Investigation of ammonia ignition delay at low temperatures and lean conditions

Maxime Pochet[*,a,b,c], Véronique Dias[a], Bruno Moreau[d], Fabrice Foucher[d], Hervé Jeanmart[a], Francesco Contino[b,c]

[a] *iMMC, Université catholique de Louvain, Louvain-la-Neuve, Belgium*
[b] *Department of Mechanical Engineering, Vrije Universiteit Brussel, Brussels, Belgium*
[c] *BURN Joint Research Group, Vrije Universiteit Brussel & Université Libre de Bruxelles, Brussels, Belgium*
[d] *Laboratoire PRISME, Université d'Orléans, Orléans, France*

Introduction

Worldwide interest is growing for ammonia as an alternative fuel obtained from renewable energy. Indeed, massive penetration of renewables will lead to electricity excess that could be advantageously stored as a fuel through Power-to-Fuel (P2F). Being carbon-free, easily produced from hydrogen and the nitrogen in the air, ammonia is fairly easily stored and transported (liquid under 9 bar of pressure) [1].

In the search for higher efficiencies and lower emissions, the use of Low Temperature Combustion (LTC) mode for ammonia combustion has been suggested and investigated first by Van Blarigan with a 40:1 compression ratio free piston Homogeneous-Charge Compression-Ignition (HCCI) engine [2] and more recently by the authors with a 15:1 compression ratio HCCI engine [3, 4]. These studies put forward the high resistance of ammonia to auto-ignition: it needs to be promoted by another fuel (e.g. hydrogen) or to be brought to a high temperature by a high compression ratio or a high inlet temperature. However, increasing the compression ratio increases the friction and heat losses, and a high inlet temperature affects the power density. Therefore the knowledge for a potential use of ammonia in LTC engine is incomplete: the conditions under which ammonia could be used alone in an LTC engine.

Several mechanisms have been built to represent ammonia oxidation kinetics. The two main applications and origin for the development of these mechanisms are the DeNOx process and the combustion in Spark Ignition (SI) engine. It is legitimate to question their suitability/representativeness for ammonia ignition delay under LTC mode (mid-range temperature).

The present study uses a Rapid Compression Machine (RCM) to fill the gap in ammonia ignition delay data at representative conditions for the LTC mode: low temperatures (1000 K - 1100 K), without dilution, at lean conditions (equivalence ratios, ϕ, of 0.2, 0.35, and 0.5), and at high pressures (43.4 bar and 65.5 bar). The addition of small fractions of hydrogen (10 and 25%vol.) will also be done. The objective of this paper is to answer the following questions: (1) how is ammonia ignition delay evolving in LTC conditions? and (2) how do the five most-developed ammonia mechanisms found in the literature compare against the experimental results.

Methodology

The experimental set-up used in this study is the single piston RCM of the Université d'Orléans, PRISME laboratory. It has a compression ratio of 24.3:1, a compression time of 35 ms and a t_{50} of 4 ms (i.e. time between compression pressure and the half of it). The high crevice volume allows a strong absorption of the boundary layer to have a minimal roll-up vortex formation during the compression. Following the crevice validation methodology of Bourgeois et al. [5], the crevice volume is 13% below the conservative volume that guarantees the absence of a vortex. Still neither ammonia nor hydrogen have negative temperature coefficient regions, therefore the effect off a small vortex located near the crevice region will not impact the ignition delay since the auto-ignition onsets in the core region.

Several sensors are needed to measure the ignition delay, τ, defined as the time between the end of the compression (i.e. maximum compression pressure) and the combustion Maximum Pressure Rise Rate (MPRR). The intake pressure is controlled by a KELLER PAA-33X/80794 piezoresistive tranducer and the in-cylinder pressure by a piezoresistive AVL QH32C transducer.

With well designed RCM crevices, the temperature and chemical composition can be considered uniform outside of the boundary layer. Therefore a 0-Dimensional model can be used to represent the RCM when using and assessing the five mechanisms. The thermodynamic state that has to be captured is the one relevant for the chemical kinetics, that is the core zone

[*]Corresponding author
Email address: max.pochet@uclouvain.be

(i.e. the hottest region) of the RCM. The widely-used model of the *effective adiabatic core volume* has been implemented to capture this core zone [6, 7]. Based on an experimental non-reactive pressure curve, the *effective volume* of the RCM combustion chamber is the volume that will give -for an isentropic compression- the exact same pressure as the experimental non-reactive one. Therefore the hottest core zone is correctly modelled and the heat losses (and other machine-related effects) are implicitly taken into account by the *effective volume*.

This model is used together with five ammonia-hydrogen kinetic mechanisms. The mechanism of Konnov and De Ruyck **(KD)** [8], the mechanism of Zhang et al. **(ZH)** [9], the mechanism of Song et al. **(SO)** [10], the mechanism of Dagaut-Kéromnès **(DK)** [11], and finally the mechanism of Nakamura et al. **(NK)** [12].

Main results

The pure ammonia ignition delay as a function of the compression temperature is depicted in Figure 1. Given the obtained range of ignition delays (3 ms - 30 ms), these measurements show the suitability of pure ammonia use in a slightly pre-heated intake (~60°C to 100°C) LTC engine with a compression ratio of 25:1. Regarding the mechanisms, they globally all fail predicting accurately ammonia ignition delays under LTC conditions. SO and DK capture ammonia ignition delays best, probably as they originate from the DeNOX process study (mid-range temperatures). KD is over-reactive (as observed by Mathieu and Petersen [13]) and ZH under-reactive. Finally NK is over-reactive as well and very similar to KD, athough based on a DeNOx mechanism.This might be an evidence of the predominance of the N_2H_x chemistry added by NK.

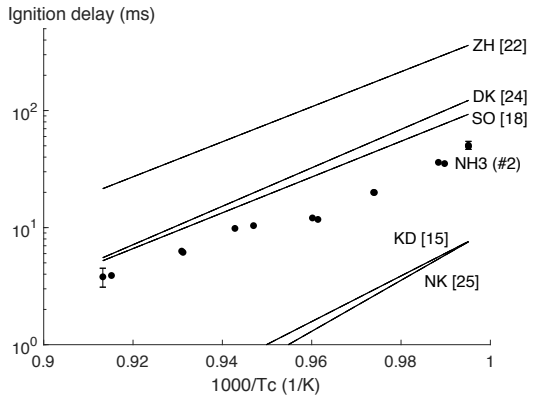

Figure 1: Experimental and numerical ammonia ignition delays as a function of the compression temperature, and for an equivalence ratio of 0.35 and a compression pressure of 65.5 bar.

Conclusion

The ignition delays measured for ammonia prove its suitability for LTC engines with a high compression ratio (~25:1), with a slight intake pre-heating around 200°C. Next to being both achievable, these parameters allow to minimize the intake temperature and consequently the heat losses even though the high compression ratio. Three out of the five mechanisms were found under-reactive for ammonia auto-ignition (DeNOx-based mechanisms), and two over-reactive (flame-based mechanisms), stressing out the need for an adapted ammonia kinetic mechanisms to LTC pressures and temperatures.

The future steps of this study are the exploitation of the other experimental results (equivalence ratio, compression pressure, and hydrogen addition) in addition to a sensitivity analysis that will allow to identify the reactions that are responsible for globally under- or over-reactive mechanisms.

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