Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 105 (2017) 1532 – 1538

Energy Procedia

The 8th International Conference on Applied Energy – ICAE2016

# Multifuel CHP HCCI engine towards flexible power-to-fuel: numerical study of operating range

Maxime Pochet[1abc], Véronique Dias[a], Hervé Jeanmart[a], Sebastian Verhelst[d], Francesco Contino[bc]

[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] *Department of Flow, Heat and Combustion Mechanics, Ghent University, Belgium*

**Abstract**

The transition towards 100% renewable electricity production already raises several challenges at only 20-30% of renewable share. To match energy production and consumption, there will be a need for massive daily and seasonal electricity storage, in particular for fluctuating sources such as wind and solar. Power-to-fuel is one of the energy storage systems that allows long term storage such as season shifting. Electricity can be stored into fuels that are gaseous (hydrogen or methane), easily liquefiable (ammonia), or liquid (methanol). Still, these four fuels are regarded separately in terms of energy production, which reduces the flexibility of the power-to-fuel technology and its potential use as a storage mean. Our approach is to integrate these four fuels into a single technology for power and heat production: Homogeneous-Charge Compression-Ignition (HCCI) engines. Therefore, we developed a 0-Dimensional model to assess the suitability of a unique HCCI engine for the combustion of the four fuels of interest. This paper reports the feasibility of compression-ignition within achievable intake conditions (temperature and pressure) for various engine compression ratios, equivalence ratios and exhaust gas recirculation rates.

For the four fuels, we obtained a proper ignition within a single engine design and for intake conditions (temperature and pressure) that can be sustained by recovering the heat losses of the engine only. As a consequence, power-to-fuel can effectively be used as a storage system when combined to a multifuel HCCI engine for the fuel reconversion to energy. Yet the low power densities estimated require further work on increased equivalence ratio and boosting conditions, as well as on the ringing risks associated with such techniques.


Peer-review under responsibility of the scientific committee of the 8th International Conference on Applied Energy.

Keywords: HCCI, power-to-fuel, hydrogen, methane, ammonia, methanol

## 1. Introduction

Increasing the share of renewable energy in the present energy mix is a key step to meet the objective of $CO_2$ neutrality by 2050. Still, it will eventually lead to the need of significant electricity storage capacities, from a daily to a seasonal time scale. Indeed, renewable energy production depends on the time in the day and in the year. Power-to-fuel has raised great interest as part of a range of storage technologies like pumped hydro, batteries, compressed air, etc. Its long term storage capabilities (months) added to its low storage costs (2 to 3 orders of magnitude lower than the other storage technologies [1]), and its low installation constraints give a perfect fit to the increasing need for decentralized seasonal storage options. Regarding the fuels coming from power-to-fuel systems, they are all based on hydrogen.

[1]* Corresponding author.
*E-mail address:* max.pochet@uclouvain.be


Peer-review under responsibility of the scientific committee of the 8th International Conference on Applied Energy.
doi:10.1016/j.egypro.2017.03.468

Hydrogen is obtained from water electrolysis, as done industrially in more than 30 power-to-fuel plants over the world [2]. Hydrogen can be further processed into ammonia by combining it with nitrogen (Haber-Bosch process), as done in commercially available units [3]. Moreover, during the transition period to 100% renewables there will still be carbon dioxide emitted in the atmosphere. This carbon dioxide can be captured and, using hydrogen, upgraded to methane or methanol [4,5]. Hydrogen is the easiest and most efficient fuel to produce. But its low volumetric energy density makes it rather difficult to store in large quantities. This is the reason for which the three other fuels are unavoidable : methane can be injected into the natural gas network without any restriction, methanol is liquid at atmospheric conditions and ammonia is liquid under 9 bar of pressure.

Unfortunately, due to the unpredictability of renewable energies, the identity of the fuel that is going to be produced at a certain place and time cannot be predicted. Moreover, each fuel has a limited use which makes the power-to-fuel system a very specialized storage solution that fits only in rare conditions. Instead, if we consider the fuels all together by working out a multifuel power-production technology, the system becomes more resilient and flexible hence increasing its potential applications, see Fig. 1.

Additionally, in order to maximise the efficiency of the whole system (power-to-power), a combined heat and power (CHP) unit is preferred. This allows the system to valorize the heat losses associated with the production of electricity. Moreover, a CHP system fits perfectly into a decentralized storage-production system due to the proximity of heat consumers and renewable electricity producers, see Fig. 1.

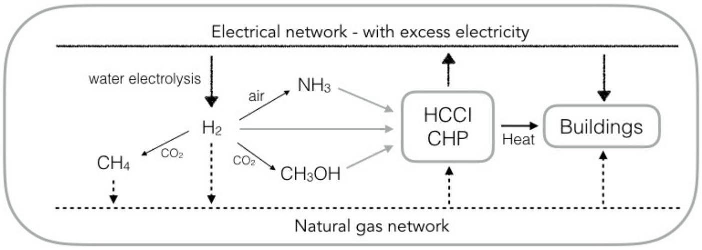


Fig. 1. Entire power-to-power system. From excess renewable electricity, to storage, to electricity and heat. Gaseous hydrogen and methane and liquid methanol and ammonia are the four energy vectors considered. These fuels are used in a CHP HCCI engine.

The Homogeneous-Charge Compression-Ignition (HCCI) engine has been chosen for this system since many studies have demonstrated its multifuel capability, as long as the fuel are admitted under gaseous phase [6–8]. Moreover, HCCI engines deliver high efficiencies (Diesel-like), low $NO_x$ emissions (few ppm) and are well-suited for CHP applications. Although hydrogen, methane and methanol have already been thoroughly studied in HCCI conditions [9-16], we couldn't find any experiment or simulation of an ammonia HCCI engine. Indeed, as shown in Fig. 2, ammonia has a higher resistance to auto-ignition than the three other fuels. Fig. 2 displays the intake temperature needed for having the CA5 (Crank Angle at which 5% of the combustion energy has been released, i.e. the combustion timing) at 0 CAD after the Top Dead Center (aTDC).

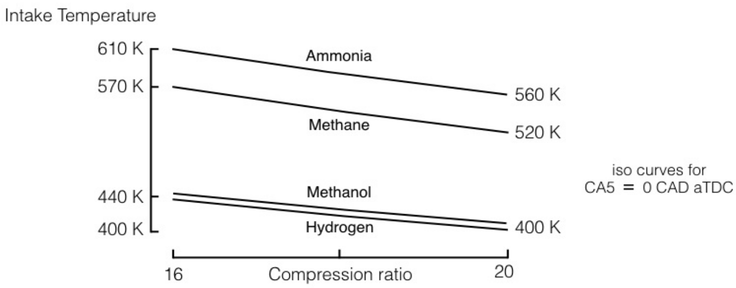


Fig. 2. Calculated intake temperature required for having a proper combustion of the selected fuels as a function of the compression ratio of a naturally aspirated HCCI engine. The equivalence ratio for these simulations is 0.4. Methane and ammonia are particularly resistant to auto-ignition, but increasing the intake temperature allows a proper combustion.

Nonetheless, operating an HCCI engine raises two issues that are the control of the ignition timing and a low power density. The combustion occurring by auto-ignition, the onset of combustion is controlled by the kinetics of the fuel. Thus, we only have an indirect control on the combustion timing through the in-cylinder temperature. The second challenge is caused by the global auto-ignition. The fuel content has to be leaned to avoid too fast or violent reactions hence a low Indicated Mean Effective Pressure (IMEP) i.e. indicated work per motoring cycle [J/m$^3$]. IMEP is also referred to as power density in this paper.

To increase the power density, the fuel quantity inside the cylinder has to be raised. This will be assessed by either increasing the equivalence ratio or by increasing the intake pressure. Still, increasing the equivalence ratio will eventually lead to ringing (HCCI knocking). Therefore, Exhaust Gas Recirculation (EGR) will be assessed in order to damp the high combustion rates associated with high equivalence ratios. The recirculated gases (partially composed of $H_2O$, and $CO_2$ if the fuel contains carbon atoms) are replacing part of the intake air. $H_2O$ and $CO_2$ having higher heat capacities than the air, the temperature rising rate inside the cylinder diminishes and therefore the auto-ignition timing is delayed. This delay causes the ignition to happen after the TDC and therefore damps the combustion rate. Moreover, the reduced oxygen availability slows down the kinetics hence a damped combustion rate [17].

## 2. Methodology and simulation

In this study, we want to determine the operating conditions under which a single engine geometry allows to use the four storage fuels. Table 1 shows the values of the different variables of interest that are going to be studied. The chosen ranges, based on the available experimental and theoretical references [9-17], allow to cover the operating range of the four fuels in a HCCI engine. The rotational speed is fixed at 1500 rpm since our interest lies in stationary applications. The EGR rate is defined in our study as a volumetric proportion of the exhaust gases. The volume recirculated replaces an equivalent volume of intake air. Doing so, EGR rate does not affect the fuel quantity hence simplifying the comparison of the EGR effect. Given the high number of possible combinations to assess, we used a 0-Dimensional (0D) model with a differentiate form of the conservation of energy, and imposing the piston motion in OpenFOAM-3.0.x. The assumption of ideal gas was made.

Table 1. Parameter ranges and engine dimensions used for the 0D numerical investigation.

| Parameter | Range | Step |
|---|---|---|
| Compression Ratio CR | 16-20 | 2 |
| Intake pressure [bar] | 1-2 | 0.5 |
| Equivalence ratio φ | 0.2-0.4 | 0.1 |
| EGR rate [%] | 0-40 | 10 |
| Intake temperature [K] | t.b.d. | 10 |

| Engine characteristics | Value |
|---|---|
| Bore diameter [m] | 0.086 |
| Crank radius [m] | 0.0375 |
| Conrod length [m] | 0.1204 |
| Intake valve close [CAD aTDC] | -127 |
| Exhaust valve open [CAD aTDC] | +127 |

The target of our 0D model is to correctly predict the timing of combustion (CA5) as HCCI engines control is based on it. As the auto-ignition is triggered in the, hotter, core zone, the objective is thus to correctly describe the evolution of the core temperature. Hence heat losses have to be taken into account.

### *2.1. Core temperature estimation – Heat losses*

In a 0D model, the temperature is a scalar representative of the whole bulk gas. Thereby, a heat loss model will slow down the temperature rise of the entire mixture at the same rate. However, in a real compression it is the boundary layer that exchanges heat with the cylinder walls. This leads to a hotter core zone, that 0D models cannot depict. Convective correlations dissipate the correct amount of heat through the walls during one cycle [18], but they do not influence correctly the core temperature. Moreover, the combustion mode of HCCI engines is very different from spark -or compression- ignition engines. Broekaert et al. decided to adapt usual convective correlation by fitting experimental heat losses measured from an HCCI engine [18]. By modifying the scaling factor of Hohenberg's convective coefficient correlation, Broekaert et al. were able to correctly estimate the peak convective coefficient at the TDC. The drawback was that the heat losses were underestimated during the compression stroke. Nevertheless, in our 0D model this underestimation induces a higher in-cylinder temperature: the result sought for. This type of correction on the convection coefficient was tested within our 0D model and compared to experimental temperature curves [10-12]. The ideal scaling factor for the core temperature estimation was found to be varying around 66, instead of Hohenberg's original coefficient of 130.

### *2.2. Chemical kinetic models*

The kinetic mechanisms must be validated for HCCI conditions, i.e. in ignition delay and for high pressures and lean mixtures. For methanol, we used the mechanism from Li et al. [19] that was validated in a Shock Tube (ST) and in a Rapid Compression Machine (RCM) for an equivalence ratio of 0.5 and for pressures of 20 and 50 atm [20]. For ammonia, we used the mechanism from Mathieu and Petersen that was constructed with ST experiments at 0.5 of equivalence ratio and for pressures of 11 and 30 atm [21]. Finally, for methane and hydrogen we used the mechanism from Metcalfe et al. [22] that was validated in a RCM and in a ST for equivalence ratios of 0.3 and 0.5 and for pressures of 10 and 30 atm [23].

## 3. Results and discussion

We obtained a proper combustion for the four fuels in our simulated HCCI engine (Fig. 2). Still, ammonia and methane required intake temperatures higher than 500K. This has an effect on both the feasibility of the system and the power density. Indeed, such temperatures are not easy to provide and they reduce the density of the intake mixture hence the quantity of fuel admitted. Although an increase in compression ratio from 16 to 20 allows to reduce the intake temperature by 40K (Fig. 2), a further reduction of the intake temperature is desirable.

### *3.1. Influence of the equivalence ratio and intake pressure on the engine intake temperature*

Fig. 3 shows the effect of intake pressure (a) and of the equivalence ratio (b) on the intake temperature required for having the onset of combustion (CA5) at TDC. Intake pressure obviously has an influence as a 2 bar intake allows to reduce the intake temperature by 40K for ammonia. For the equivalence ratio, the influence is of lesser magnitude because it only affects the mixture heat capacity. The heat capacities of ammonia and methanol being higher than the one of air explains their reversed slopes in Fig. 3(b). However, a 0D model being unable to depict the combustion duration, the simulations cannot predict the combustion duration reduction as the equivalence ratio rises. Eventually, even though the intake temperature needed is reduced by pushing the operating conditions as far as a classical engine can bear (maximal in-cylinder pressure), a lot of energy still must be provided to the intake mixture.

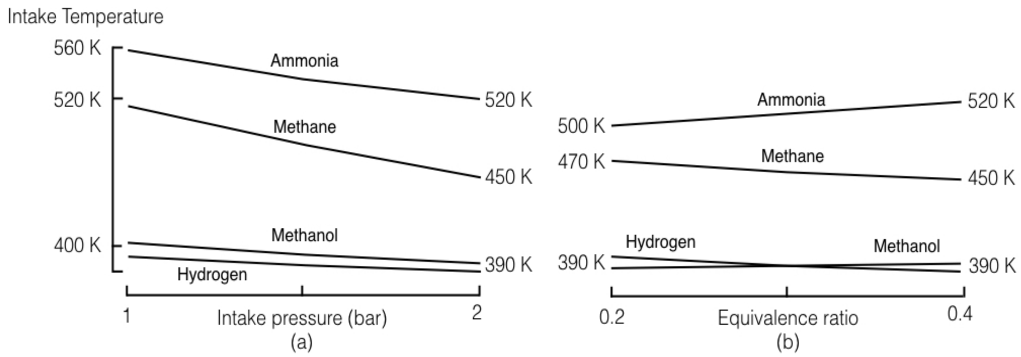


Fig. 3. Intake temperature needed for having a combustion with CA5 at TDC as a function of (a) the intake pressure and (b) the equivalence ratio. The engine compression ratio is set at 20 for both cases, with an equivalence ratio of 0.4 for (a) and an intake pressure of 2 bar for (b). Boosting the intake pressure from 1 bar to 2 bar promotes the auto-ignition as much as increasing the compression ratio from 16 to 20.

### *3.2. Influence of the equivalence ratio on the system feasibility*

To be feasible as well as autonomous and efficient, our system will need to provide the necessary intake conditions (temperature and pressure) by itself. Using a turbo-compressor and a heat exchanger allows to provide the intake conditions by recovering energy from the exhaust gases, without reducing the electrical efficiency. For hydrogen and methanol, all the considered intake conditions are achievable with this system. On the other hand, methane and ammonia cannot be operated in any condition because they require intake temperatures that are too high in comparison to the energy available at the exhaust. In order to have enough energy at the exhaust, the equivalence ratio has to be higher than 0.32 for methane and higher than 0.41 for ammonia (Fig. 4). These results derive from a thermodynamic analysis of a turbo-compressor with a heat exchanger. We assumed an isentropic efficiency of 60% at the turbine and 75% at the compressor, a mechanical efficiency of 95%, a pinch of 30K at the gas-phase heat exchanger and finally 10% heat losses are accounted for. As a consequence to ammonia auto-ignition resistance, we might not use pure ammonia but rather mix it with hydrogen or methanol. Indeed, equivalence ratios higher than 0.4 might lead to ringing or to the production of thermal $NO_x$.

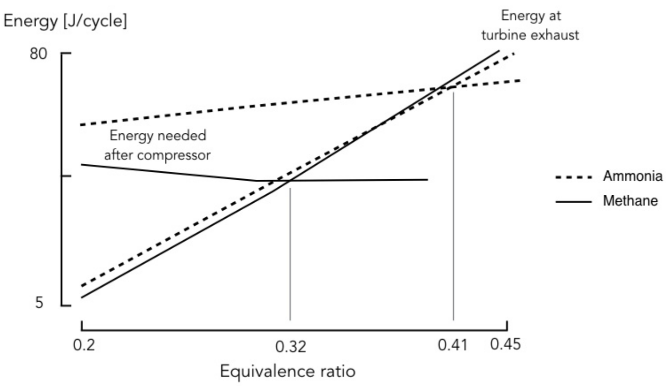


Fig. 4. Energy available at the exhaust of the system (after the turbine) against the energy that still needs to be transferred to the mixture after its compression. The results are shown for a 2 bar intake pressure, an equivalence ratio of 0.4 and a compression ratio of 20. For this system to operate, methane and ammonia require equivalence ratios higher than 0.32 and 0.41, respectively.

### *3.3. Achievable power density and limitations*

The power density achievable by our system depends strongly on the fuel, the equivalence ratio and the intake pressure. The compression ratio, as one can expect, has only a small and indirect influence on the power density through the efficiency. Fig. 5 shows the predicted IMEP for our four fuels as a function of the equivalence ratio and intake pressure. The power density doubles for a doubled equivalence ratio or intake pressure. The IMEP absolute value is, on the other hand, overestimated by 0D models.

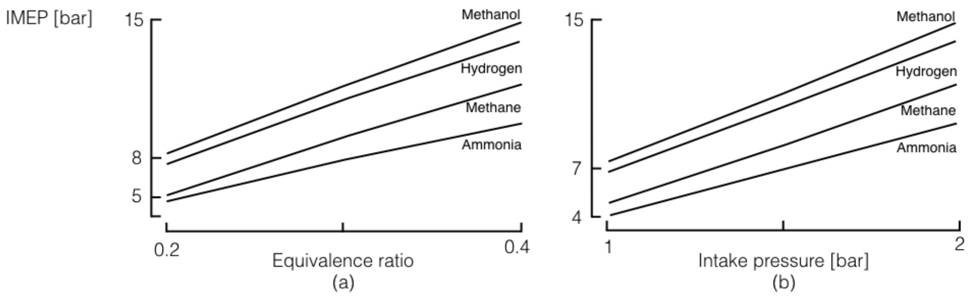


Fig. 5. Indicated Mean Effective Pressure (IMEP) as a function of (a) the equivalence ratio and (b) the intake pressure. The engine compression ratio is 20. The operating conditions are an intake pressure of 2 bar for (a) and an equivalence ratio of 0.4 for (b).

The mechanical and pumping losses being fixed for a given engine and operating conditions, a low IMEP means a low overall efficiency and a larger engine for the same power. So the highest equivalence ratio and intake pressure are desirable. Yet, ringing conditions are known to appear with high equivalence ratios. For fuels that auto-ignite easily like hydrogen, ringing conditions are likely to happen with equivalence ratios higher than 0.3 [14]. To prevent the combustion from ringing, one must decrease the maximum pressure rise rate. This can be done either by shifting the combustion later in the expansion stroke or by reducing the kinetics of reaction. Both effects can be achieved by using EGR. Fig. 6 shows the effect of EGR on combustion timing: from 0 to 40% of EGR, the combustion is delayed by 7 CAD for methanol and 2 CAD for hydrogen. Unfortunately, a 0D model is not able to depict the combustion duration.

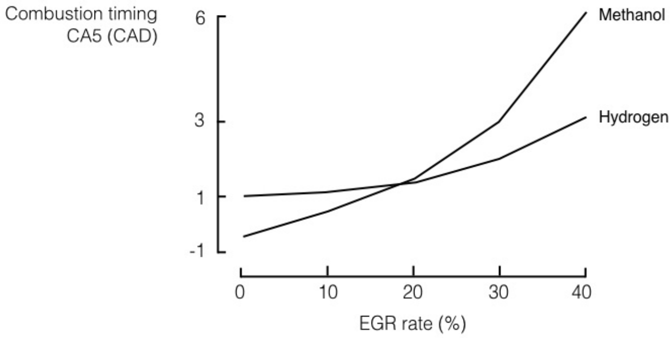


Fig. 6. CA5 as a function of EGR rate for methanol and hydrogen. The simulations are done for identical intake conditions and engine characteristics. The combustion is delayed through the use of EGR for both fuels.

## 4. Conclusions and future work

The HCCI engine technology studied in this paper is able to run with the four fuels of interest (hydrogen, ammonia, methane and methanol) within a single engine. Such HCCI-CHP system is a step further to give economical and industrial interest to power-to-fuel electricity storage. Still, some operating conditions are not yet achievable. First, hydrogen and methanol are likely to experience ringing if the power density is maximized by increasing the equivalence ratio to higher values than 0.3. Consequently, EGR use will be needed to damp the reaction rate. Nevertheless, a model that predicts ringing conditions is required to assess and optimize the effectiveness of EGR to damp the combustion rate. Secondly, very high equivalence ratios (~0.41) are needed with ammonia in order for the exhaust gases to contain enough energy to supply the intake pressure and temperature required. However, ringing is likely to occur at such equivalence ratios. Yet, in this case, using EGR is not a solution as it would raise the required intake temperature. A solution might be to mix ammonia with combustion promoters such as hydrogen or methanol. Still, ideal proportions of mix are to be determined. As a conclusion, a flexible and autonomous HCCI engine can be achieved for the utilization of the four fuels of interest. Nevertheless, a pure ammonia operating condition seems unsustainable and mixing conditions needs to be studied. Finally, EGR and turbo-compressed technologies must be modeled more accurately to assess their precise effect on the timing and duration of the auto-ignition.

## Acknowledgements

The investigations presented in this paper are obtained within a doctoral research funded by the FRIA (F.R.S.-FNRS) and supported by ENGIE Electrabel to whom we are grateful.

## References

[1] Walker S B, Mukherjee U, Fowler M, Elkamel A, Benchmarking and selection of Power-to-Gas utilizing electrolytic hydrogen as an energy storage alternative, *International Journal of Hydrogen Energy*, in press 2016.

[2] Gahleitner G. Hydrogen from renewable electricity: An international review of power-to-gas pilot plants for stationary applications. *International Journal of Hydrogen Energy*, 38(5):2039–2061, 2013.

[3] Fuhrmann J, Hülsebrock M, Krewer U. Energy Storage Based on Electrochemical Conversion of Ammonia. *Transition to Renewable Energy Systems*, doi: 10.1002/9783527673872.ch33, 2013.

[3] Proton Ventures. *NFuel*. http://www.protonventures. com/, 2014. Accessed on 2015-08-28.

[4] Audi AG. Première mondiale: l'usine "power-to-gas" à l'échelle industrielle. http://www.audi.fr/fr/web/fr/vorsprung_durch_technik/content/2013/10/tournant_energetique.html, 2015. Accessed on 28-08- 2015.

[5] LeanShips EU and Verhelst S. LeanShips, towards the energy-efficient and very low emission vessel. https://eu-ems.com/event_images/presentations/ SebastianVerhelst13- OCT.pdf, 2015. Accessed on 29-03-2016.

[6] Christensen M, Hultqvist A, Johansson B. Demonstrating the Multi Fuel Capability of a Homogeneous Charge Compression Ignition Engine with Variable Compression Ratio. *SAE Technical Papers*, 1999-01-36, 1999.

[7] Jeuland N, Montagne X, Duret P. New HCCI /CAI Combustion Process Development : Methodology for Determination of Relevant Fuel Parameters. *Oil & Gas Science and Technology*, 59(6):571–579, 2004.

[8] Tanaka S, Ayala F, Keck JC, Heywood JB. Two-stage ignition in HCCI combustion and HCCI control by fuels and additives. *Combustion and Flame*, 132(1- 2):219–239, 2003.

[9] Fiveland SB, Agama R, Johansson B, Christensen M, Hiltner J, Mauss F, Assanis DN. Experimental and simulated results detailing the sensitivity of natural gas hcci engines to fuel composition. *SAE Technical Papers*, 2001-01-36(August):1–12, 2001.

[10] Kozlov VE, Chechet IV, Matveev SG, Titova NS. Modeling study of combustion and pollutant formation in HCCI engine operating on hydrogen rich fuel blends. *International Journal of Hydrogen Energy*, 41(5):3689–3700, 2015.

[11] Neshat E, Saray RK. Effect of different heat transfer models on HCCI engine simulation. *Energy Conversion and Management*, 88:1–14, 2014.

[12] Komninos NP, Hountalas DT, Rakopoulos CD. A parametric investigation of hydrogen hcci combustion using a multi-zone model approach. *Energy Conversion and Management*, 48:2934– 2941, 2007.

[13] Sharma P, Dhar A. Development of chemical kinetics based hydrogen HCCI combustion model for parametric investigation. *International Journal of Hydrogen Energy*, pages 1-7, 2015.

[14] Ibrahim MM, Ramesh A. Investigations on the effects of intake temperature and charge dilution in a hydrogen fueled HCCI engine. *International Journal of Hydrogen Energy*, 39(26):14097–14108, 2014.

[15] Masurier J-B, Fourcher F, Dayma G, Dagaut P. Ozone applied to the homogeneous charge compression ignition engine to control alcohol fuels combustion. *Applied Energy,* 2015.

[16] Zhang C, Wu H. Combustion characteristics and performance of a methanol fueled homogeneous charge compression ignition (HCCI) engine. *Journal of the Energy Institute*, pages 1-8, 2015.

[17] Oh C H, Jamsran N, Lim O T, A numerical investigation about the EGR effect under the condition of boost pressure on HCCI autoignition. *Energy Procedia,* 68:398-408, 2015.

[18] Broekaert S, De Cuyper T, Chana K, De Paepe M, Verhelst S. Assessment of Empirical Heat Transfer Models for a CFR Engine Operated in HCCI Mode. *SAE Technical Papers*, 2015-01-17, 2015.

[19] Li J, Zhao Z, Kazakov A, Chaos M, Dryer F L, Scire J J Jr, A comprehensive kinetic mechanism for CO, $CH_2O$, and $CH_3OH$ combustion, *International Journal of Chemical Kinetics*, 39: 109–136. doi:10.1002/kin.20218

[20] Burke U, Metcalfe W K, Burke S M, Heufer K A, Dagaut P, Curran H J, A detailed kinetic modeling, ignition delay time and jet-stirred reactor study of methanol oxydation, *Combustion and Flame,* 165:125-136, 2016.

[21] Mathieu O, Petersen E L, Experimental and modeling study on the high-temperature oxidation of ammonia and related $No_x$ chemestry, *Combustion and Flame*, 162:554-570, 2015.

[22] Metcalfe W K, Burke S M, Ahmed S S, Curran H J. A hierarchical and comparative kinetic modeling study of C1-C2 Hydrocarbon and oxygenated fuels. *International Journal of Chemical Kinetics*. 45(10):638-675, 2013.

[23] Donohoe N, Heufer A, Metcalfe W K, Curran H J, Davis M L, Mathieu O, Plichta D, Morones A, Petersen E L, Güthe F, Ignition delay times, laminar flame speeds, and mechanism validation for natural gas/hydrogen blends at elevated pressures, *Combustion and Flame,* 161:1432-1443, 2014.

**Biography**

Maxime Pochet started his PhD in October 2015 at the Université catholique de Louvain and Vrije Universiteit Brussel, in Belgium. He is a FRIA fellow and his reasearch focuses on HCCI engines using blends of renewable fuels.