of ammonia and hydrogen ignited via a hydrogen-scavenged pre-chamber with a spark plug,
- Third, diffusive ammonia combustion with high pressure direct injection (HPDI)

For the first two concepts both, experiments and simulations are introduced and discussed, and results are compared. The third concept was investigated up to now only by means of CFD simulations. The decision not to perform experiments for the latter was made, as we trust in the reliability and predictivity of the simulation after having it validated on various cases including the first and the second concept described in this paper.

Based on the displayed results (experiments, simulations), the focus of this paper is comparing the three listed concepts as potential solutions contributing to the MPEC CO_2-emission reduction targets.

Measurement results of the first and the second combustion concept will be discussed regarding their impact on engine performance and emissions. The comparison of engine maps is presented, illustrating challenges associated with high levels of unburned ammonia and emissions of nitrous oxide (N_2O) as a by-product in the exhaust gas. Recognizing N_2O as a potent greenhouse gas, the paper underscores the necessity of minimizing its emissions through combustion system development or by deploying exhaust gas aftertreatment systems.

Additionally, the paper discusses simulation results of mixed hydrogen-ammonia fuel operation. Insights to mixture preparation and combustion are provided, especially looking at NO_x and N_2O emissions, along with unburned ammonia. Based on simulation and experimental data the potential for enhancing air/fuel mixing and combustion is elaborated.

The seamless integration of the displayed advanced 0D/1D/3D CFD simulation methodology in combination with experimentally obtained data, provides a holistic view on ammonia combustion systems and sets the stage for further improvements of ammonia powered internal combustion engines.

2 ASSESSMENT OF COMBUSTION CONCEPTS FOR AMMONIA

The characteristics of different gas and dual fuel combustion concepts have already been discussed in previous papers [4], [5], [6], [10], [11], [12], [13].

The concepts introduced in this paper are shown in Figure 2.

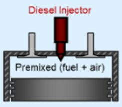
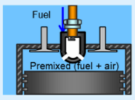
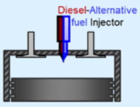
Strategy	Quick 'time-to-market'		
Mixture formation	Pre-mixed		Direct injection
Ignition	Diesel	Spark plug	Diesel
Combustion Concept			

Figure 2: Ammonia combustion concepts

Most large gas engines employ spark-ignited pre-mixed combustion and apply either an open chamber or a pre-chamber concept. These engines can be converted in a relatively simple manner into carbon-neutral engines. This requires adopting the needed changes to, for example, the gas supply system or the piston design, as needed for the operation with the new fuel.

Considering the ammonia properties, namely low heating value, high ignition energy and low combustion speed (refer to Table 2), the open chamber concept seems to be less favourable for pure ammonia combustion. Instead, such design would require adding hydrogen to ammonia to assure stable ignition and combustion.

Pre-chamber engines with spark ignition are better suited to realize stable ammonia combustion, but mixing of hydrogen may still be necessary at engine start and at low load operation.

A combustion concept with diesel ignited premixed ammonia could be realized relatively easily by adapting the gas supply system to the requirements of the new fuel. The diesel pilot fuel provides sufficient ignition energy and therefore, additional hydrogen admixing is not necessary. The associated challenges, such as achieving exhaust emission targets, limiting maximum substitution rate and thus the actual potential for reducing greenhouse gas emissions, are still to be resolved. The concept of diffuse combustion could prove to be a better solution here.

Ammonia diffusion combustion has the potential for a significant reduction of unburned NH_3 emissions compared to pre-mixed combustion systems. Injectors and high-pressure pumps for ammonia, however, are still at an early phase of the development and available to a limited extent. Also, the significantly increased complexity of such engine and its subsystems is challenging.

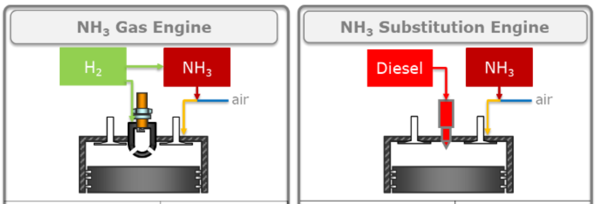
3 TEST ENGINE

The AVL high-speed single cylinder test engine SCE175 shown in Figure 3 was used for the experimental investigations described in this paper. AVL designed this new single cylinder unit from a clean sheet of paper to serve as platform for testing performance and mechanical developments. With the Diesel version of the test carrier AVL successfully demonstrated a BMEP of 35 bar and a BSFC of 168 g/kWh at 1500 rpm. The gas engine version provides a BMEP of 32.5 bar at 1500rpm, and a brake thermal efficiency of 50% at the same engine speed. Engine-out emissions have been capped at 500 mg/Nm^3 NO_x at 5% residual O_2 [7].

The engine is characterized by a maximum peak firing pressure capability of 330 bar while retaining state-of-the-art durability requirements. The engine can be operated as a diesel engine, gas engine or dual fuel engine with a common rail injection system for liquid fuel and with a port gas admission valve or venturi mixer for gaseous fuel. Each cam segment for intake and exhaust valves can be replaced or adjusted separately.

Figure 3: AVL High-Speed Single Cylinder Test Engine SCE175

For the present study, the engine was adapted to investigate the characteristics of pre-mixed ammonia combustion with two different ignition concepts. The schematic diagram of the engine configurations tested in the following measurements and their high-level specifications are given in Figure 4. The gaseous fuel was mixed with the air using a venturi gas mixer. For the spark-ignited combustion concept, a mixture of hydrogen and ammonia was mixed with the air and additionally, a small quantity of pure hydrogen was supplied to the pre-chamber. For the Diesel-ignited concept, only ammonia was mixed with air by the venturi gas mixer.



Bore	175 mm
Stroke	215 mm
Displacement	5.2 l/cylinder
Rated speed	1500 rpm
BMEP NH3	25 bar
Rated power	162 kW
Compression ratio	13.5:1
Intake valve timing	Miller 490 °CRA
Combustion system	Quiescent

Bore	175 mm
Stroke	215 mm
Displacement	5.2 l/cylinder
Rated speed	1350 / 1800 rpm
BMEP	25 bar
Rated power	195 kW
Compression ratio	16.5:1
Valve timings	Miller 490 °CRA
Combustion system	Quiescent

Figure 4: Schematic diagram and specifications of SCE175 used for testing in this study

4 PRE-MIXED AMMONIA WITH DIESEL PILOT IGNITION

The ammonia/air mixture in the combustion chamber was ignited by injecting diesel fuel. The diesel injector is capable to provide sufficient fuel for a rated output of 35 bar BMEP when the engine is running in pure diesel mode. Although this concept offers the advantage of maintaining full load capability in diesel operation, the maximum possible substitution by ammonia is limited by ignition stability at low injection quantities.

Figure 5 shows the influence of diesel energy ratio and excess air ratio on unburned ammonia emission and nitrous oxide emission.

The excess air ratio shown in the figure 6 is a global excess air ratio considering both diesel and ammonia. The measurement was conducted within the shown operating range but the outer contour of the map is not necessarily the operational limit. Towards the lower excess air ratio and the higher diesel energy ratio (top left corner of the diagram), the operational limits are the exhaust gas temperature and CO emissions due to incomplete combustion of the diesel fuel. Towards the higher excess air ratio and the lower diesel energy ratio (bottom right corner of the diagram), the operational limits are the high unburned ammonia emission and the low combustion stability.

At excess air ratio above 1.8 and diesel energy ratio above 50%, the unburned ammonia emission as well as nitrous oxide emission increases significantly when the diesel substitution rate is increased. In this area, the influence of the global excess air ratio is rather moderate because the excess air ratio of ammonia only is still quite high (3.5 to 5). Lean ammonia/air mixture in the vicinity of the diesel flame burns well and a considerable portion of the ammonia/air mixture located outside diesel flame remains unburned. Thus, a small variation of the global excess air ratio does not improve the ammonia combustion sufficiently (Figure 10).

If the excess air ratio and the diesel energy ratio are further decreased, the unburned ammonia as well as nitrous oxide emissions decrease significantly. In this area the excess air ratio of ammonia only becomes below 2.5 and the combustion of ammonia/air mixture between the diesel flames improves.

Figure 6 shows the break thermal efficiency of the single cylinder engine and the CO_2 -equivalent emissions of the same measurement campaign. The values of the baseline diesel operation are indicated in the diagrams too. Note, that the values of diesel operation were measured with the same engine configuration as the ammonia substitution measurements and do not represent the optimum diesel performance of this engine platform.

The efficiency decreases as the ammonia energy ratio is increased mainly due to unburned ammonia emissions. It slightly improves although at low excess air ratio and low diesel energy ratio because of the decreasing unburned ammonia emission.

CO_2 equivalent emissions reflect the emission of nitrous oxide. The Global Warming Potential (GWP) of nitrous oxide is 265 in 100 years scale according to the 5th assessment of the IPCC [8]. It therefore has a significant influence on the CO_2 equivalent emissions. This is why a diesel energy ratio of above around 40% is even worse than the baseline diesel operation in terms of CO_2 equivalent emissions. The benefit of the combustion concept can therefore only be seen at low excess air ratio and low diesel energy ratio where the nitrous oxide emissions can be kept low.

Therefore, it can be concluded that it is important for the pre-mixed ammonia combustion with diesel ignition to maximize the ammonia substitution rate and minimize the excess air ratio to optimize to realize a low amount of unburned ammonia and low nitrous oxide emission.

If a diesel injector with high full load capability is carried over, its ability for stable injection of small quantities is one of the key success factors for this combustion concept. In addition, the turbocharger layout and the air path control system are important elements, as they allow (or not allow) realizing a

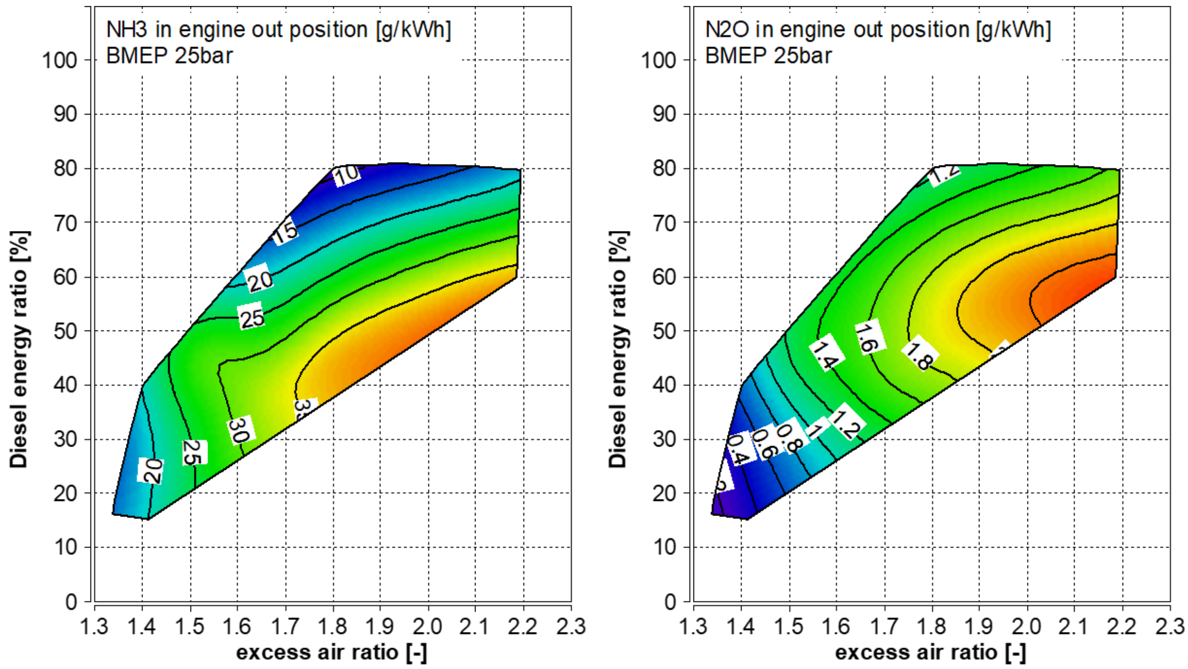


Figure 5: Unburned ammonia emission (left) and nitrous oxide emission (right) as a function of diesel energy ratio and excess air ratio measured at engine out at BMEP 25 bar and 1350 rpm

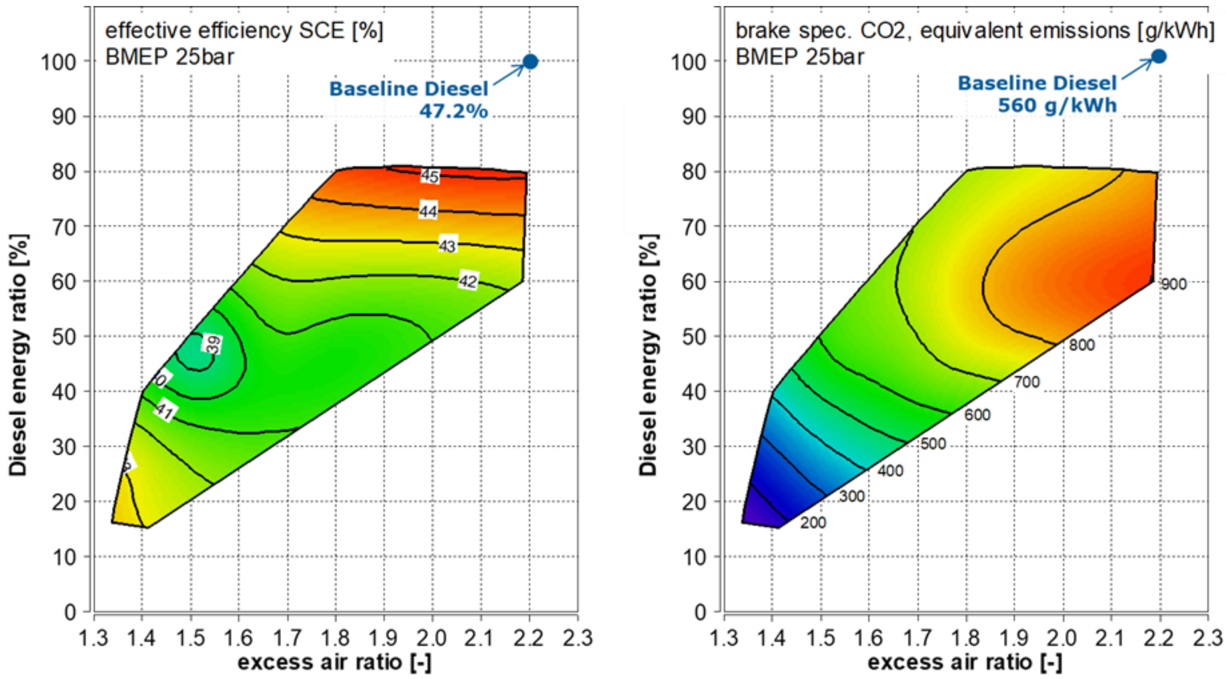


Figure 6: Brake thermal efficiency (left) and CO_2 equivalent emission (right) as a function of diesel energy ratio and excess air ratio measured at engine out at BMEP 25 bar and 1350 rpm

low excess air ratio which is required for the ammonia combustion and high excess air ratio in diesel operation mode. Furthermore, optimizing the transition from diesel to ammonia operation is a challenge, as a gradual increase in the ammonia ratio may fail due to excessive unburned ammonia and excessive nitrous oxide emissions.

4.1 3D CFD Simulation

As already mentioned, for a better understanding of the physical phenomena and to support combustion concept development respectively, 3D CFD simulations were conducted by using the AVL finite volume CFD simulation solution FIRE™ M. A computational model was setup for the operating point 25bar BMEP at 1350rpm. The simulations have been performed for two operating modes –

using pure diesel as a fuel and using 20%e of diesel and 80%e ammonia. The given percentage describes the share in the total energy introduced into the combustion chamber. While the first operating condition reflects the standard diesel operating mode of the engine, the other one with 20%e Diesel and 80%e NH_3 represents conditions close to the limit where stable combustion still can be achieved. The computational model is presented in a Figure 7 and the operating conditions in Table 1.

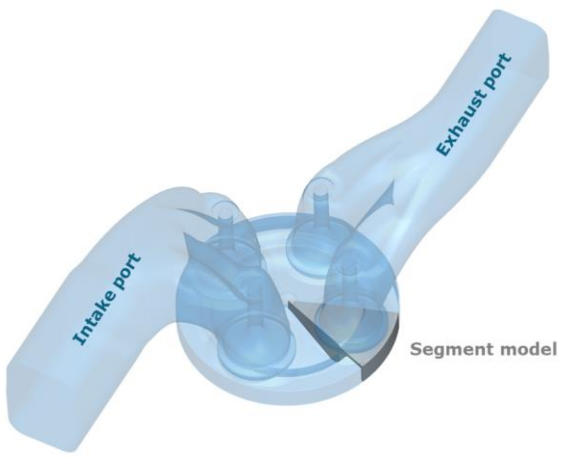


Figure 7: CFD simulation model

Table 1: Simulated operating conditions

Parameter	*Diesel / Ammonia = 100 / 0 energy %*	*Diesel / Ammonia = 20 / 80 energy %*
BMEP [bar]	25.0	25.0
Rated speed [rpm]	1350	1350
Diesel SOI [°CA bTDC]	4.80	13.30
Diesel DOI [°CA]	8.60	6.00
Diesel rail pressure [bar]	2200	1400
Total air excess ratio [-]	2.22	1.47

As per design of the engine, a mixture of ammonia and air is supplied to the intake port through a venturi mixer. This can be assumed to result in an almost ideal homogeneity of the mixture. Therefore, the CFD Model was initialized with a homogeneous mixture in the intake ports at start of the simulation and the same mixture is supplied through the inlet boundary of the intake ports during the simulated cycles.

The engine utilizes an injector with nine injection holes. To minimize the required computational resources, the simulation model was setup as a cylinder segment of 40°, as seen in Figure 7. This segment features only one nozzle hole and allows simulating the high-pressure cycle including compression, diesel injection and combustion.

The combustion itself was simulated deploying a general gas phase reaction solver, applied to a chemical kinetic mechanism able to handle NH_3, H_2 and n-heptane combustion under engine-like conditions [9]. This mechanism consists of 69 species and 389 chemical reactions. To speed up solving the chemical kinetics, an acceleration technique, called multi-zone model, was enabled. With this, cells having similar conditions (temperature and equivalence ratio) are grouped into zones for which the chemistry is solved at once rather than for each individual cell. The simulations performed in this study use a 5K limit for temperature and 0.01 limit for the equivalence ratio to define the zones. This specification enables a significant acceleration of the simulation while preventing a visible deterioration of the simulation result accuracy.

Simulations of both operating modes were conducted. Cylinder mean pressure and rate of heat release curves are presented in Figure 8.

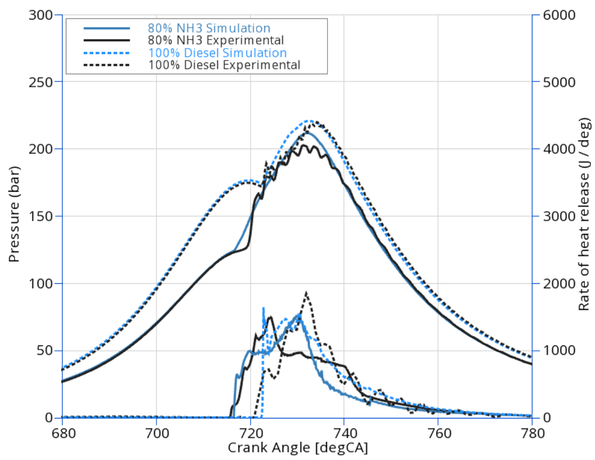


Figure 8: Simulated vs. experimental cylinder mean pressure and ROHR for two operating modes

A good agreement between simulated and experimental results can be observed, which indicates, the simulation realistically reflects related physical phenomena.

3D results obtained for fuel injection and combustion are presented in Figure 9. Diesel starts to evaporate earlier and more intense if it is injected into pure air. In this particular case, the rail pressure is significantly higher. Consequently, also the combustion starts earlier and a bit closer to the injection nozzle. The observed combustion progress is typical for a diesel diffusion flame, driven by the injection. Flow inertia from diesel injection and the aerodynamics of the piston bowl redirects the flame front from the piston bowl rim to the cylinder head.

In the dual fuel case, the evaporation of the diesel starts later. Also, ignition is taking place significantly later compared to the pure diesel

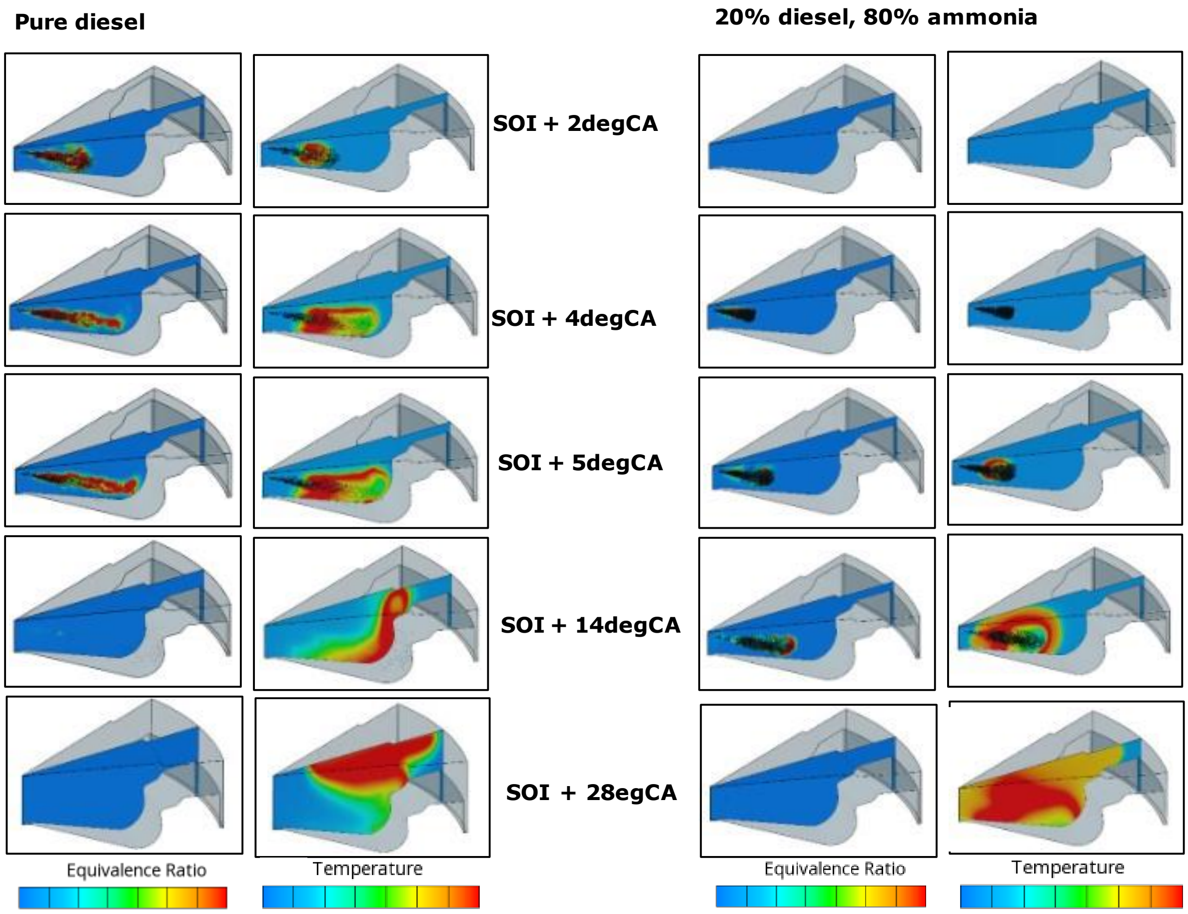


Figure 9: Comparison of fuel injection and combustion for both simulated operating modes

mode. There are several reasons for that. Injecting diesel into ammonia, means, there is less oxygen available for ignition and combustion. Due to the lower rail pressure and, consequently, the lower kinetic energy of the fuel jet, there is weaker jet breakup and slower evaporation. The lower injection velocity also results in a weaker mixing process. Furthermore, the diesel/ammonia mixture has elongated auto-ignition time compared to pure diesel. Therefore ignition starts at a time, when the kinetic energy of the jet is almost neutralized. The ignition point is in a mixed fuel region.

From this ignition kernel, the combustion spreads like from a fictitious spark plug, which is typical for pre-mixed cases. The aerodynamics of the bowl loses on importance. Once the flame reaches pure ammonia regions (this is when it moves towards the squish area), the flame propagation slows down due to the low laminar flame speed of ammonia. This is happening after the exhaust valves opened. Some of the remaining ammonia is propagating into the exhaust system. This is a reason for the high ammonia slip related to this concept, please refer to the Figure 10.

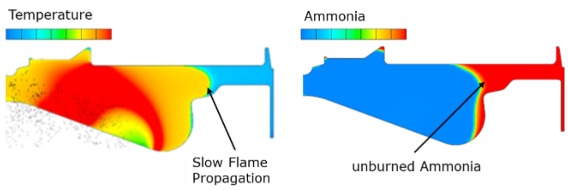


Figure 10: Slow combustion in pure ammonia region

5 AMMONIA AND HYDROGEN IGNITED VIA HYDROGEN SCAVENGED PRE-CHAMBER WITH SPARK PLUG

For the spark-ignited combustion concept, hydrogen and ammonia are mixed with air through a venturi mixer. For the experiments discussed in this section, the energy fraction of hydrogen was kept constant at 15%e. During the compression stroke, the ammonia/hydrogen/air mixture is forced into the pre-chamber and mixed with the pure hydrogen, which is supplied separately, directly into the pre-chamber. The quantity of this additional hydrogen was about 1% compared to the energy of the totally supplied fuel. This extra enrichment of

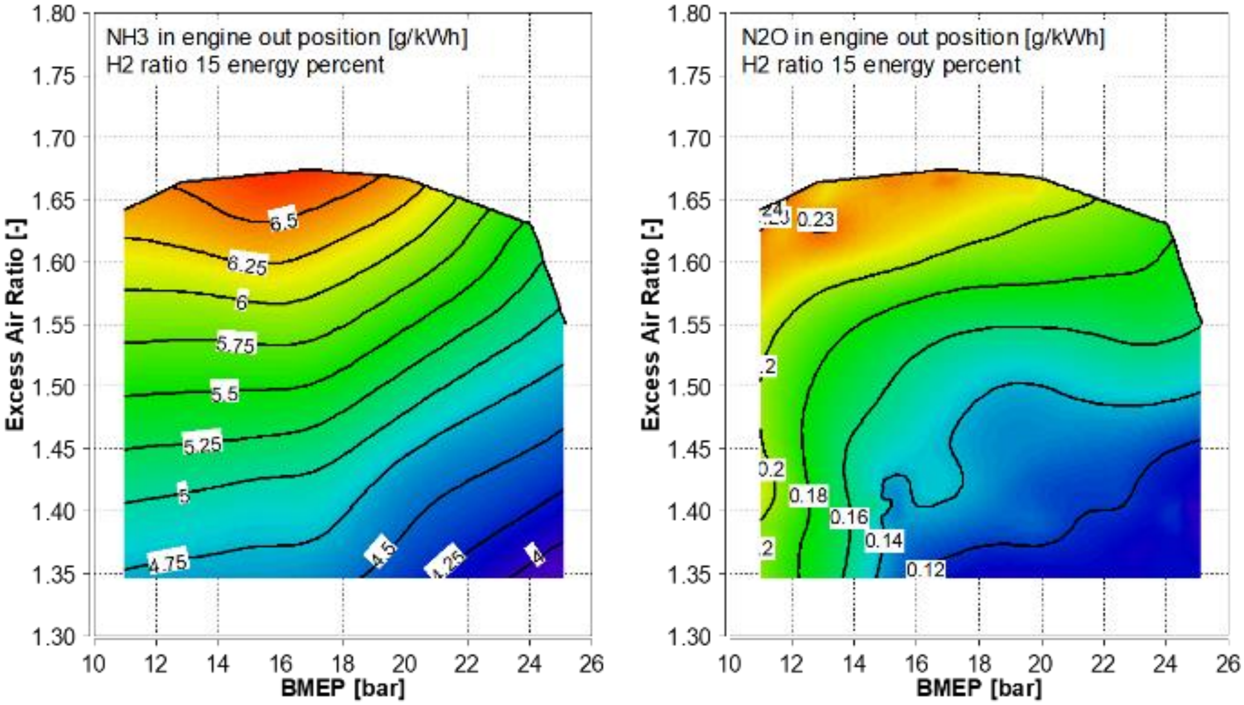


Figure 11: Unburned ammonia emission (left) and nitrous oxide emission (right) as a function of BMEP and excess air ratio measured at engine out at 1500 rpm with a constant hydrogen energy fraction of 15%

the pre-chamber by the pure hydrogen is to ensure a stable start of combustion by a spark ignition.

Figure 11 shows the unburned ammonia emission and nitrous oxide emission as function of the BMEP and the excess air ratio. The excess air ratio shown in the figures is a global excess air ratio considering ammonia and hydrogen. At first glance it can be noticed that the level of unburned ammonia emission and nitrous oxide emission is considerably lower than that of diesel-ignited combustion concept shown in the Figure 5. Due to the absence of the diesel fuel, the excess air ratio of the spark-ignited concept can generally be set lower without suffering from incomplete combustion and CO emissions. In addition, the mixing of hydrogen significantly supports the ammonia combustion and reduces the emissions of unburned fuel. Nevertheless, the trend itself is similar to the diesel-ignited combustion and the lower excess air ratio results in the reduction of the emissions.

Figure 12 shows the effective engine efficiency of the single cylinder engine and the CO_2 equivalent emissions of the same measurement campaign. The efficiency is not significantly influenced by the excess air ratio but increases as the engine load is increased. The trend of the CO_2 equivalent emission follows that of the nitrous oxide emissions but is at a very low level compared to the diesel-ignited concept shown in the Figure 5. The fuel is carbon free and thus, the CO_2 emission, resulting from the combustion of lubricating oil, is at a very low level.

A drawback of the tested concept were the very high NO_x emissions, NO_x values above 35 g/kWh were measured, due to the compact heat release enabled by the hydrogen and due to the high combustion temperature caused by the low excess air ratio. The level of NO_x emission is much higher than that of the unburned ammonia emission. This means that an SCR exhaust gas aftertreatment system with additional AdBlue injection is mandatory for this engine.

A reduction of the hydrogen energy ratio and an optimization of the excess air ratio are further conceivable development steps to reduce the NO_x emissions at engine out. In addition, supplying the pre-chamber with the same fuel as the main chamber could be investigated. In this study, pure hydrogen was supplied to the pre-chamber for simplicity. This although is likely to have an influence on the resulting NO_x emission. In the actual application, however, partially cracked ammonia is likely to be supplied to both the main chamber and the pre-chamber to avoid installing an additional fuel tank for the pure hydrogen.

Figure 13 compares the engine performance and emissions of four different combustion concepts, namely, diesel, natural gas, ammonia spark-ignited

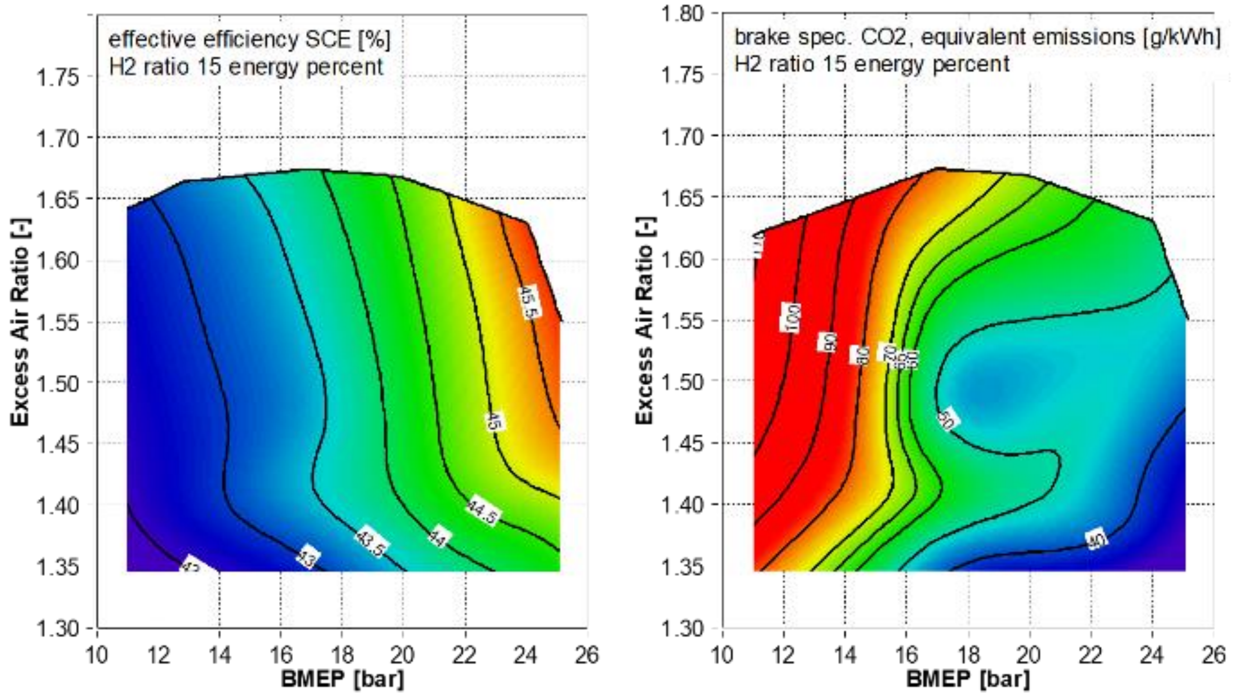


Figure 12: Brake thermal efficiency (left) and CO_2 equivalent emission (right) as a function of diesel energy ratio and excess air ratio measured at engine out at BMEP 25 bar and 1350 rpm

and ammonia diesel-ignited, at a BMEP of 25 bar. The engine configuration for the diesel engine is different from that of the ammonia diesel-ignited concept. The diesel engine is optimized for the single fuel operation, especially in terms of the compression ratio. On the other hand, the engine configuration for the natural gas engine is the same as that of the ammonia spark-ignited concept.

The diesel engine has the highest brake thermal efficiency (BTE) of 48.6 % but at the same time emits the highest CO_2 emission. The natural gas engine follows with the BTE of 47% measured at NOx 500 mg/Nm3 at residual O_2 of 5%. The CO_2 emission from the gas engine is lower by more than 20% compared to the diesel engine. However, the benefit is partially compensated by the CH_4 emission, which has a GWP of 28 according to the 5th assessment of the IPCC, resulting in only 10% reduction in the CO_2 equivalent emission compared to the diesel engine.

The ammonia spark-ignited concept shows a remarkable potential for the reduction in the CO_2 equivalent emissions benefitting from the carbon free fuel and very low nitrous oxide emission. It emits only 6 to 6.6% of CO_2 equivalent emissions compared to the diesel and the gas engine, respectively. As discussed above, however, the excessive NO_x emission is a challenge and requires further development steps.

It is clearly visible that the BTE of the ammonia diesel-ignited concept is remarkably lower than the others, mainly due to the high unburned ammonia emission of around 20 g/kWh. While the CO_2 emission itself is about 20% compared to the diesel engine, the CO_2 equivalent emission counts for 36% of the diesel engine. This is because of the nitrous oxide emission. Even though the nitrous oxide emission was reduced to a low level of about 0.3 g/kWh, the contribution to the CO_2 equivalent emission is still quite high due to its high GWP of 265. A further increase of the ammonia energy fraction and an optimization of the excess air ratio to minimize the nitrous emission are the key development targets for this combustion concept.

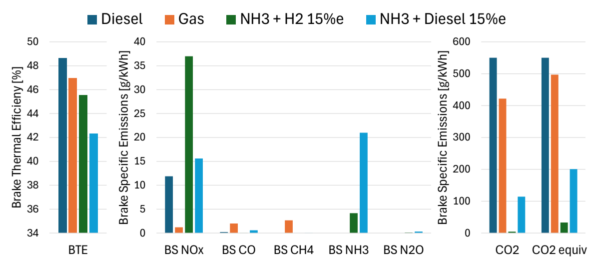


Figure 13: Comparison of brake thermal efficiency and emission performances among diesel, gas, NH_3 spark ignited and NH_3 diesel ignited at BMEP 25 bar

5.1 3D CFD Simulation

Also for the spark-ignited hydrogen/ammonia combustion system 3D CFD simulations have been conducted for a better understanding of the relevant physical phenomena and to support the development of the concept.

The computational model was setup for one representative engine operating condition: 1500rpm, air excess ratio = 1.44 and indicated mean effective pressure = 24.6 bar. This point was selected to be comparable with the diesel-ignited pre-mixed ammonia combustion concept.

Ammonia and hydrogen are supplied to the intake port through a venturi mixer. This results in almost ideal homogeneity of the mixture. Therefore, a homogeneous mixture was initialized in the intake ports at start of the simulation and is supplied through the inlet boundary of the intake ports during the simulation.

The energy share of the hydrogen was kept constant at 15%e. An additional 1%e energy share of pure hydrogen is supplied into the pre-chamber to enrich the mixture in the spark plug area for stable ignition and fast propagation of the flame into the main chamber. The computational model with its main elements is presented in a Figure 14. A key role in this combustion concepts plays the pre-chamber.

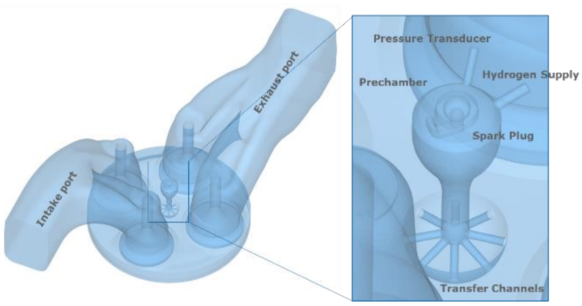


Figure 14: Simulation model

Simulating the combustion of the spark-ignition concept, again general gas phase reaction kinetics and multi-zone accelerator have been enabled.

A CFD simulation of a selected operating condition was conducted. The mean cylinder pressure and the accumulated heat release curves for the simulated operating condition are presented in Figure 15. Good agreement between simulated and the experimental results can be observed, which indicates that the simulation results realistically reflect the relevant physical phenomena.

Compared to the experimental data, although, the simulation result shows a slightly faster reaction rates, which relates to the also slightly overpredicted mean cylinder pressure. Otherwise, simulated and experimental results are consistent.

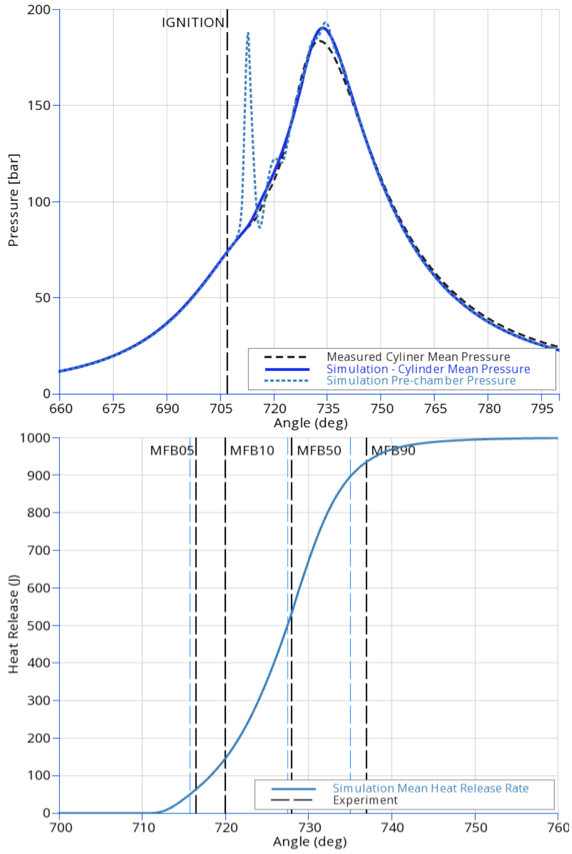


Figure 15: Simulated vs. experimental cylinder mean pressure and accumulated heat release

The pre-chamber is the key element to make this combustion concept work. For the hydrogen supply into the pre-chamber a non-return valve is used. It operates based on the pressure difference on both sides of the valve, which makes a bit challenging to exactly control the supplied mass. The dynamic of the hydrogen propagation into the pre-chamber and the hydrogen mass-fractions in the vicinity of the spark plug area are displayed in Figure 16. It can be observed that the pre-chamber gets almost completely filled with hydrogen during the intake stroke and later a significant part of it propagates back to the cylinder. However, a sufficient amount of hydrogen remains within the pre-chamber and around the spark plug region thus enabling stable ignition and fast combustion within the pre-chamber.

In Figure 17 the combustion progress is shown. The flame front visualization nicely demonstrates how the concept works. Ignition is initiated by the spark in the pre-chamber. Due to the relatively high hydrogen concentration there, it is stable and the flame propagates quickly. The pressure in the pre-chamber rises therefore to a level significantly higher compared to the main chamber, soon after ignition. Consequently, hot, high-speed gas jets exit the pre-chamber through each of the individual transfer channels into the main chamber.

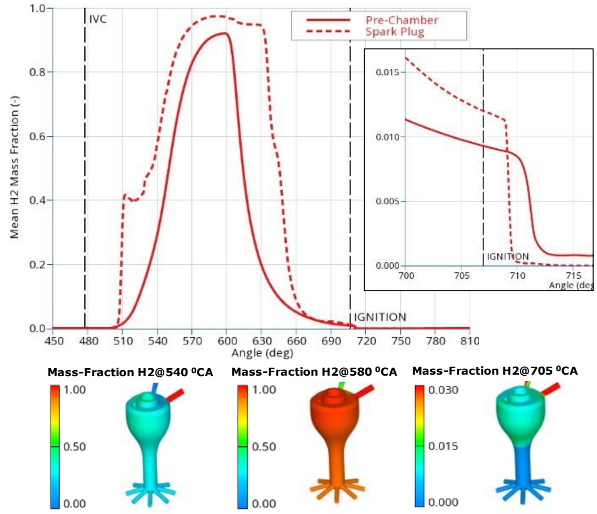


Figure 16: Hydrogen mass-fractions in the pre-chamber and spark plug area

There the energy intense jets ignite the remaining lean ammonia/hydrogen/air mixture simultaneously in almost the complete volume.

The pressure difference between the pre-chamber and the cylinder can be observed in Figure 15.

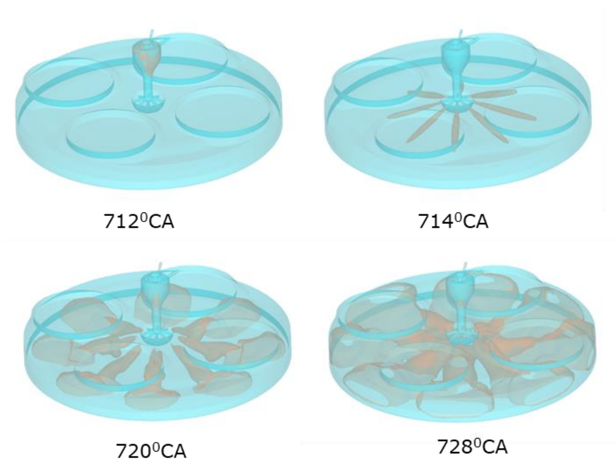


Figure 17: Flame visualization

6 DIFFUSIVE AMMONIA COMBUSTION WITH HIGH PRESSURE DIRECT INJECTION

The diffusive combustion concept offers a good solution for the challenges of auto-ignition and high exhaust gas emissions. It requires although, to well know the fuel properties. A comparison between diesel, hydrogen and ammonia is presented in Table 2.

As the lower calorific value of ammonia is less than half of the diesel value, a significantly higher mass must be injected to achieve comparable performance. This is possible only with a prolonged

Table 2: Selected diesel, hydrogen and ammonia properties

Property	Unit	Diesel	Hydrogen	Ammonia
Density @ 1 bar/0°C	kg/m3	833	0.09	0.79
Lower calorific value	MJ/kg	45	120	18.7
Stoichiometric AF ratio	kg/kg	14.5	34.3	6.1
Min. ignition energy	mJ	0.24	0.017	>10
Flammability limit λ	-	1.5~7	0.13~10	0.83~1.81
Auto-ignition temperature	°C	210	585	650
Latent Heat	MJ/kg	0.25	gas	≈ 1.4
Laminar Flame Speed	cm/s	≈86	230	≈ 7

injection duration. The latent heat is about five times higher than that of diesel, which makes it challenging to get a significant amount of ammonia burned properly. Ignition delay is long, and enough energy must be available for achieving reasonably fast and stable ignition. A well-defined injection strategy is therefore mandatory.

The previously introduced engine design was used as a basis for deriving the model for the model shown in Figure 18.

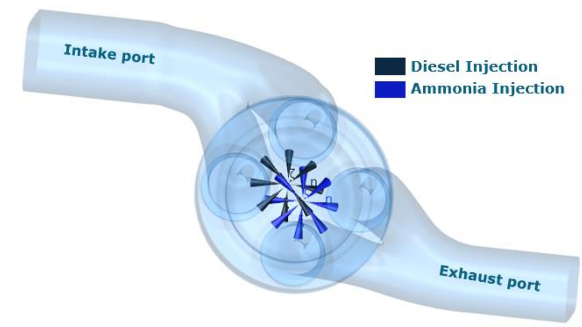


Figure 18: Model for high pressure direct fuel injection

Two injection strategies have been initially elaborated:

- two individual injectors, one for diesel and one for ammonia. The advantage of such system is that the injector positions, targeting and injection timing as well as the fuel ratio can easily be varied. Arguments speaking against such design are a potential packaging problem and the anticipated higher cost

- one injector enabling the supply of both fuels. The advantage of this system is that it requires less space. The disadvantage is that it provides less freedom in terms of ignition strategies.

Eventually, the decision was made to go for one injector with two needles. Several injection strategies were simulated. Injector positioning, orientation, targeting, timing and fuel ratios have been varied. The modelled engine geometry is as much as possible similar compared to the previously discussed cases.

The simulated operating point is more or less the same, compared to the diesel-ignited premixed and the spark-ignited premixed ammonia cases, to be able to directly compare the simulation results obtained for all strategies. An overview about all simulated cases is provided in Table 3.

Table 3: Simulated fuel supply strategies and operating conditions

Parameter	Premixed ammonia with diesel pilot ignition	Mixture of NH_3 and H_2 ignited via H_2 scavenged pre-chamber with a spark plug	Diffusive ammonia combustion with HPDI
Rotational speed	1350rpm	1500rpm	1350rpm
BMEP	25bar	24.6bar	25bar
Diesel / Ammonia / Hydrogen Energy %	20 / 80 / 0	0 / 84 / 16	10 / 90 / 0
Diesel SOI [°CA bTDC]	13.3	Spark ignition	16.5
Diesel DOI [°CA]	6.0	-	7.0
Diesel Rail Pressure [bar]	1400	-	1000
Firing Peak Pressure [bar]	210	190	205
Total Air Excess Ratio	1.47	1.44	1.5

In Figure 19 the simulated cylinder mean pressure and rate of heat release curves are presented for the ammonia premixed and the ammonia high pressure direct injection (HPDI) concept. A very similar behaviour can be observed. The HPDI concept although allows to control the combustion behaviour in a relatively easy way. This guarantees smooth engine operation.

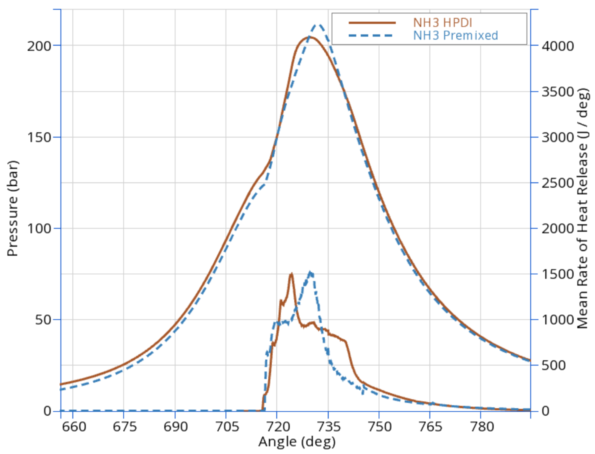


Figure 19: Cylinder mean pressure and rate of heat release curves for ammonia premixed and HPDI injection concepts.

Figures 20 and 21 display the whole working principle of the diesel-ignited ammonia HPDI concept. First, diesel is injected and ignites. The ammonia injection is optimised in a way that the energy transfer from the already ignited diesel to the not yet ignited ammonia is seamlessly ensured. A sufficiently high temperature in the region of the ammonia injection enhances atomization and evaporation. High injection velocity and a suitable level of turbulence are favourable for the diffusion flame as these parameters counteract the low laminar flame speed and the high ignition energy demand of ammonia.

7 COMPARISON OF ALL THREE AMMONIA COMBUSTION CONCEPTS

With a growing interest in switching from fossil fuels to carbon-neutral alternatives, this paper discusses dual-fuel combustion concepts in combination with the expected use of diesel, hydrogen and ammonia.

It appears feasible to adapt existing engines with relatively low effort and cost, to enable ammonia pre-mixed combustion concepts. However, this concept typically suffers from high emissions of unburned fuel. A diffusive combustion concept would solve this issue but poses the challenge of increased engine complexity with two high-pressure fuel injection systems and is more costly too.

Three different ammonia combustion systems were introduced:

- Premixed ammonia with a diesel pilot ignition
- A mixture of ammonia and hydrogen ignited via a hydrogen-scavenged pre-chamber with a spark plug
- Diffusive ammonia combustion with high pressure direct injection

For the first two concepts experimental results obtained from physical tests with the AVL SCE175 are presented and compared with the respective simulation results. The third concept has been extensively studied by means of CFD simulations. A comparison of some performance and setup parameters can be seen in Table 3. A comparison of the emission behavior can be seen in Figures 22 to 24.

In Figure 22 the main challenge of the pure ammonia premixed concept is demonstrated. Once the flame propagates from the dual fuel (diesel and ammonia) mixed zone to the pure ammonia region, the flame propagation drastically slows down, eventually resulting in a significant ammonia slip.

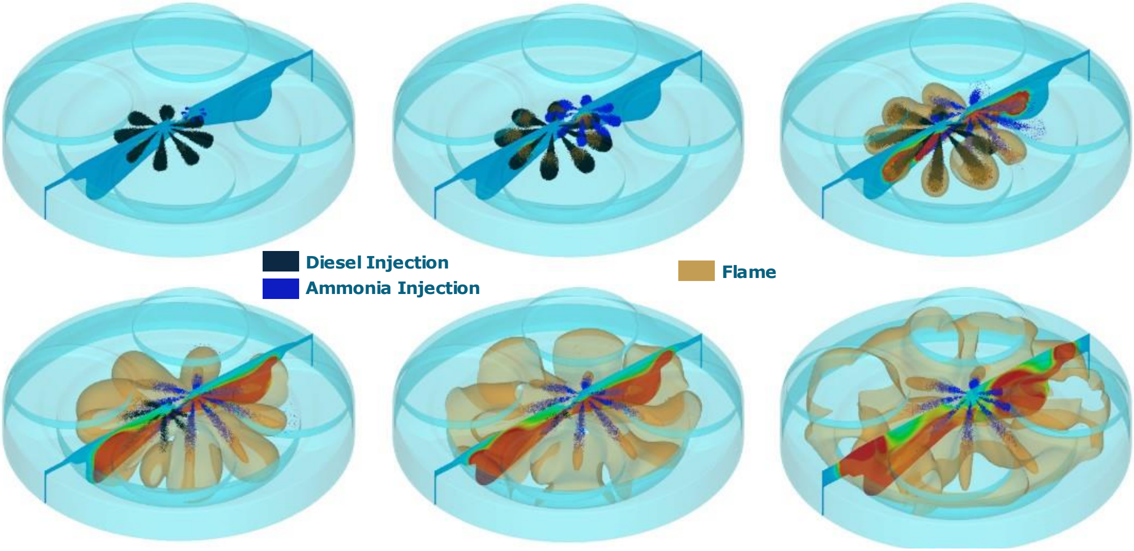


Figure 20: Fuel injection, ignition and flame propagation with the ammonia HPDI concept – isometric view

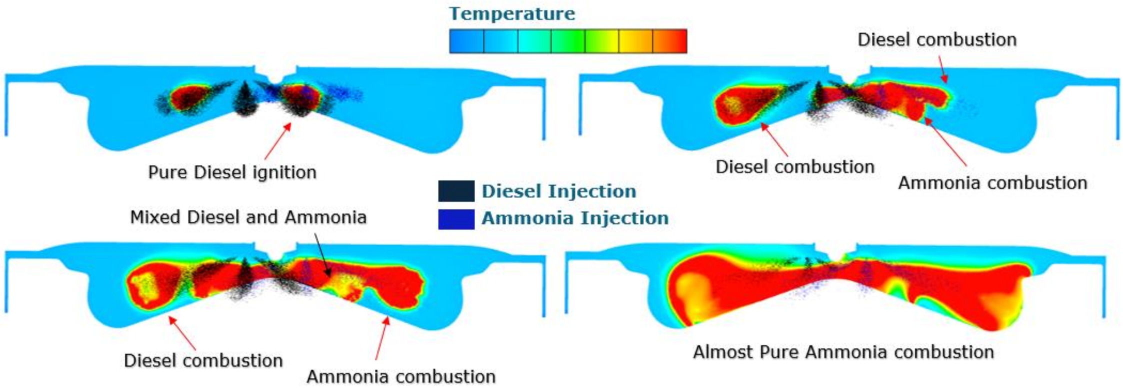


Figure 21: Fuel injection, ignition and flame propagation with the ammonia HPDI concept – cross-section through the injection axes

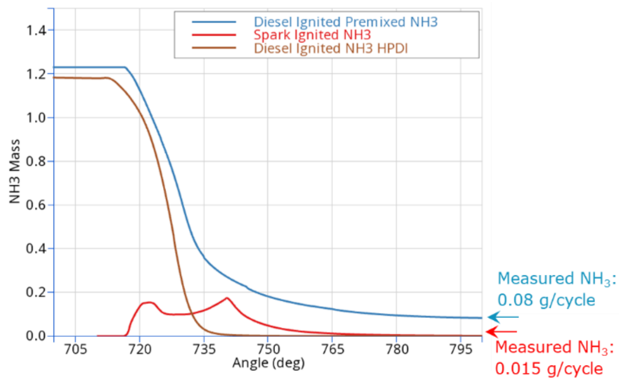


Figure 22: Comparison of ammonia emissions for all three ammonia combustion concepts

Figure 23 demonstrates NO and N_2O emissions for the different ammonia combustion concepts. Simulated and experimental results are presented. Clearly the benefits of an HPDI concept can be seen. The data also provide evidence for the good predictivity of the simulation models.

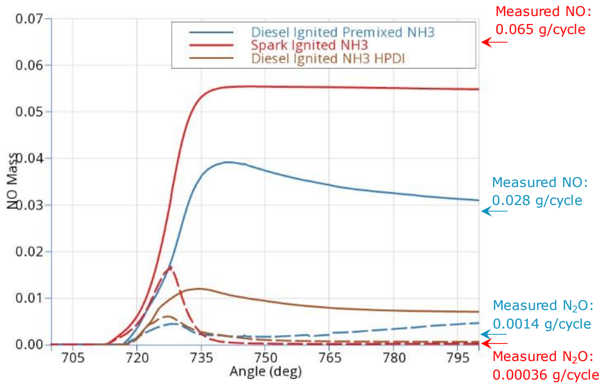


Figure 23: Comparison of NO and N_2O emissions between different ammonia combustion concepts

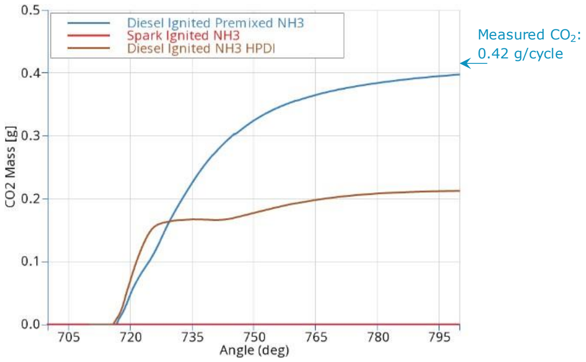


Figure 24: Comparison of CO_2 emissions between all three ammonia combustion concepts

Finally, the whole discussion is about CO_2 (and CO_2 equivalent) emissions. The comparison of experimental and simulation results for different combustion strategies is shown in Figure 24.

The spark ignited concept is the only feasible approach when targeting zero CO_2 emissions. However, the other two concepts still show a clear reduction of CO_2 emissions when compared to the pure diesel operating mode. For the latter CO_2 emission of about 2g/cycle had been measured. The savings are about 80 to 90%.

8 SUMMARY AND OUTLOOK

The paper described three different ammonia combustion concepts for high-speed engines, as investigated by AVL by means of experiment and CFD simulations. The first combustion concept represented a retrofittable approach of a premixed ammonia combustion with diesel pilot ignition. The second concept pursued a pure zero-carbon fuel strategy by utilizing a mixture of ammonia and hydrogen ignited via a hydrogen-scavenged pre-chamber with a spark plug. The third concept demonstrated a diesel ignited high pressure direct injected ammonia concept.

The measurements conducted on the AVL high-speed single cylinder test engine SCE175 with the new clean sheet engine power cylinder unit designed by AVL, enabled a fair comparison of the engine performance and emissions achieved with the different fuel setups and the different combustion concepts revealing the potential and challenges of ammonia combustion.

All experiments have been supported with 1D thermodynamic and 3D CFD simulations for clear understanding of the physical and chemical processes. On the other hand, the experimental results have been used for the validation of numerical models. The ability to model complex physical and chemical processes and to simulate them predictively, has been proven and enables an efficient, reliable and timely evaluation of concepts and variants.

This is particularly important and helpful in the development of large engines, as the production of prototypes for physical testing is associated with immense costs and time, if not impossible at all.

Looking at the combustion concepts, the diesel-ignited ammonia concept, which would require only simple modifications of a base engine, showed a reasonable reduction of the CO_2 equivalent emissions. But there is still potential for further optimization by maximizing the ammonia energy ratio and minimizing the excess air ratio. A reduction in unburned ammonia emissions and nitrous oxide emissions are the key success factors.

The spark-ignited ammonia concept showed an excellent potential for the reduction of the CO_2 equivalent emissions with low unburned ammonia emissions and low nitrous oxide emissions. However, an excessively high NO_x emission was recognized and further optimizations of operational parameters, especially the energy ratio of the additional hydrogen, are required.

For both, diesel- and spark-ignited premixed NH_3 combustion, a trade off is evident. A leaner mixture will increase unburnt NH_3 and N_2O, but reduce NO_x. On the contrary possibilities to enrich the mixture are limited. For the diesel-ignited concept, the lower limit is the increase of CO emission, due to insufficient availability of oxygen, which is required for the combustion of the diesel. For the spark-ignited concept, the lower limit is the increased thermal load and the temperature limit of specific engine components (fire deck, valves and seats, liner, piston). The trade off between NO_x and other emissions, as described above, is relevant for the layout of an exhaust gas aftertreatment system. As a next step, our development therefore focusses on substrate characterization, considering the extremes in NH_3/NO_x ratio occurring with both, the diffusive and the premixed ammonia combustion concepts. This is necessary because only an optimized thermodynamic design of the engine and the exhaust aftertreatment system makes it possible to exploit the full potential of ammonia-powered combustion engines.

In this context, a simulation-driven development approach seems to be the right way to understand and optimize concepts for CO2-neutral combustion engines on the one hand and to meet the need for shorter and less costly development cycles on the other.

9 ACKNOWLEDGEMENTS

For the ammonia test program, the authors would like to acknowledge the financial support of the "COMET - Competence Centers for Excellent Technologies" Program of the Austrian Federal Ministry for Climate Action, Environment, Energy, Mobility, Innovation and Technology (BMK) and the Federal Ministry for Digital and Economic Affairs (BMDW) and the Provinces of Styria, Tyrol and Vienna for the COMET Centre (K1) LEC EvoLET. The COMET Program is managed by the Austrian Research Promotion Agency (FFG).

The authors would like to thank the AVL colleagues Maik SUFFA, Simon Bezensek, Martin KIRSTEN and Martin HOEPPNER for their support.

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