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A spark ignited combustion concept for ammonia powered high-speed large engines – Test bed and 3D CFD simulation results

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Abstract

The ongoing energy transition and the global shift towards carbon-free fuels and e-fuels derived from renewable energy sources has sparked a significant interest in the application of ammonia. Ammonia, being a carbon free alternative fuel with some challenging attributes, shows great potential for marine propulsion systems and other high-power applications.

The paper explores two different ammonia combustion concepts for high-speed engines, as investigated by AVL. The first combustion concept involves a retrofittable approach of a premixed ammonia combustion with a Diesel pilot ignition, while the second concept pursues 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. Following a comprehensive comparison of these two concepts, the focus of the paper shifts to the analysis of the spark ignited ammonia engine.

The exploration commences with an introduction to AVL's single-cylinder high-speed engine featuring a 175 mm bore size and specific test configurations. Measurement results will be discussed regarding their impact on engine performance and emissions. Engine maps showing ammonia-nitrogen oxides ratio and excess air ratio values of NH_3-only consideration are 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 those laughing gas emissions through combustion system development or by deploying exhaust gas aftertreatment systems with highest efficiencies, further illustrating N_2O emissions in CO_2 equivalent for emphasis.

In the subsequent section, the paper discusses simulation results of mixed hydrogen-ammonia fuel operation. Insights to mixture preparation and combustion are provided, with a specific focus on NO_x and N_2O emissions, along with unburned ammonia. The discussion focuses on the potential for enhancing air/fuel mixing and combustion based on simulation results, incorporating comparisons with experimentally obtained data whenever feasible.

As a conclusion, the paper finally summarizes key findings and is offering an outlook on future developments, encompassing ongoing work on combustion concepts like ammonia high-pressure direct injection, exhaust aftertreatment, and related simulation toolchain and its application. The seamless

integration of advanced 1D/3D CFD simulation methodology combined with the experimental results provides a holistic view of the ammonia combustion processes and sets the stage for further improvements for the development of ammonia powered combustion engines.

1. Introduction

Marine transportation is a critical facilitator of the global economy, but its contribution to total anthropogenic greenhouse gas (GHG) emissions has grown. This contribution increased from 2.76% in 2012 to 2.89% in 2018 [1]. In response, various initiatives have emerged to reduce shipping emissions, including the International Maritime Organization's (IMO) initial GHG strategy adopted in 2018. This strategy has spurred increased research and development of alternative fuels and hybrid propulsion systems for the maritime sector. Building on these efforts, the IMO's Marine Environment Protection Committee (MEPC 80) in July 2023 adopted a revised GHG Strategy with ambitious emissions reduction targets. These targets include a 20% reduction by 2030, a 70% reduction by 2040 (compared to 2008 levels), and ultimately, achieving net-zero emissions by 2050, as shown in Figure 1.

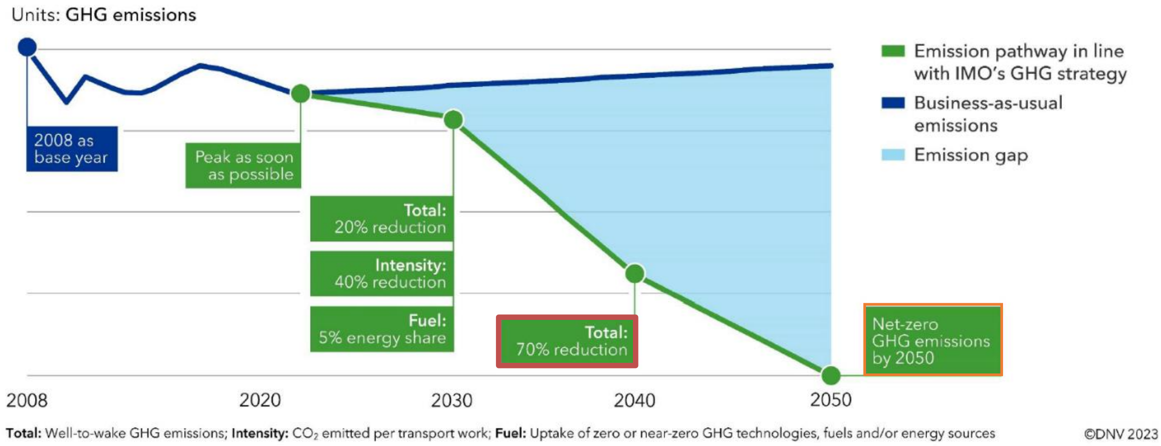


Figure 1: Revised IMO GHG strategy, Source DNV [3]

Ammonia is a zero-emission carbon free fuel and can be processed on board of vessels without producing any direct 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 (100 gCO_2/kWh-GWP100) as e-Methane, e-Methanol and e-LH2 [3]. The attractiveness of ammonia for the maritime industry is not only based on the zero direct GHG emissions, but also on the already established infrastructure as ammonia is a commonly sea-traded good and many ports worldwide can provide ammonia infrastructure already today. This is however still limited to fossil ammonia requiring huge effort to transform to green ammonia. As a bridging solution, fossil ammonia will likely be used, and the green ammonia infrastructure build-up plans are readily accessible, and there is serious commitment to be observed from key stakeholders.

This paper explores two different ammonia combustion concepts for high-speed engines, investigated by AVL. The first combustion concept involves a retrofittable approach of a premixed ammonia combustion with a Diesel pilot ignition, while the second concept pursues 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. Following a comprehensive comparison of these two concepts, the focus of the paper shifts to the analysis of the spark ignited ammonia engine.

Measurement results of both combustion concepts will be discussed regarding their impact on engine performance and emissions. Engine maps showing ammonia-nitrogen oxides ratio and excess air ratio values of NH_3-only consideration are 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 those laughing gas emissions through combustion system development or by deploying exhaust gas aftertreatment systems with highest efficiencies, further illustrating N_2O emissions in CO_2 equivalent.

Additionally, the paper discusses simulation results of mixed hydrogen-ammonia fuel operation. Insights to mixture preparation and combustion are provided, with a specific focus on NO_x and N_2O emissions, along with unburned ammonia. The discussion focuses on the potential for enhancing air/fuel mixing and combustion based on simulation results, incorporating comparisons with experimentally obtained data whenever feasible.

The seamless integration of advanced 1D/3D CFD simulation methodology combined with the experimental results provides a holistic view of the ammonia combustion processes and sets the stage for further improvements for the development of ammonia powered combustion engines.

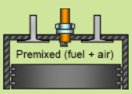
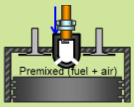
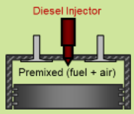
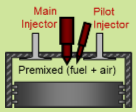
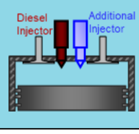
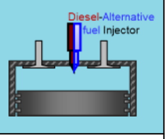
2. Assessment of Combustion Concept for Ammonia

The characteristics of different gas and dual fuel combustion concepts have already been discussed in previous papers [4], [5] and [6]. Their tolerance for the utilization of ammonia as alternative fuel are summarized in Table 1.

One possible and presumably simpler way is to employ a premixed combustion concept. The ammonia can be mixed with the air upfront of the combustion chamber, e.g. in the intake port via gas admission valves (port fuel injection, PFI). The pre-mixed air-fuel mixture will then be ignited either by a spark plug or by injecting diesel fuel. The spark ignition system or diesel injection system of the baseline engine can be carried over. This concept therefore allows a relatively simple conversion of an existing diesel or gas engine by simply applying an additional ammonia injection system, which would not only enable a quick introduction of ammonia-fueled engines into market but also a retrofit of already introduced engines whose lifetime exceeds the targeted timeframe for CO_2 reduction.

The other option is a diffusive combustion concept, in which ammonia is injected directly into the combustion chamber at high pressure of around 500 bar and higher. The injected ammonia will then be ignited by injecting the pilot diesel fuel. This concept generally offers an opportunity to solve the problems associated with premixed combustion, such as combustion anomaly or unburned ammonia emissions, but poses a challenge of engine complexity with two high-pressure fuel injection systems. Another challenge is the current availability of high-pressure pumps and fuel injection equipment for ammonia.

Table 1: Combustion Concepts for Ammonia

Strategy	**Quick 'time-to-market'**				**Dedicated 'Flex Fuel'**	
Mixture formation	**Port gas admission**				**Direct injection**	
Combustion & Ignition Concept	**Pre-mixed combustion Spark ignition**		**Pre-mixed combustion Diesel pilot injection**		**Diffusive combustion Diesel pilot injection**	
						
Substitution rate	**100%**		**30 ~ 90%**	**> 95%**	**~95%**	
Diesel back up capability	**N.A.**		**100%**		**30 ~ 100%**	

2.1. Pre- mixed combustion with spark ignition

The majority of large natural gas engines on the market employ spark-ignited pre-mixed combustion concept and apply either an open chamber concept or a pre-chamber combustion concept. These natural gas engines can be converted in a relatively simple way to carbon-neutral engines by adapting the relevant components such as gas supply system to those compatible to the selected alternative fuel.

Considering the lower heat value of ammonia compared to the natural gas, an appropriate sizing of gas admission valve is required. In addition, the ammonia compatibility of the materials used in the entire gas supply system as well as in the components that come in contact with ammonia (e.g. combustion chamber, exhaust system, crankcase and blowby system) must be carefully checked.

Both of the combustion concepts with or without pre-chamber can tolerate ammonia well to a certain extent. Open chamber spark-ignited (OCSI) concept, however, may suffer from the low reactivity characteristics of ammonia due to its limited ignition energy and a mixing of hydrogen to ammonia is necessary to assure a stable ignition and combustion.

The pre-chamber spark-ignited (PCSI) concept has a higher chance to realize a good ammonia combustion, but an admixing of hydrogen is still necessary at least at engine start and low load operation. Highlights from the measurement results on a single cylinder test engine will be given in a later section of the paper.

In both OCSI and PCSI, high levels of unburned ammonia emissions and nitrous oxide emissions as well as very high NO_x emissions are expected and thus, exhaust aftertreatment system is mandatory.

2.2. Pre- mixed combustion with diesel injection

By adding or adapting the gas supply system, it is feasible in a relatively simple manner to burn ammonia in diesel or dual fuel engines. One of the biggest advantages of such diesel substitution or dual fuel engines is the redundancy of engine operation in diesel mode. It is possible to continue the engine operation independently of the availability of the ammonia or even in case of troubles of ammonia-related subsystems.

Ammonia can be tolerated quite well by the diesel-ignited pre-mixed combustion concept. The strong ignition energy made available by the pilot diesel injection assures a stable ignition of the mixture.

Combined with a proper setting of the excess air ratio, 90 to 95% (energy based) substitution rate can be realized. Similar to the spark-ignited combustion, however, quite high unburned NH_3 emissions and very high NO_x emissions force an application of exhaust aftertreatment. Highlights from the measurement results on a single cylinder test engine will be given as a comparison basis to the spark-ignited pre-mixed combustion concept in a later section of the paper.

2.3. Diffusive combustion with diesel pilot injection

While the pre-mixed combustion concept could be realized in a relatively simple manner by adapting the gas supply system, the associated challenges such as combustion anomalies and exhaust gas emissions pose a limitation on the achievable substitution rate and potential reduction of GHG gas emissions. Diffusive combustion concept could offer a good solution to these known challenges of the pre-mixed combustions whereas the availability, reliability and durability of high-pressure injectors and high-pressure pumps that are compatible for the selected alternative fuel as well as the significantly increased complexity of the engine and subsystems are the main challenges.

From the diffusive combustions of ammonia, a significant reduction of unburned NH_3 emissions is expected compared to pre-mixed combustions. Injectors and high-pressure pumps for ammonia, however, are still at an early phase of the development and available to a limited extend.

3. Single Cylinder Engine Test Results

3.1. Test engine

The AVL high-speed single cylinder test engine SCE175 shown in Figure 2 was used for the investigations described in the following section of the paper. AVL designed a new clean sheet engine power cylinder unit to be used as a platform for the performance and mechanical development testing and successfully demonstrated a BMEP of 35 bar and a BSFC of 168 g/kWh at 1500 rpm in diesel engine version and a BMEP of 32.5 bar and a brake thermal efficiency of 50% at 1500 rpm with and engine-out emissions cap of 500 mg/Nm3 NO_x at 5% residual O_2 in gas engine version [7].

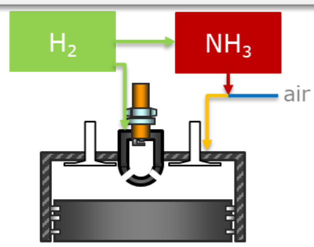
The engine is characterized by a high peak firing pressure capability of up to 330 bar while retaining state-of-the-art durability requirements. The engine can be operated as a diesel engine, gas engine or dual fuel engine with a common rail injection system for liquid fuel and with a port gas admission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

Figure 2: 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 Table 2. The gaseous fuel was mixed with the air by a venturi gas mixer and an air/fuel mixture was supplied to the engine. 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 the air by the venturi gas mixer.

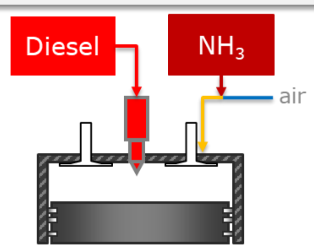
Table 2: Schematic diagram and specifications of SCE175 used for testing in this study

NH_3 Gas Engine



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

NH_3 Substitution Engine



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

3.2. Diesel-ignited pre-mixed ammonia combustion test result

The ammonia air mixture supplied to the combustion chamber was then ignited by an injection of diesel fuel through a common rail diesel injector that is capable of the rated output in diesel operation mode i.e. 35 bar BMEP. While this concept has an advantage of being able to maintain the full load capability in diesel operation mode, the maximum possible substitution rate by ammonia is typically limited by the injection stability at low injection quantities.

Figure 3 shows the influences of diesel energy ratio and excess air ratio on unburned ammonia emission and nitrous oxide emission. The excess air ratio shown in the figure is a global excess air ratio considering both diesel and ammonia. The measurement was conducted within the shown operating area 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 typically are the exhaust gas temperature and CO emissions due to incomplete combustion of diesel fuel. Towards the higher excess air ratio and the lower diesel energy ratio (bottom right corner of the diagram), the operational limits typically 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) and the very lean ammonia air mixture only vicinity of the diesel flame burns and a considerable portion of ammonia air mixture between the diesel flames remains unburned. Thus, a small variation in decimals of the global excess air ratio do not improve the ammonia combustion sufficiently.

As the excess air ratio and diesel energy ratio are further decreased, however, the unburned ammonia as well as nitrous oxide emission decreases significantly. In this area the excess air ratio of ammonia only becomes below 2.5 and it can be understood that the combustion of ammonia air mixture between the diesel flames also starts improving.

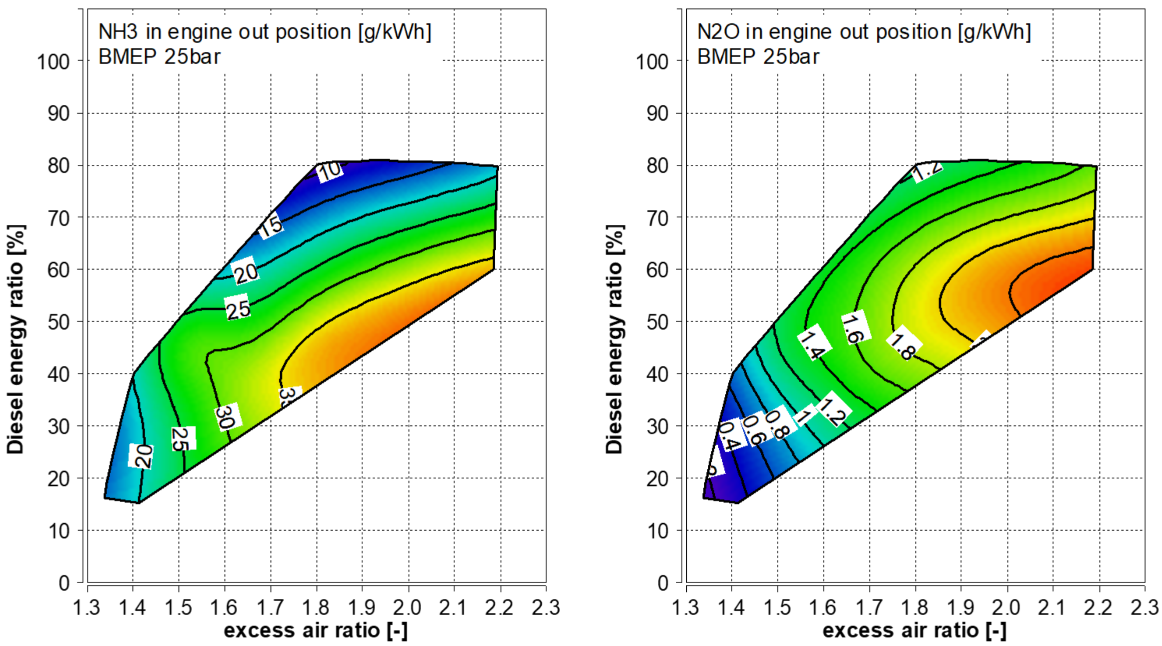


Figure 3: Unburned ammonia emission (left) and nitrous oxide emission (right) as a function of diesel energy ratio and excess air ratio measured at engine out at BMEP 25 bar and 1350 rpm

Figure 4 shows the effective engine 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. Note that these values of diesel operation mode were measured with the same engine configuration as the ammonia substitution measurement and do not represent the optimum diesel performance measured on this engine platform.

The efficiency decreases as the ammonia energy ratio is increased mainly due to unburned ammonia emissions and slightly improves at the low excess air ratio and the low diesel energy ratio as the unburned ammonia emission decreases in this area.

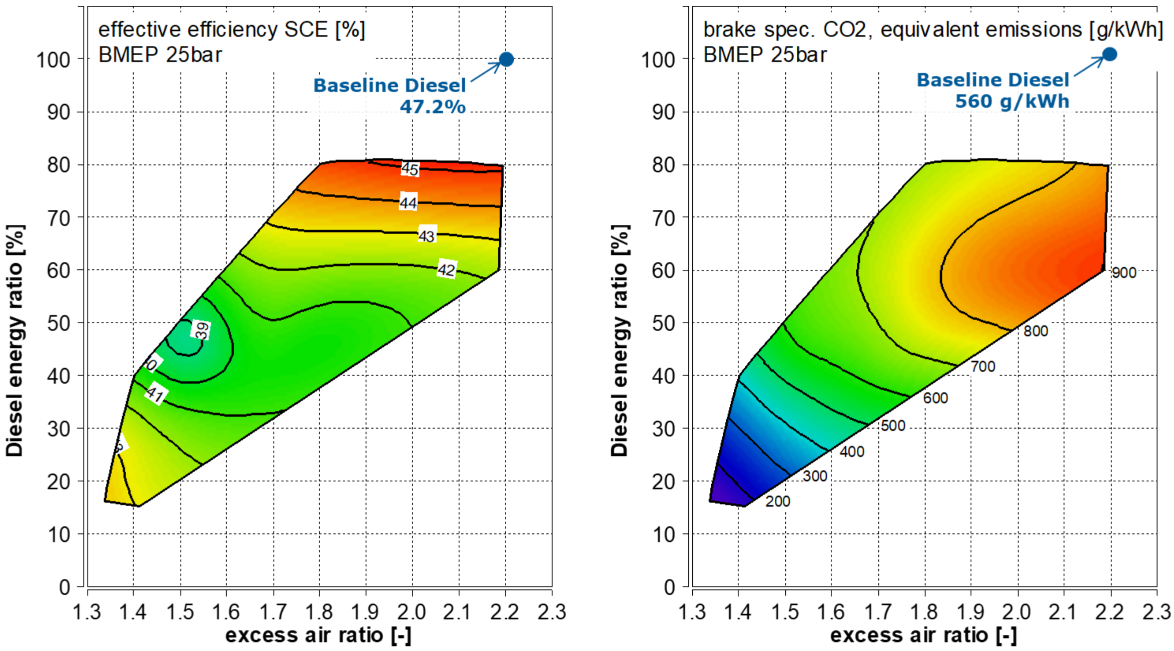


Figure 4: Brake thermal efficiency (left) and CO_2 equivalent emission (right) as a function of diesel energy ratio and excess air ratio measured at engine out at BMEP 25 bar and 1350 rpm

CO_2 equivalent emissions reflect the trend of the nitrous oxide emissions as the global warming potential of the nitrous oxide is 265 in 100 years scale according to the 5th assessment of the IPCC [8] and has a significant influence on the CO_2 equivalent emissions. Diesel energy ratio of above around 40% CO_2 equivalent emissions is even worse than the baseline diesel operation. The benefit can only be seen in the area of the low excess air ratio and the low diesel energy ratio where the nitrous oxide emissions can be decreased.

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 in order to realize a low unburned ammonia and a low nitrous oxide emission.

When the diesel injector with the full load capability is carried over, the injector capability for stable injections of small quantities is one of the key success factors for this combustion concept. In addition, the turbocharger layout including the air path control system to realize the low excess air ratio required for ammonia combustion and high excess air ratio in diesel operation mode is an important development topic. Furthermore, the optimizing the transition from diesel to ammonia operation is another development challenge, as the gradual increase in the ammonia ratio may fail due to excessive unburned ammonia and excessive nitrous oxide emissions.

3.3. Spark-ignited pre-mixed ammonia combustion test result

For the spark-ignited combustion concept, a mixture of hydrogen and ammonia was mixed with the air through a venturi mixer. The energy fraction of hydrogen mixed to ammonia was constant at 15% in the measurements discussed in this section. 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 and directly into the pre-chamber. The quantity of the additional hydrogen to the pre-chamber was about 1% in energy fraction of the total fuel. This extra enrichment of the pre-chamber by the pure hydrogen is to ensure a stable start of combustion by a spark ignition.

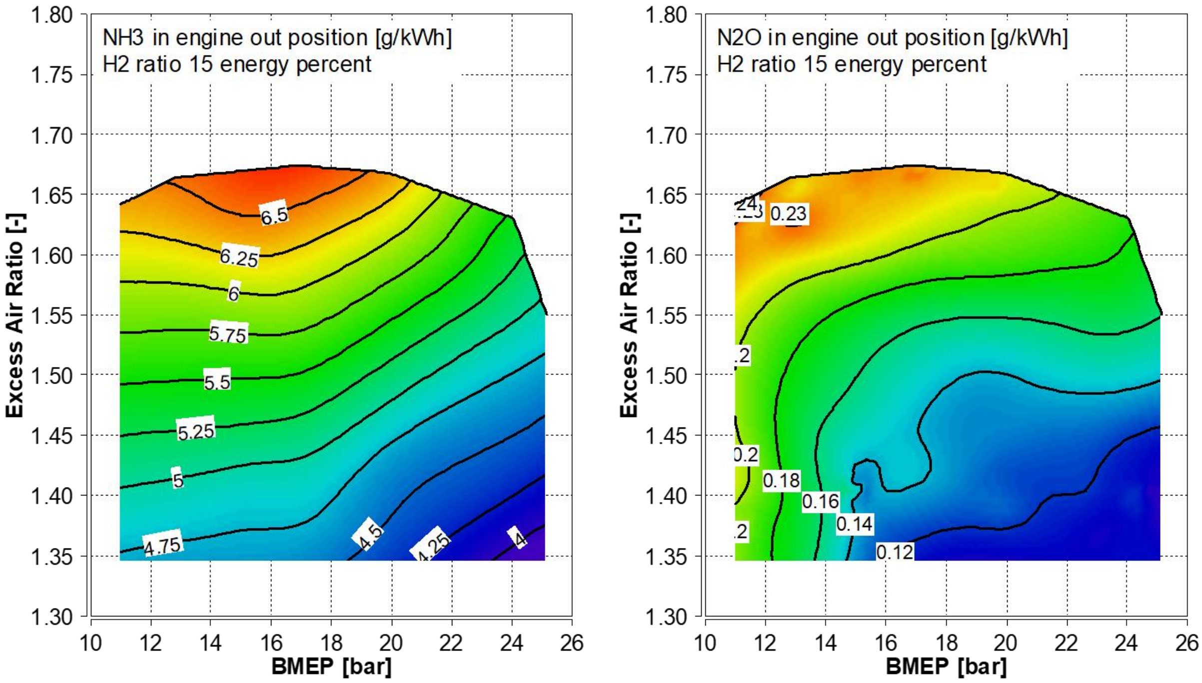


Figure 5: Unburned ammonia emission (left) and nitrous oxide emission (right) as a function of BMEP and excess air ratio measured at engine out at 1500 rpm with a constant hydrogen energy fraction of 15%

Figure 5 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 as shown in the Figure 3. 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 the incomplete combustion and CO emissions. In addition, the mixing of hydrogen significantly supports the ammonia combustion and reduces the unburned emissions. Nevertheless, the trend itself is similar to the diesel-ignited combustion and the lower excess air ratio results in the reduction of the emissions.

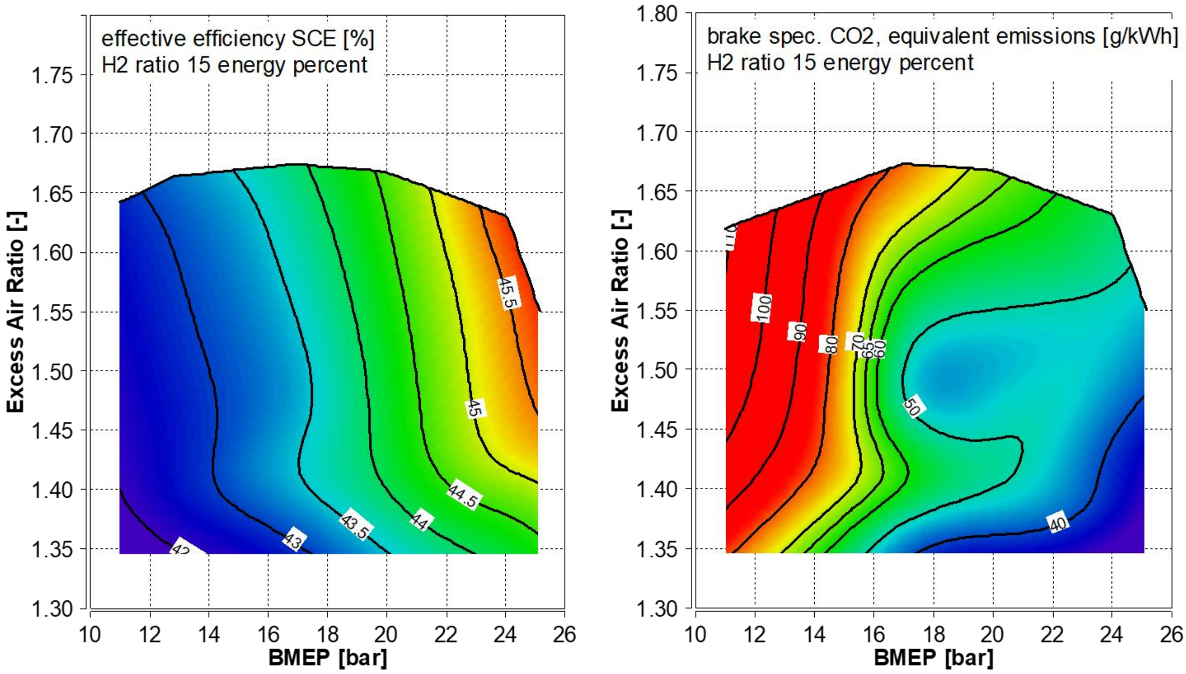


Figure 6: Unburned ammonia emission (left) and nitrous oxide emission (right) as a function of BMEP and excess air ratio measured at engine out at 1500 rpm with a constant hydrogen energy fraction of 15%

Figure 6 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 for the CO_2 equivalent emissions follows nitrous oxide emissions, but is at very low level compared to the diesel-ignited concept as shown in the Figure 4. The fuel is carbon free and thus, the CO_2 emission from the engine is at a quite low level and resulting from the combustion of the lubricating oil.

A drawback of the tested concept were the very high NO_x emissions, NO_x values above 35 g/kWh were measured, due to compact Rate of heat release as enabled by the hydrogen admixing and due to high temperature caused by the low excess air ratio. The level of NO_x emission is much higher than that of the unburned ammonia emission meaning that an additional urea injection would be required at SCR. Ideally, the levels of NO_x emission and NH_3 emission at engine out are balanced so that the additional urea injection at SCE can be avoided or minimized.

A reduction of 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 must be investigated. In this study, pure hydrogen was supplied to the pre-chamber for simplicity, and this must have had a certain influence on the resulting high NO_x emission. In the actual application, however, the 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 7 compares the engine performance and emissions of four different combustion concept, namely, diesel, natural gas, ammonia spark-ignited 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 NO_x 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 global warming potential (GWP) of 28 according to the 5th assessment of the IPCC, resulting in 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 emissions. It emits only 6 to 6.6% of CO_2 equivalent emissions compared to the diesel and gas engines, respectively. As discussed above, however, the excessive NO_x emission is the challenge of this combustion concept and further development steps are necessary.

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 from this concept is about 20% compared to the diesel engine, the CO_2 equivalent emission counts for 36% of the diesel engine 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. Further increase of the ammonia energy fraction and optimization of the excess air ratio to minimize the nitrous emission are the key development targets for this combustion concept.

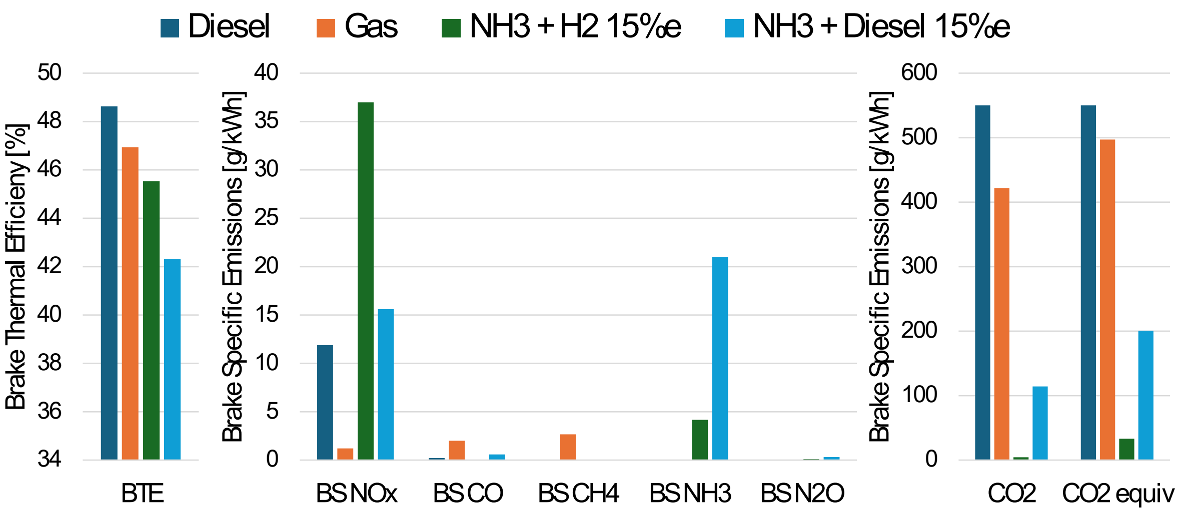


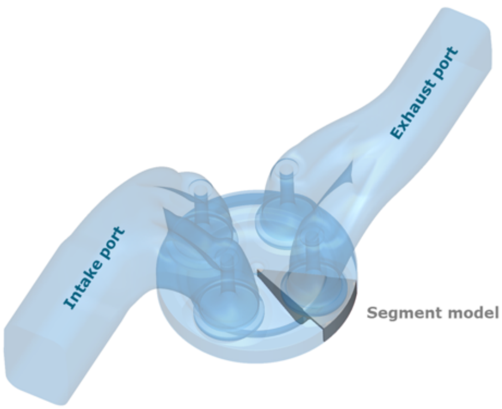
Figure 7: Comparison of brake thermal efficiency and emission performances among diesel, gas, NH_3 spark ignited and NH_3 diesel ignited at BMEP 25 bar

4. 3D CFD Simulation

For a better understanding of the physical phenomena and to potentially support further combustion concepts development, 1D thermodynamic and 3D CFD simulations of the diesel-ignited pre-mixed ammonia combustion and the spark ignited pre-mixed ammonia concept, were conducted. A computational model was setup for each concept separately and some selected operating conditions were simulated by means of CFD, while 1D thermodynamic simulation was performed for the complete engine operating map using the AVL Simulation solutions FIRE™ M und CRUISE™ M respectively.

4.1. Diesel-ignited premixed ammonia combustion concept simulation

The computational model was setup for the operating point 25 bar BMEP at 1350 rpm. The simulations have been performed for two operating conditions – one for using pure diesel as a fuel and the other one using 20 energy percent of diesel and the rest ammonia. The given percentage describes the share in the total energy introduced in the combustion chamber. While the first operating condition reflects the standard diesel operating mode of the engine, the other one with 20% Diesel and 80% NH_3 represents conditions close to the limit where stable combustion still can be achieved. The computational model and the simulated operating conditions are presented in Figure 8.



	100% Diesel	20% Diesel, 80% NH_3
Rotational speed [rpm]	1350	1350
IMEP [bar]	24.5	23.5
Diesel SOI BTDC [ºCA]	4.8	13.3
Diesel DOI [ºCA]	8.6	6.0
Rail pressure [bar]	2200	1400
Total air excess ratio [-]	2.22	1.47

Figure 8: Simulation model and simulated operating conditions

A mixture of ammonia and air is supplied to the intake port through a venturi mixer. This results in almost ideal homogeneity of the mixture. Therefore, homogeneous mixture was initialized 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. In order to minimize the required computational resources, only a cylinder segment of 40°, featuring one nozzle hole was simulated for the high-pressure cycle featuring compression, diesel injection and combustion as shown in Figure 8.

The combustion process was simulated deploying a general gas phase reaction solver. This requires the use of a chemical kinetic mechanism suitable for NH_3, H_2 and n-heptane combustion simulation [9]. The mechanism deployed in this study 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 5 K limit for temperature and 0.01 limit for the equivalence ratio to define the model 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. Diesel injection and combustion were calibrated to the experimental data. Cylinder mean pressure and rate of heat release curves are presented in Figure 9.

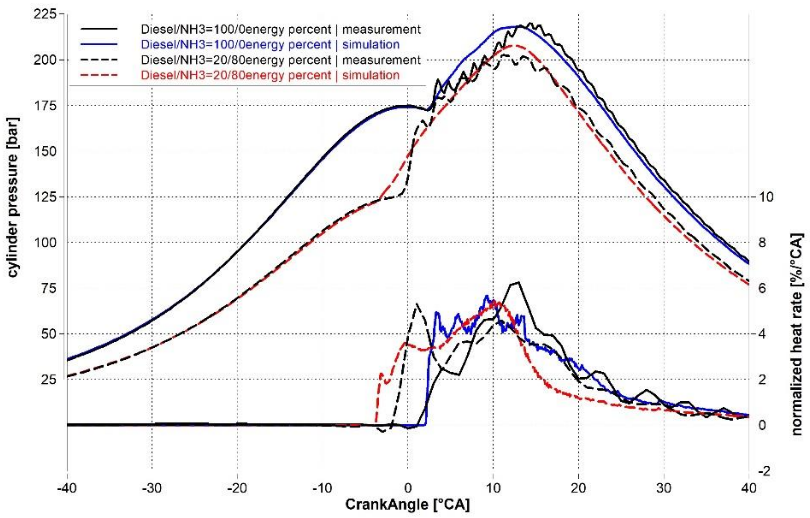


Figure 9: Simulated vs Experimental cylinder mean pressure and ROHR for two operating modes

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 10. Diesel starts to evaporate earlier and more intense if it is injected into a pure air. In this particular case the rail pressure is significantly higher. Consequentially 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.

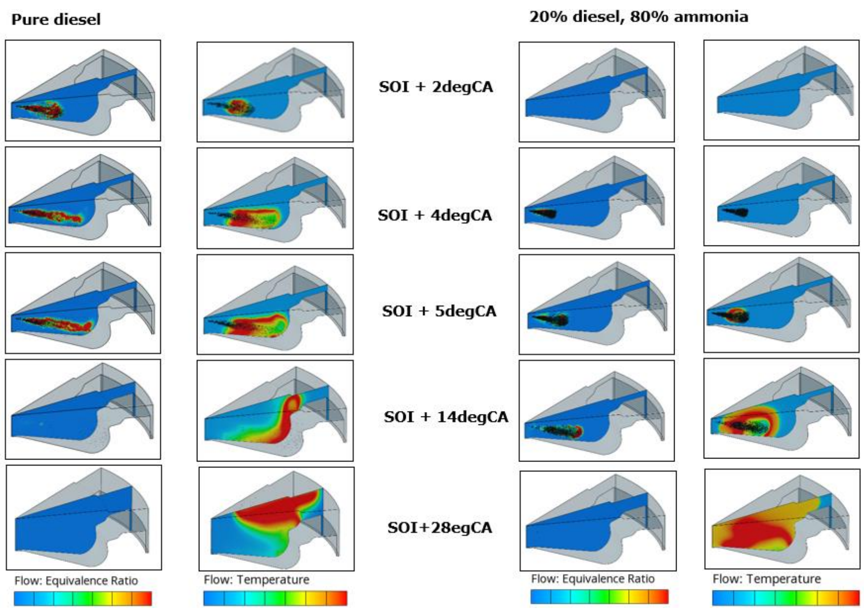


Figure 10: Comparison of fuel injection and combustion for both simulated operating modes

In the dual fuel case, the evaporation of the diesel starts later. Also, ignition is taking place significantly later compared to the pure diesel 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 evaporation is slower. The lower injection velocity also results in a weaker mixing process. Furthermore, the diesel-ammonia mix has elongated auto-ignition time, therefore ignition starts at a time, when the jet kinetic energy is almost neutralized. The ignition point is in a mixed fuel region. From this ignition kernel, the combustions 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 into the squish area), the flame propagation slows down due to the low laminar flame speed of ammonia. This slow combustion is also a reason for the high ammonia slip related to this concept. Please refer to the Figure 11.

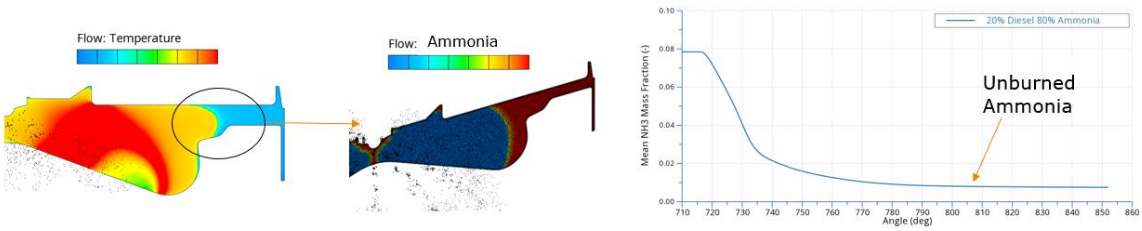


Figure 11: Slow combustion in pure ammonia region

4.2. Spark ignited premixed ammonia combustion concept simulation

The computational model was setup for three operating conditions. They represent load and an air excess ratio variation at constant engine speed, see Table 3.

Table 3: Simulated operating conditions

Operating condition	369	378	381
Rotational speed [rpm]	1500	1500	1500
IMEP [bar]	18.5	24.6	27.8
Air excess ratio	1.46	1.44	1.40

As written above, the mixture of ammonia and hydrogen is supplied to the intake port through a venturi mixer. This results in almost ideal homogeneity of the mixture. Therefore, 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%. An additional 1% 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 including important geometry parts is presented in Figure 12. A key role at this combustion concepts plays the pre-chamber.

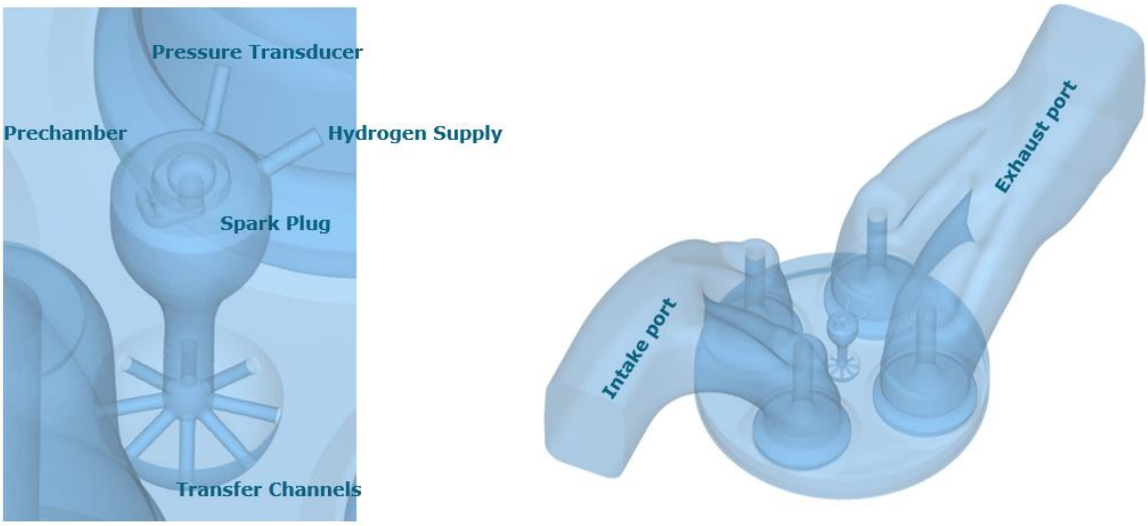


Figure 12: Simulation model (© AVL)

Simulating the combustion of the spark-ignition concept, the same models (general gas phase reaction kinetics and multi-zone accelerator) have been used as for the diesel-ignition concept.

CFD simulations of all selected operating conditions were conducted. Minor calibration of the combustion process was required in order to match mean cylinder pressure and rate of heat release curves from the experimental data. The calibration was done by means of variation of the combustion reaction rate. The mean cylinder pressure and the accumulated heat release curves for all simulated operating conditions are presented in Figure 13. Good agreement between simulated and the experimental results can be observed, which indicates that the simulation results realistically reflect the involved physical phenomena.

Slightly too fast reaction rates can be observed, which relates to the slightly overpredicted mean cylinder pressure for all simulated operating conditions. Simulated and experimental results are consistent for all modelled operating conditions, which indicates a high level of robustness of the simulation model and its potential to correctly predict in-cylinder flow conditions for a large variety of operating points.

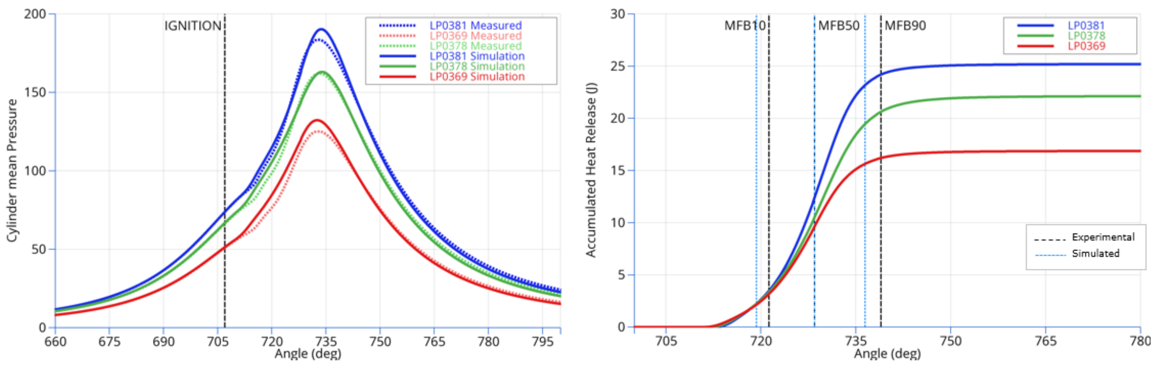


Figure 13: Simulated vs. experimental cylinder mean pressure and accumulated heat release

As already mentioned, the key role in this combustion concept plays the pre-chamber design and the enrichment of the pre-chamber mixture with additional hydrogen. 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 it a bit difficult to control the supplied mass. The dynamic of the hydrogen propagation into the pre-chamber and mass-fractions in the spark plug area are displayed in Figure 14. It can be observed, that the pre-chamber gets almost completely filed with hydrogen during the intake stroke and later a significant part of it propagates to the cylinder. However, a considerable mass-fraction of hydrogen remains within the pre-chamber and in the spark plug region thus helping to achieve stable ignition and combustion within the pre-chamber.

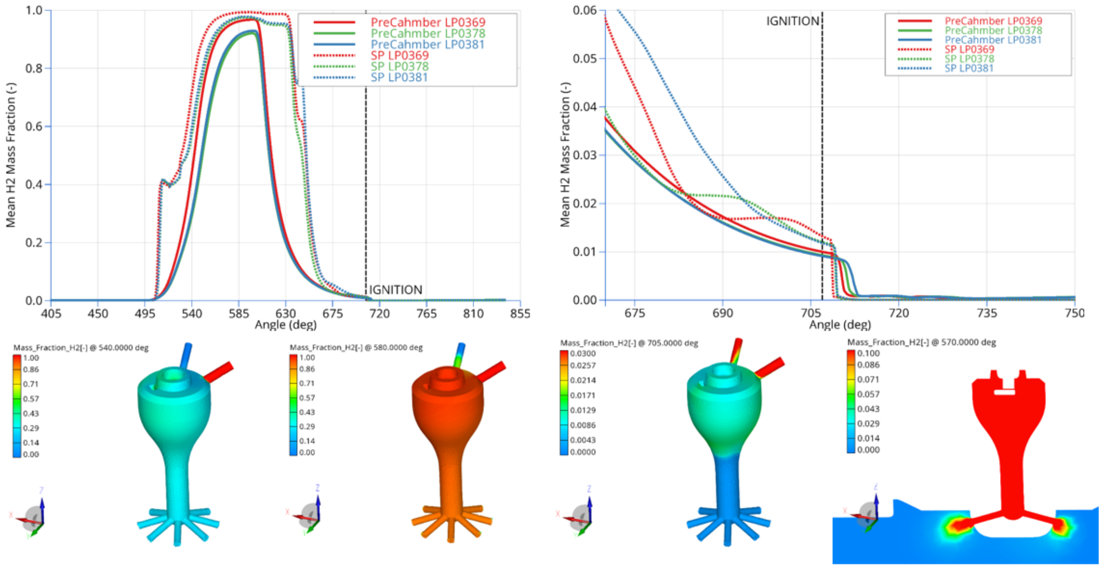


Figure 14: Hydrogen mass-fractions in the pre-chamber and spark plug area

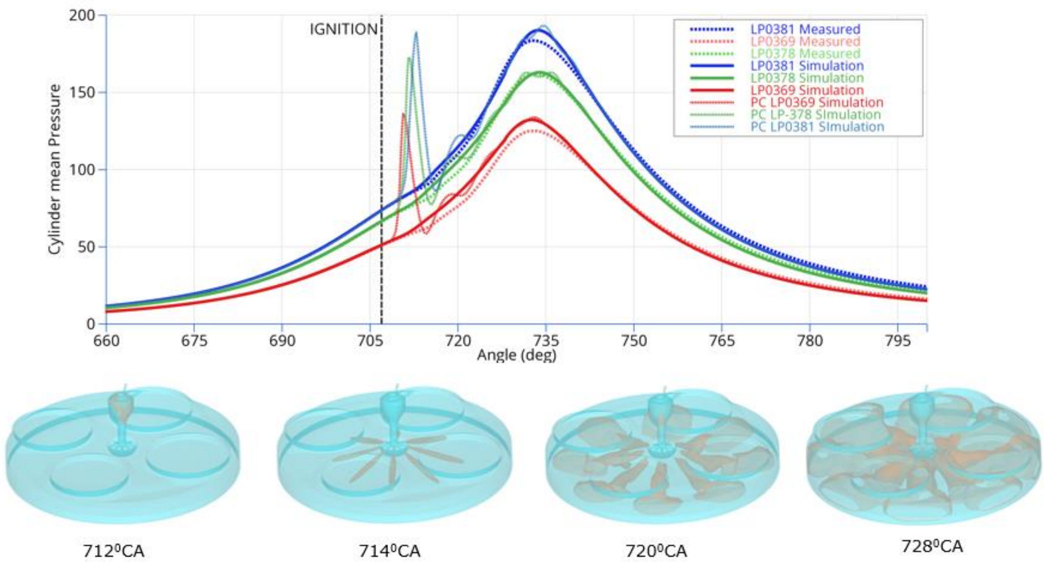


Figure 15: Pre-chamber pressure vs. cylinder mean pressure (top) and flame visualization (bottom)

In Figure 15 the combustion behaviour is shown. The flame front visualization nicely demonstrates the working engine concept. Ignition is initiated by the spark in the pre-chamber. Due to the relatively high hydrogen concentration there, it is stable and reliable. High pressure appears in the pre-chamber after ignition (significantly higher than in a cylinder). Therefore, a strong flow and flame propagation from the pre-chamber to the main chamber through the transfer channels can be observed. The high-speed and energy intense jets entering the main chamber ensure ignition and combustion of the lean ammonia/hydrogen/air mixture in the cylinder volume.

5. Summary and Outlook

The paper described two different ammonia combustion concepts for high-speed engines, as investigated by AVL. The first combustion concept represented a retrofittable approach of a premixed ammonia combustion with a diesel pilot ignition, while 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 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 from the different fuels and different combustion concepts revealing the potential and challenges of the ammonia combustions.

While the diesel-ignited ammonia combustion concept already showed a reasonable reduction in the CO_2 equivalent emissions by a relatively simple engine modification, there is still a good potential for the further optimization by a maximization of the ammonia energy ratio and a minimization of excess air ratio. A reduction in unburned ammonia emissions and nitrous oxide emissions are the key success factors.

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

For specific applications, hydrogen is derived from Ammonia via an onboard cracking process. Further combustion development and optimizations will focus on the admission of N_2/H_2 mixtures to the pre- and main chamber.

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 (combustion byproduct) and reduce NO_x. On the contrary an enrichment of the mixture is limited. For the diesel ignited concept, the lower limit is the increase of CO, due the missing oxygen content for the combustion of Diesel.

For the spark ignited concept, the lower limit is the increased thermal load and the temperature limit of specific engine core components (fire deck, valves and seat rings, liner, piston). The trade off as described above is relevant for the layout of the aftertreatment system as determining the composition of the raw missions varying over speed and load of the engine.

As a next step, our developments are focused on substrate characterizations considering the low and high NH_3/NO_x ratio to cover diffusive and premixed ammonia combustion. The overall thermodynamic layout of the engine and aftertreatment is a key element enabling Ammonia engines to be a promising solution for the near future.

CFD simulations (in conjunction with other simulation models and disciplines) represents a suitable means of understanding and optimizing concepts for CO_2-neutral combustion engines. The ability to model complex physical and chemical processes and to simulate them predictively in a timely manner allows concepts and variations to be assessed efficiently and reliably. This is a decisive argument for the use of simulation, especially in the development of large engines, since the construction of components and system prototypes for physical testing is associated with immense costs and time expenditure.

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