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Specific Challenges for Ammonia Engines

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ABSTRACT

Despite several trials of ammonia-powered vehicles in the past, no vehicles are currently on the road. Theoretical studies in the 1960s highlighted the various technological challenges to be overcome. Now that the world is aware of the need to move towards a low-carbon society, the cards have been reshuffled: not only ammonia is considered as one of the vectors of clean electricity for the future, but it can also be a fuel in its own right, even if its fundamental combustion characteristics are not advantageous. Some various aspects ranging from control of injection, in the gaseous or liquid phase, ignition and combustion itself, to pollutant emissions and their possible post-treatment are summarized.

1. Introduction

In despite of some successful stories about ammonia engines, no ammonia-powered vehicles are currently on the road. In fact, during the 60s', the theoretical studies concluded that ammonia, due to its pure combustion characteristics, is so different in comparison to hydrocarbon fuels that it would induce too many changes and development to be implemented in a vehicle. But since these last 6 years, it becomes more evident that ammonia is not only an excellent hydrogen carrier due to its higher volumetric energy density (as 15.6 MJ/L for liquid ammonia, compared to 5.6 MJ/L at 70 MPa, for compressed hydrogen), but also a possible carbon-free fuel for internal combustion engines. Ammonia engines could be not only for road vehicles but also for marine transport, rail and for genset and auxiliary power units and even aircrafts. In 2014, researchers from Oxford University announced that ammonia is a clean and secure hydrogen-containing energy source, proposing the idea 'to use it directly in engines' [2]. Ammonia is an ideal fuel since it is not a greenhouse gas and its complete combustion forms only N_2 and H_2O [3].

First, ammonia, containing 17.8% by weight of hydrogen, can be stored in the liquid phase at approximately 9 bar at 20°C or -33°C at ambient pressure. Its high auto-ignition temperature and research octane number (RON=130) guarantee no occurrence of knock phenomenon if it is used without other fuels. But in the other hand, it limits its use in current engines. As suggested in [4], a compression ratio of 35:1 has to be used to obtain auto-ignition of ammonia. But as underlined in Kurien and Mittal [5], higher compression ratios (>35:1) are impractical in the case of conventional engines since the permissible compression ratio in real world applications is in the range from 12:1 to 24:1. Therefore, to enhance the ignition, spark plug and/or pre- or local mixing with other fuel is needed. In the case of premixed combustion, the low laminar flame speed of ammonia [6] also induces the requirement of boosted conditions or promoting its burning with other fuels.

It is therefore evident that ammonia cannot be considered suitable as a drop-in replacement for conventional fossil fuel. Development of combustion strategies to optimize ammonia performance in engines is necessary. From the past, many studies focused on ammonia sharing with other fuels without reaching level higher than 90% of energy fraction. These results remain interesting as it

could be convenient for practical uses to have 'flex-fuel' engine, in case of no sufficient availability of ammonia. Moreover, in the longer perspective, a 100% sustainable fuel supply is desired to fully decarbonize the transport and energy sectors. Therefore, in this review, will be considered recent studies where at least 98% of energy from ammonia is used as fuel.

Therefore, the development of Internal combustion engines with ammonia as the main fuel follows mainly 3 directions:

- to consider conventional SI Spark ignition engine). From recent studies, it is stated that addition of small quantities of H_2 can strongly enhance the stability of NH_3 combustion [7, 8] and can reach similar efficiency than natural gases engines.

- to consider compression ignition engine by 2 ways [5, 9]: (i) adding a spark plug to help the combustion ignition even if the compression ratio is more about 16-18; (ii) igniting ammonia charge with high reactive fuel (hydrocarbons), as Diesel, biodiesel, DME...

A summary of various challenges from ammonia/air mixture preparation, with gaseous or liquid injection, ignition and combustion itself, to pollutant emissions and their possible post-treatment are addressed in the following.

2. Injection of ammonia in engine

As for any fuel, the injection process is one key parameter to optimize local air/fuel mixture inside the combustion chamber, to enhance combustion development and limit the pollutant emission itself [10]. In the case of ammonia, no universal solution seems to come off as the potential of different injection systems remain to be studied. Therefore, as schematized in Figure 1, all configurations could be chosen in liquid or gaseous form, port fuel or direct injection, split or not. This becomes more complex when the injection of one other fuel as combustion booster has to be done.

Table 1 : comparison of different fuels properties

Fuel	NH_3	H_2	CH_4	C_8H_{18}	$C_{12}H_{24}$
air/fuel stoichio	3.57	2.38	9.52	59.50	88.06
mass air/fuel ratio	6.06	34.32	17.16	15.05	15.11
energy (KJ/Kg air)	3078.04	3494.46	2913.75	2823.92	2812.71

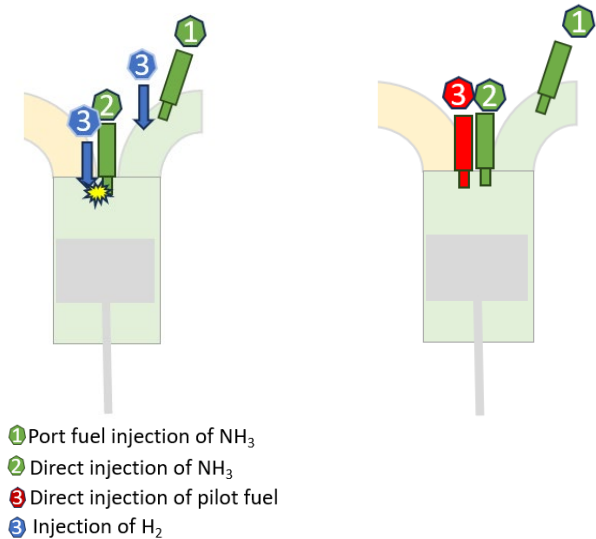


Figure 1: different configurations of ammonia injection with other fuels for SI or CI engines.

In the past, different studies used classical port-fuel gaseous injectors as is, but . It was only recently concluded that the dynamic of the ammonia gaseous jet is similar to gaseous methane [11]. The main difference will be at the end the local air/fuel ratio as indicated in Table 1 due to the strong different stoichiometric air/fuel ratio. . Therefore, even if the choice of gaseous direct injection could be justified, nthe flow rate to ensure sufficient ammonia amount is not usual.

Since this type of injection is mainly for spark ignition engine, the laminar flame speed and the interaction with turbulence will be the major properties that drive the combustion process. As concluded in [12], as the laminar flame speed is very low in the case of classical SI engine conditions, the turbulence flow affects a lot the combustion process. One consequence is the difficulty to stabilize the combustion for low load as well as for low and high rpm as in [8].

The advantage of direct liquid injection compared to port fuel is not only to help the filling of the engine but also to vaporize as fast as possible the fuel inside the chamber by breaking up the fuel spray into droplets. Then, the vaporization of droplets is greatly significant for the spatial distribution of fuel vapor/air, the ignition, and the combustion itself. Generally, the use of high-pressure injection systems favors the atomization in small droplets which enhances the liquid-air interface, the vaporization, and the fuel/air mixing to avoid NH_3 trap. However with ammonia, atomization can be mainly driven by flash-boiling process which requires to be more studied before being controlled for engine applications. Some recent studies started to focus on ammonia liquid spray as for example in [13]. As it can be seen in Figure 2, the examples of liquid spray morphology for ammonia in comparison for gasoline indicate the challenge to ensure optimum fuel/air mixture inside the combustion chamber.

$\rho_{\text{air}}, T_{\text{air}}$	$2.38 \cdot \text{kg/m}^3$ 20°C	$2.38 \cdot \text{kg/m}^3$ 80°C	$2.38 \cdot \text{kg/m}^3$ 120°C	$8.32 \cdot \text{kg/m}^3$ 20°C	$8.32 \cdot \text{kg/m}^3$ 80°C	8.32kg/m^3 120°C
NH_3						
Gasoline						

Figure 2: example of liquid spray shapes for ammonia and gasoline with a Gasoline Direct Injector (120 b injection pressure).

Some first CFD modelling indicated the difficulties to predict well ammonia vaporization process and especially the droplet size to help engine design [14]. First results in SI engine provided as conclusion that injection strategies (late, early and split injections) need also to be more explored before choosing a right one [15].

In the case of Reactivity Controlled Compression Ignition, i.e. the ignition of ammonia combustion by local distribution of a more reactive fuel, as in Figure 1 (right), most of recent studies considered premixing of ammonia with air in the intake as in [16]. For that, current common-rail injector for the reactive fuel is used even if to control small quantities, very low injection pressure is required, resulting some difficulties to control efficiently the amount of pilot fuel. A recent study evaluated the dual-fuel concept with premixed ammonia and direct-injected n-heptane but by using a gasoline direct injector to investigate the possibility of running a CI-engine with higher ammonia-energy share than previously seen. The GDI injector allows small, quick injections with rapid atomization of the pilot fuel [17]. It is really hard to predict what best solution will be chosen in the future as it is dependent to the engine architecture, the operating conditions and the pollutant emissions trade-off. Other interesting alternatives are to directly inject ammonia near the reactive fuel as recently in [18].

3. Combustion in ICE

- Spark ignition

In the case of premixed combustion, the ignition tool and the laminar-turbulence interaction are key parameters to favor the combustion development itself. The laminar flame speed of ammonia is approximately 1/5th of gasoline at stoichiometric and ambient conditions. Therefore, the ammonia combustion requires larger spark advance and yields to longer combustion durations compare to a conventional gasoline fuel. Therefore, the flow dynamics between the spark ignition and the end of combustion has more effect on flame development itself. From a combustion standpoint, turbulence ahead of the flame front tends to increase the flame surface area and increases the fuel consumption rate. As highlighted in [13], the turbulence enhances more ammonia flame than ammonia/hydrogen or ammonia/methane ones. This is due to the low value of laminar flame speed, which induces the flame development in the 'broken reaction zone' of the Turbulent Combustion regime diagram as indicated in Figure 3 (blue points). However, as indicated in [19, 20], using diesel engine architecture with the

addition of spark-plug is interesting as neat ammonia can be in a wider range of operating conditions (low load, low and high speed), despite of the low level of turbulence in diesel combustion chamber, due to the swirl motion. This is totally different to what it can be observed with same engine running with ‘classical fuel’ as gasoline, where in fact the spark increases locally the temperature, inducing one strong peak of pressure following by another main heat release rate. This is in fact considered as two-steps combustions. In the case of ammonia, the heat release rate evolves exactly as in current SI engine. The increase of compression ratio has no sufficient impact on laminar flame speed (less than 10% of improvement) to explain the stability of combustion. This is due to the turbulence level and vortices size which affect more the ammonia flame.

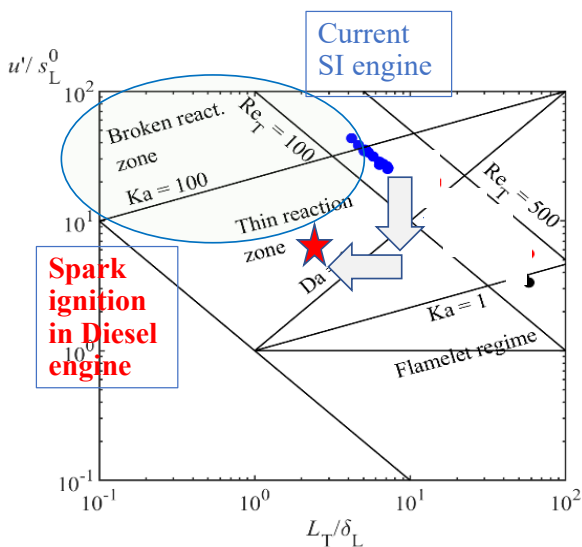


Figure 3 – difference of ammonia flame regime between current Spark Ignition engine and Diesel engine ignited by a spark-plug (from conditions in [12, 19]).

Recently, different turbulence dynamics have been tested using different piston shapes [20]. The conclusions are not so evident as even if high turbulent kinetics energy is needed to enhance sufficiently ammonia flame, unburnt ammonia can be obtained also because of the piston shape.

- Ignition by pilot reactive jet

In the case of pilot fuel ignition, a minimum CR around 15 seems to be sufficient from previous studies to guarantee a good ignition. It is surely dependent on the cetane number of the pilot fuel [22], but remains one promising solution to retrofit diesel engines, usually used in ships, gensets and construction machines by slightly modifying the intake port to supply ammonia. But most of previous studies are not focused on high ammonia energy share as in [15]. The example of pressure trace presented in Figure 4 between RCCI and Spark ignition for the same engine (Compression ratio 16) indicates that clearly for this case, the more reactive fuel is ignited before allowing the combustion of the premixed ammonia/air mixture. This combustion mode is interesting as it is possible to run at leaner conditions, down to 0.5 of equivalence ratio for this case with a high indicated ammonia combustion efficiency. However the

range of operating conditions and different injection strategies are so wide, as for spark-ignition engines, that it is difficult to provide a clear vision of the best strategies. In addition, as emphasized in [16], the more viscous the pilot fuel, the more difficult very small injections are and the larger the spray droplets are.,

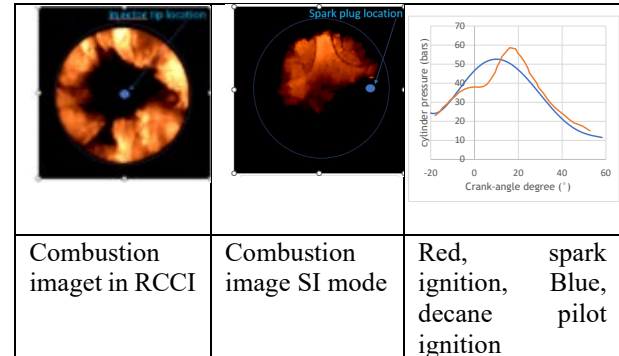
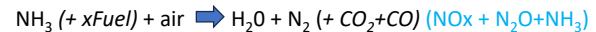


Figure 4 – Different combustion developments: ammonia/air equivalence ratio 0.9 – decane : 2.2% energy share

Recently some studies started to consider prechamber igniter as another way to help ammonia combustion in engine as for example in [23, 24], but the question remains what the best solution is to fill the prechamber with ammonia, hydrogen, cracked mixtures etc.

4. Pollutants and post-treatment

If one considers ammonia combustion equation, without no carbon content fuel, no CO or CO₂.



As underlined in [25], the emissions are additional challenges of NH₃/air combustion. Indeed, if the combustion is complete, no unburnt NH₃, and as a function of local equivalence ratio, temperature and pressure, NO_x and N₂O could be or not important.

The relationship between NO_x and ammonia slip is not monotonous: NO_x emissions tend to be produced at high combustion temperatures (for CI engines) or lean equivalence ratio (for SI engines), and unburnt ammonia at low temperatures or rich equivalence ratio respectively. No “ideal” temperature level eliminating both emission species were determined as underlined in [9]. Moreover, emissions of unburnt ammonia can occur during unstable combustion conditions or also due to fuel trapping, especially in the case of retrofitted CI engine with port-fuel injection of ammonia. In Figure 5 [20], a scheme of emissions evolution at the exhaust for ammonia SI engine is suggested as a function of air/fuel ratio. Therefore, for post-treatment systems, 2 strategies are possible: to run in slightly rich conditions with unburnt ammonia and H₂ (due to internal cracking) as underlined in [19, 26] or slightly lean conditions with NO_x but small quantities of NH₃.

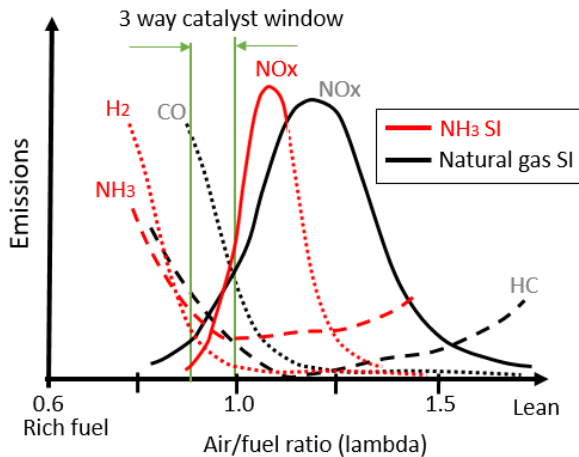


Figure 5: comparison of emissions from ammonia SI engines and Natural gas ones [20].

In the case of RCCI engine, one main question is about CO₂ emissions due to the reactive fuel. But it has to be considered that in the case of ammonia combustion as a function of the operating conditions N₂O specie can be also produced. Even if the level is low (around 50 ppm), its global warming potential is 265 times that of CO₂ with a lifetime in the atmosphere of over 100 years. The comparison of ammonia CI engines, ignited by a small decane pilot injection or a spark plug shows that the level of N₂O emissions is similar (less than 50 ppm) without any visible effect of the equivalence ratio. Moreover, in Figure 6, N₂O level was converted in CO₂ equivalence. Therefore, even if decane contributes to enhance CO₂ emissions, CO₂ emissions are in the same order of magnitude for both spark and pilot ignition for lean mixture up to the stoichiometry where N₂O and CO₂ are slightly increased in the case of RCCI condition because of the increase of diesel energy share to guarantee engine stability.

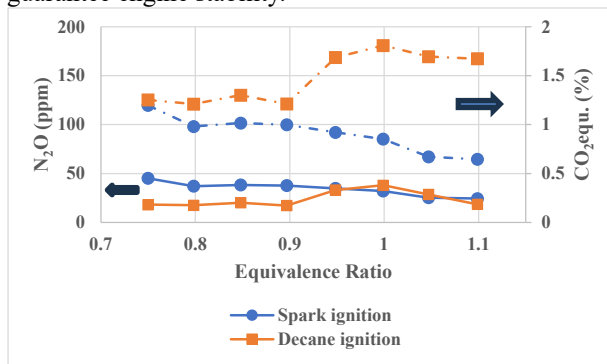


Figure 6 : comparison of CO₂ eq. emissions from pilot diesel ignition versus spark ignition in ammonia CI engines.

5. Conclusions

Even if there are several announcements from companies to deliver ammonia engines soon, the studies about ammonia engines remain sparse, especially for direct injection configurations or pilot reactive ignition. Moreover, most of studies are more and more done by CFD modelling. Unfortunately due to the lack of knowledge as ammonia is a particular fuel, it is not

possible until now to design engines with ammonia by only considering classical injection, atomization, combustion and kinetics modeling. The development of optimized post-treatment requires accurate predictions of pollutant species. But as underlined in [27], not only NH₃ oxidation chemistry presents still many open issues, especially at high-pressure as in engines, but also the sensitivity of NH₃ to other chemistries as DeNO_x, NO-NO₂ loop, and N₂O. Last the addition of fuel promoters has also a direct effect on the oxidation chemistry and needs more understanding to predict ICE combustion.

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