Simulation of ammonia combustion in dual-fuel compression-ignition engine

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Abstract. Ammonia is regarded as an attractive alternative fuel for combustion engines with a great potential to replace currently used petroleum-based energy carriers. Its direct combustion does not result in emission of carbon dioxide and it can be produced from renewable sources. The energy density of ammonia is reasonable, it is relatively easy to store and has well established infrastructure for production, storage, handling and distribution. However, ammonia is corrosive to some materials, difficult to ignite due to high octane number and high autoignition temperature, and has low heating value. Therefore theoretical and experimental studies are needed to enhance the performance and expand the operating range of ammonia-fuelled engines. This study investigates the feasibility of introducing ammonia to dual-fuel compression-ignition engine, where a pilot dose of diesel oil initiates the ignition of ammonia-air mixture. Numerical simulations of the combustion process were carried out using a one-dimensional model, parametrized according to the specifications of a four-cylinder, turbocharged compression-ignition engine with conventional direct injection supply system, modified slightly for ammonia induction. The model was validated by comparison with empirically determined data. The simulations were performed for different combinations of ammonia-diesel oil ratios at various engine load. Ammonia was treated as an energy replacement for diesel oil. Engine performance and emissions of selected pollutants in dual-fuel operation mode were compared to that with diesel oil only. The results showed that different ammonia–diesel oil ratios can be used to achieve the same engine torque. A higher than rated power, depending on engine load conditions, can be obtained with the addition of an extra dose of ammonia. The influence of ammonia on the emissions of particular pollutants varied and was discussed in detail. Acquired combustion characteristics and engine performance parameters allow for a positive verification of the proposed model. The drawn conclusions may be useful for the development of dual-fuel engine control algorithms.

1. Introduction
In the upcoming decades the world transportation industry is expected to develop in the direction of substituting fossil fuels with other energy sources, including carbon-free alternatives. The trend to make transportation vehicles independent of carbon-based fuels has both short and long term explanation. In the short term, decarbonisation of transportation has a great potential to reduce engine pollutant emissions originate from carbon combustion, including carbon dioxide (CO₂) – the most stigmatized greenhouse gas, carbon monoxide (CO), hydrocarbons (HC) and particulate matter (PM) – one of the most problematic pollutants when it comes to the impact on health. From the long term
perspective, it is clear that the fossil fuels reserves are likely to be depleted and their domination in world transportation has an end date. Therefore currently much effort is being spent on the evaluation of other energy carriers with a particular emphasis on their sustainability [1–4].

Among the many options being considered, ammonia (NH₃) has some distinct advantages [5]. Its large-scale implementation is regarded as relatively easy comparing to other alternative fuels. Currently ammonia is one of the most synthetized chemicals in the world and already has well established infrastructure for production, handling and distribution. It can be produced from both fossil and renewable sources. It is inconvenient to store as a gas or in liquid form at low pressure (approx. 1 MPa) and room temperature (298 K).

The only products of ammonia combustion are water (H₂O) and nitrogen (N₂). Theoretically, no CO₂ is formed in the engine cylinder, unless it comes from the combustion of lubricating oil or hydrocarbon fuel in dual-fuel systems. However, exhaust gases may contain remnants of unburnt ammonia, which poses a threat to the environment, because of its toxicity and contribution to the formation of secondary PM that has been related with adverse health effects [6]. Therefore appropriate exhaust after treatment is needed, e.g. ammonia scrub by water bath or selective catalytic reduction (SCR) [7].

The effective application of ammonia as a fuel for direct combustion in engines requires some technical and operational challenges to be overcome [5, 7, 8]. This is a consequence of certain physiochemical properties of ammonia. The most relevant properties from this perspective are summarized in table 1 and compared with the properties of diesel oil and gasoline.

### Table 1. Selected properties of ammonia and fossil fuels [9, 10].

| Properties                          | Ammonia | Diesel oil | Gasoline |
|-------------------------------------|---------|------------|----------|
| Formula                             | NH₃     | –          | –        |
| Storage method                      | Liquid  | Liquid     | Liquid   |
| Approximate AKI° octane rating      | 120     | –          | 87–93    |
| Cetane rating                       | –       | 40–55      | –        |
| Storage temperature [K]             | 298     | 298        | 298      |
| Fuel liquid density [kg/m³]         | 602.8   | 832.0      | 745.0    |
| Lower heating value [MJ/kg]         | 18.61   | 42.38      | 44.0     |
| Latent heat of vaporization [kJ/kg] | 1370.0  | 232.4      | 348.7    |
| Stoichiometric air-fuel ratio       | 6.0466  | 14.322     | 15.291   |
| Energy content of stoichiometric mixture [MJ/kg] | 2.64 | 2.77 | 2.58 |
| Ignition temperature [K]            | 924     | 527–558    | 548      |
| Ignition limit (vol.) [%]           | 15.8–28.0 | 1.0–6.0 | 1.4–7.6 |

°Anti Knock Index

One major problem is lower energy content (low lower heating value) of ammonia than that of conventional hydrocarbon fuels. However, ammonia exhibits lower stoichiometric air-fuel ratio, which means that more ammonia than hydrocarbon fuel can be burned with the same amount of air. Therefore low energy content of ammonia can be compensated with inducting greater dose of fuel into the engine. This makes energy content of stoichiometric mixtures of air and ammonia, diesel oil and gasoline comparable. Nonetheless, ammonia is a demanding fuel in terms of burning. Other factors like high resistance to autoignition (high octane rating), high latent heat of vaporization and slow flame speed make it difficult to control combustion process in both spark-ignition (SI) and compression-ignition (CI) engines. Ammonia handling maybe problematic when it comes to its toxicity. Even at low
concentration level (150–300 ppm) it is considered to be harmful to human health [10]. Last but not least, ammonia is corrosive to some materials like copper, brass, nickel and rubber.

Despite the above mentioned disadvantages, numerous studies have proved that ammonia combustion in engines can be successfully achieved if proper combustion strategies and fuel supply system modifications are implemented. Direct and indirect injection of ammonia have been attempted in SI and CI engines. The best results have been obtained for combination of ammonia with another fuel, usually gasoline or diesel oil, to counteract ammonia’s unfavourable combustion properties. Secondary fuel is needed mainly to lower high energy demand of ammonia ignition. The detailed review of previous works in this field can be found in other papers [5, 8–10].

The aim of this study is to investigate the feasibility of introducing ammonia to dual-fuel compression-ignition engine, where a pilot dose of diesel oil initiates the ignition of ammonia-air mixture. Engine performance simulations have been conducted, computing the operation parameters of an engine for a given geometry with variable operating conditions. This research has a preliminary character and is intended to build a basis for future empirical investigation.

2. Materials and methods
Investigation of the combustion process was carried out with the use of a one-dimensional numerical model of dual-fuel CI engine supplied with diesel oil and ammonia. The model was validated based on results of engine testing on dynamometer. Numerical simulations of an engine operation were performed for three fuelling modes characterized by different combinations of ammonia-diesel oil flow rates.

2.1. Model assumptions
The model of dual-fuel engine was developed in AVL BOOST software and parametrized according to the specifications of Perkins 1104C-E44T engine. Detailed information on the engine is given in table 2.

| Parameter                | Data                        |
|--------------------------|-----------------------------|
| Manufacturer             | Perkins                     |
| Model                    | 1104C-E44T                  |
| Type                     | Four-stroke, compression-ignition |
| Cylinder layout          | In-line                     |
| Number of cylinders      | 4                           |
| Compression ratio        | 18.23:1                     |
| Displacement volume      | 4400 cm$^3$                 |
| Bore and stroke          | 105 mm, 127 mm              |
| Valves per cylinder      | 2                           |
| Aspiration               | Turbocharged                |
| Maximum power            | 85 kW @ 2000 rpm            |
| Maximum torque           | 415 N·m @ 1400 rpm          |

Engine fuel supply system in the model was modified to allow delivery of ammonia into the intake manifold, while a dose of diesel oil was injected directly into the cylinder. The idea behind those modifications was to make the engine run in dual-fuel mode without introducing significant changes to the overall construction. The general structure of the model developed in AVL BOOST is shown in figure 1.
Figure 1. The structure of the engine model developed in AVL BOOST: SB1, SB2 – system boundaries; MP1–MP7 – measuring points; TC1 – turbocharger; CO1 – air cooler; R – reference point for volumetric efficiency; I1 – gas injector; PL1–PL2 – plenums; C1–C4 – cylinders; E1 – engine; 1–14 – connecting pipes.

The heat release rate in engine cylinders was modelled by means of two-phase Wibe function, parametrized individually for actual engine working conditions [12]. This function differentiates the mass fraction burned in kinetic and diffusion combustion stages, according to the formulas [13]:

\[ x_b = b_1 \cdot \left\{ 1 - \exp \left[ -a \left( \frac{\alpha - \alpha_0}{\Delta \alpha} \right)^{m_1+1} \right] \right\} + b_2 \cdot \left\{ 1 - \exp \left[ -a \left( \frac{\alpha - \alpha_0}{\Delta \alpha} \right)^{m_2+1} \right] \right\} \]

(1)

\[ b_1 + b_2 = 1 \]

(2)

where: \( \alpha \) – crank angle, \( \alpha_0 \) – crank angle corresponding to the start of combustion, \( \Delta \alpha \) – crank angle corresponding to total combustion duration (from \( x_b = 0 \) to \( x_b = 1 \)), \( a \) – the completeness of combustion (for complete combustion \( a = 6.908 \)), \( b_1 \) – mass fraction burnt coefficient for kinetic combustion, \( b_2 \) – mass fraction burnt coefficient for diffusion combustion, \( m_1 \) – combustion rate for kinetic combustion, \( m_2 \) – combustion rate for diffusion combustion.

The values of above parameters, apart from the completeness of combustion, were assumed individually for each engine working conditions. The crank angle of the start of combustion was determined by autoignition delay angle of diesel oil.

2.2. Model validation

The validation of the model concerned the case of engine supplying with diesel oil only, because of the lack of empirical data on the engine power supply with ammonia (the purpose of this work is to investigate the feasibility of conducting empirical research). The validation was accomplished by comparing the simulated course of pressure of the medium inside the cylinder with the pressure measured empirically on the engine test bed. The empirical data used for model validation was acquired from the results of research carried out by Orliński et al. The exemplary data was published in paper [14], where detailed conditions of the tests have been described.

The comparison was made for the same engine working conditions, defined by engine speed and load, with diesel oil and air consumption introduced to the model. The values of independent variable parameters of Wibe function were modified in order to ensure that the simulated course of pressure was sufficiently close to the measured one. Sample results of the comparison have been presented in figure 2. They refer to engine speed of 1400 rpm with the load set at 100% and 50% of its maximum value. The crankshaft rotation angle of 0 deg corresponds to the Top Dead Centre (TDC).
Figure 2. Comparison of simulated and measured in-cylinder pressure for engine speed of 1400 rpm, 50% and 100% of maximum load.

The comparison of the course of pressure has shown a sufficient conformity in all analysed points. However, for a more in-depth assessment of the accuracy of the estimation of measured in-cylinder pressure by the model, absolute and relative errors have been calculated using the following formulas:

\[ \Delta p = p_m - p_s \]  
\[ \delta p = \frac{(p_m - p_s)}{p_m} \]

where: \( \Delta p \) – absolute error, \( \delta p \) – relative error, \( p_m \) – measured in-cylinder pressure, \( p_s \) – simulated in-cylinder pressure.

Example error values, calculated for the pressure courses presented in figure 2, are shown in figure 3. Generally, for both engine load conditions, the absolute and relative errors can be rated as not large – their values do not exceed the range of (-0.12–0.12) MPa and (-2.0–1.5)% respectively. Taking into account the whole engine cycle, the smallest errors correspond to the compression stroke, while the largest occurs for active combustion after TDC. The analysis of absolute and relative errors confirms good quality of estimation of measured pressure by the developed model.

Figure 3. Absolute (a) and relative (b) errors of the accuracy of the estimation of measured in-cylinder pressure by the model for engine speed of 1400 rpm, 50% and 100% of maximum load.

2.3. Simulation assumptions

In this study the engine speed was held constant at 1400 rpm, which corresponds to maximum engine torque for diesel oil operation. Fuel flow intensity, brake specific fuel consumption (BSFC), engine power, engine torque and emissions of: carbon dioxide (CO\(_2\)), carbon monoxide (CO) and
nitrogen oxide (NO) were determined. The engine was supplied with either ammonia-diesel oil combination or a diesel oil alone. Three different engine operating modes were simulated:

- Constant ammonia flow rate with variable diesel oil flow rate. Diesel oil flow rates were adjusted to ensure 10%, 25%, 50%, 75% and 100% of the maximum engine load obtained exclusively with diesel oil. At each specific load condition, a small, fixed amount of ammonia was introduced into the engine.

- Constant diesel oil flow rate with variable ammonia flow rate. Diesel oil flow rate was maintained at a constant level to sustain the idling operation of the engine. Ammonia was added to obtain the desired torque output in each specific load condition (10–100% of maximum diesel oil load).

- Constant engine torque with variable flow rates of ammonia and diesel oil. Diesel oil flow rate was set to enable the engine to reach torque equal to that of single-fuel supply approach with 10–100% of maximum diesel oil load. Then ammonia was added in order to level engine torque to the same value as for 100% diesel oil load.

3. Results

The results obtained for three engine operating modes are presented in form of graphs plotting fuel flow intensity (q), brake specific fuel consumption (BSFC), engine power (P) and concentration of pollutants (C_{CO_2}, C_{CO}, C_{NO}) against the share of the maximum engine load obtained using diesel oil only (L_D). Each case includes dual-fuel and single fuel (diesel oil) supply of the engine.

3.1. Constant ammonia flow rate with variable diesel oil flow rate

This operation mode gives the effect of diesel oil being the primary fuel with ammonia added to boost the performance of the engine. Detailed results are shown in figure 4. As intended, diesel oil flow rate varied accordingly to single-fuel supply approach and ammonia flow rate was fixed. BSFC increased almost in the whole range of load conditions. It is clear that a constant increase in engine power was obtained as a result of ammonia combustion. Since the engine speed was maintained constant, power is proportional to torque. Pollutant concentration did not change significantly, because diesel oil supply was kept at original level and the dose of ammonia was small. A slight difference can be seen only in case of CO concentration.

3.2. Constant diesel oil flow rate with variable ammonia flow rate

In the second operation mode, ammonia was meant to compensate diesel oil energy allowing the engine to generate the required torque output. As can be seen in figure 5, the diesel oil flow rate was kept constant while the ammonia flow rate increased with an increase in engine load. Engine efficiency for dual-fuel approach was deteriorated (increase in BSFC) comparing to single-fuel approach. It can be explained by lower heating value of ammonia than diesel oil. The reduction in CO_2 and CO concentration for dual-fuel supply is a consequence of replacing the part of the carbon fuel with carbon-free ammonia. NO concentration is also reduced, but only for heavy engine loads.

3.3. Constant engine torque with variable flow rates of ammonia and diesel oil

In the third operation mode, different combinations of ammonia and diesel oil were used to obtain peak engine torque, equal to the maximum torque produced with diesel oil alone (figure 6). As expected, ammonia flow rate decreased with an increase in diesel oil flow rate. Constant engine speed and torque induce constant power output. BSFC for dual-fuel supply decreased almost proportionally with a decrease in ammonia flow rate. CO_2 concentration was comparable in both diesel oil and dual-fuel approaches. CO concentration was much lower when ammonia was used, while NO concentration increased slightly.
Figure 4. The results of simulation for engine operation mode of constant ammonia flow rate with variable diesel oil flow rate: fuel flow intensity (a), brake specific fuel consumption (b), engine power (c), concentration of CO$_2$ (d), CO (e) and NO (d) in exhaust gases for given share of the maximum diesel oil engine load.

Figure 5. The results of simulation for engine operation mode of constant diesel oil flow rate with variable ammonia flow rate: fuel flow intensity (a), brake specific fuel consumption (b), engine power (c), concentration of CO$_2$ (d), CO (e) and NO (d) in exhaust gases for given share of the maximum diesel oil engine load.
4. Conclusions

The following conclusions may be drawn based on the results of this study:

- It is feasible to use ammonia as a fuel in CI engine with diesel oil that initiates ignition.
- Higher than rated power and torque, depending on operating conditions, can be achieved with the addition of a small, fixed dose of ammonia to the engine supplied with diesel oil.
- The use of ammonia as a primary fuel, with diesel oil sustaining only idle operation of the engine, is possible and results in significant reduction of CO₂ and CO emission.
- Different ammonia–diesel oil ratios can be used to obtain maximum power and torque output of the engine.
- The efficiency of the engine supplied with ammonia and diesel oil is usually deteriorated, compared to diesel only operation, due to the low heating value of ammonia.
- The biggest difference in emission of NO between dual-fuel and single-fuel approaches occurs for large engine load and depends on the operation mode of the engine.

This study had a preliminary character and highlighted mainly qualitative tendencies in energetic effects of supplying CI engine with ammonia and diesel oil. Detailed examination of combustion characteristics as well as exhaust emission are necessary and will be performed in a future work.

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