Numerical assessment of the operating range for a multi-fuel HCCI engine: hydrogen, ammonia, methane and methanol

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Introduction

Increasing the share of renewable energy is a key step to meet the objective of CO_2 neutrality by 2100. Still, it will eventually lead to the need of significant electricity storage capacity, especially at a seasonal time scale. Renewable fuels (*i.e.* fuels produced with excess of renewable electricity in a process called *power-to-gas*) have raised great interest as part of a range of storage technologies like pumped hydro, batteries, etc. Indeed, their long term storage capabilities added to their decentralized suitability gives a perfect fit to the increasing installation of solar and wind power. The most promising renewable fuels (hydrogen, ammonia, methane and methanol) are currently used separately in terms of energy production, which reduces their integration capabilities into the energy market. Our approach is to integrate all these storage fuels into a single technology of power production (multiGas-to-power). The key interest is its ability to use natural gas allowing it to be connected to both storage facilities and natural gas network, hence raising interest for investments in renewable fuel storage technologies.

Internal Combustion Engines (ICE) have been chosen as our multiGas-to-power system since it is a mature and low cost technology. The fuel flexibility can be achieved by operating the ICE in homogeneous charge compression ignition (HCCI) mode, as demonstrated in [1–4]. HCCI engines have Diesel-like thermal efficiencies and very low NO_x emissions (a few ppm). Still, operating an HCCI engine, especially with blends of fuels, raises two challenges that are the control of auto-ignition timing and its low power density. The onset of combustion in HCCI mode is controlled by the chemical kinetics of the fuel, which is affected by the bulk gas temperature, mainly. Because of the global auto-ignition, the mixture is leaned to appropriate levels to avoid knocking hence reducing the power density to around 4 bar of indicated mean effective pressure for methane.

The fuels of interest have a rather high auto-ignition resistance as shown in Figure 1. This has been observed and described in many experiments and simulations with HCCI engines in [5–8] for methane, in [9–11] for hydrogen and in [12, 13] for methanol.

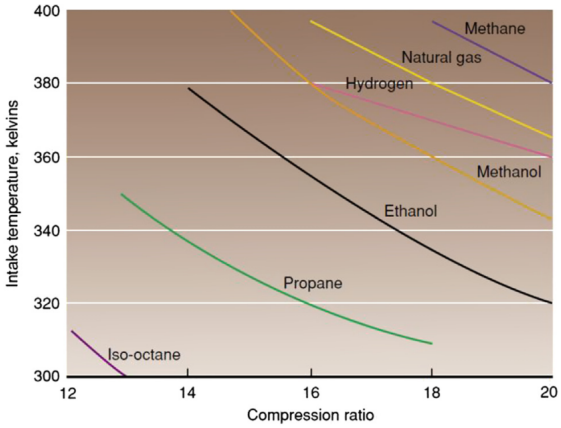

Figure 1: Conditions required for auto-ignition of several fuels in an HCCI engine. Methane is particularly resistant to auto-ignition. Reproduced from [14].

No ammonia HCCI engine has yet been claimed to run or being simulated even though ammonia can benefit from a combustion promoter whose auto-ignition tendency is high like hydrogen or methanol [15]. Increasing the intake temperature is another way to overcome auto-ignition resistance. To control the engine and maximise the efficiency, the ideal situation is to have the CA50 (crank angle where 50% of the fuel in the bulk has been burned) at -or right after- the top

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dead center (TDC) to avoid having the pressure peak working against the piston's motion and to decrease the maximum pressure rise rate hence avoiding knock [1, 16]. The CA50, depending on ignition timing and combustion duration, is mainly controlled by the intake temperature. Finally, one can proceed to exhaust gas recirculation (EGR) in order to delay the auto-ignition. Water vapour and carbon dioxide contained in the recirculated gases have higher heat capacities than the other species hence a lower bulk temperature rise. Consequently, using EGR for identical intake temperature and CA50, one can admit more fuel or increase the intake pressure leading to an increased power density and efficiency. Such process have been observed with an increase of up to a 100% in power density in [11, 16, 17]. HCCI engine control and power density are coupled when using EGR or boosting, which are a must when dealing with varying blends of auto-ignition reluctant fuels.

For this numerical study, the goal is to assess the operating range of a unique HCCI engine able to use the four fuels of interest. As the control of HCCI engines is most often based on CA50, we are interested in correctly describing the timing of combustion. The auto-ignition of the entire bulk gas is triggered in the hottest core zone, therefore the objective of our model is to correctly describe the temperature evolution during compression as it rules the chemical kinetics. Table 1 shows the range of the different variables of interest that are going to be studied. The values are based on the available experimental and theoretical references in the literature that allow to cover the potential use of the four fuels, avoiding knock and misfire. The number of simulations to perform being greater than a thousand, only a 0-Dimensional (0D) model is applicable in order to obtain the most interesting engine and intake parameters in a respectable amount of time.

Table 1: Parameters range for the 0D numerical investigation

Parameter	Range	Step
Compression ratio CR	15 - 20	2.5
Intake pressure p_{in} [bar]	1 - 2	0.5
Equivalence ratio ϕ	0.2 - 0.5	0.1
EGR rate [%]	0 - 30	15
H_2:NH_3 [%:%]	0:100 - 100:0	50
H_2:CH_4 [%:%]	0:100 - 100:0	50
CH_3OH:NH_3 [%:%]	0:100 - 100:0	50
CH_3OH:CH_4 [%:%]	0:100 - 100:0	50
H_2:CH_3OH [%:%]	0:100 - 100:0	50
CH_4:NH_3 [%:%]	0:100 - 100:0	50

The evolution of temperature in a 0D model is based on the evolution of the cylinder volume following the perfect gas model. The key parameter influencing temperature evolution is the heat loss. Indeed, in a 0D model the temperature is a single scalar representative of the whole bulk gas so adding heat losses to the model will decrease the temperature of the whole bulk at the same rate. Though, in a real case scenario it is the boundary layer that exchanges heat with the cylinder walls leading to a local temperature decrease. This induces a change in density which allows more space for the core zone to take. Finally, compared to an isentropic compression, the core zone do experience a decrease in temperature but not as much as what renders a 0D model. Indeed, heat loss models are semi-empirical rules made to fit experimental wall heat losses [18]. As they dissipate the correct amount of heat through the walls, they do not influence correctly the core temperature which is the goal of this study. Consequently, one might need a smaller convective heat transfer coefficient in order to correctly describe the maximal in-cylinder temperature before auto-ignition. This has been done by Broekaert et al. where they changed the correlation factor of several heat loss models to fit experimental measurements of the heat release in a HCCI engine [18]. Our model is based on this study as well as on a comparison and validation with numerical and experimental data found in the literature.

Conclusion

The expected results are cartographic maps of the ignition timing and CA50 versus the imposed parameters (CR, ϕ, intake pressure) and the control parameters (intake temperature and EGR rate). Based on those, we will assess if a unique engine architecture can deal with the four fuels while allowing high equivalence ratios and intake pressures (*i.e.* higher power density). We will then balance the unique engine architecture case with a case where two architectures are used to cover the four fuels and see what gains are achievable in terms of power density versus efficiency as well as in terms of ease of control.

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