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Study the impact of fuel and exhaust gas recirculation on HCCI combustion

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Abstract. This paper presents a numerical study of fuel/fuel blends impact on rate of heat release at different exhaust gas recirculation rate in case of homogeneous charge compression ignition (HCCI) combustion. A direct injection engine is used for simulation which also allows mixture preparation in intake manifold leading to premixed combustion. The numerical analysis was conducted by means of an engine model developed in advanced simulation software AVL Boost. The combustion model is based on skeletal reaction mechanism of C7H16(n-heptane) that uses 26 species and 66 reactions. Additionally, to the main fuel, methane and hydrogen was added. Thus, the influence of fuel blends was evaluated at EGR rate within the range of 0% to 40%.

1. Introduction

Conventional spark-ignition (SI) and compression-ignition (CI) engines offer high thermal efficiency in conversation the fuel energy. However, the combustion process in both engines leads to high NOx and soot formatted in the cylinder due to high local temperature and non-homogeneous charge especially in diesel engines. As a result, complex after treatment system needs to be implemented in passenger cars that leads to higher vehicle's cost as well as to restriction in the optimal engine management. Moreover, CO_2 emissions from ICEs need to be further reduced according to the new European regulation for passenger cars that was imposed in 2020. The new CO_2 reference limit is 95 g/km. In short term, replacing the gasoline by compressed natural gas (CNG) in SI engines could reduce CO_2 emissions by 25% in NEDC [1]. This study also reported around 50% reduction of NOx while CO and CH slightly increase. However, the emissions were measured after a three-way catalytic converter (TWC). Thus, TWC is still needed to respect Euro 6 limits. Methane in mixture with CO_2 in a form of biogas could be successfully used in stationary SI engines where biogas is residual product [2]. However, increased concentration of CO_2 significantly reduces the engine output power.

In order to reduce in-cylinder NO_x and soot more complex approach is needed. For that, low temperature combustion (LTC) of homogeneous mixture need to be implemented [3]. Pachiannan et al. in [4], presented a comprehensive review of performance and emission characteristics of LTC when different fuel was used. LTC combustion can be achieved by different approaches such as: homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI), partially premixed charge compression ignition (pPCCI), reactivity controlled compression ignition (RCCI) and etc. The main differences between HCCI, PCCI and pPCCI is the duration of ignition delay period. HCCI is recognised by long ignition delay while pPCCI offers ignition delay similar to conventional CI engines [5]. Operating range in terms of local temperature/air-excess ratio of HCCI for NOx and soot reduction

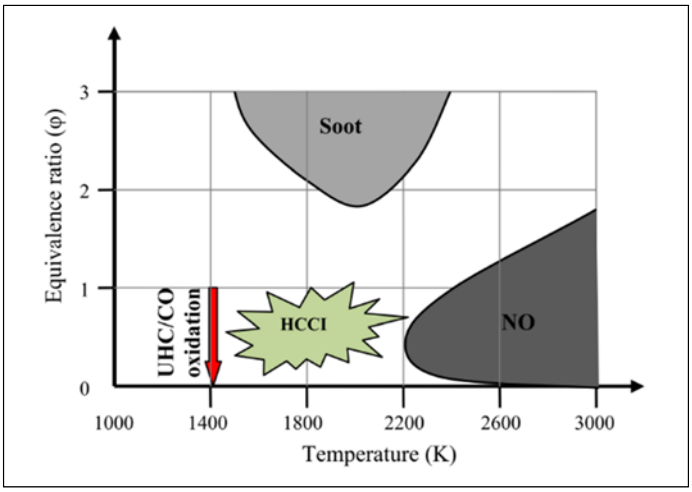

Figure 1. Operating mode of HCCI combustion on local φ-T diagram [8]

is shown in Figure 1. RCCI is a combustion process where usually two fuels with different reactivity are used [6,7]. LTC is very sensitive to numbers of factors such as: fuel reactivity, injection timing, injector characteristics, injection pressure, piston bowl geometry, intake charge temperature, exhaust gas recirculation (EGR), turbocharging, compression ratio and etc. [8–10]. The influence of fuel/fuel blends and EGR rate on combustion characteristics was widely studied in the literature [11–15]. The fuel has an impact on HCCI combustion by their reactivity. The impact of ethanol/diesel and ethanol/biodiesel blends on emissions was experimentally studied in [13]. It was reported that an average 56.5% of diesel fuel can be replaced by ethanol with 70% NOx and 61% smoke opacity reduction. Calam et al. [16] compared combustion characteristics, engine performance and emissions on several fuels to n-heptane operating in HCCI combustion. It was reported that octane number has significant impact on HCCI combustion as CA50 was more controllable with high octane fuels while E25 is more suitable for HCCI combustion with minimum pressure rise.

The combustion process in ICEs is often studied numerically by means of 1D-0D simulation approach [17]. It allows to investigate the combustion characteristics using different blends in both SI and CI engines without complex CFD simulation. However, HCCI combustion is usually two or three stage combustion with low temperature phase (LTF), intermediate phase (IF) and high temperature phase (HTF) [4,18] that cannot be expressed with conventional diesel combustion mechanism. Phenomenological HCCI combustion models are based on detailed chemistry reactions of the fuel in 0D cylinder model. The reaction mechanism on n-heptane and blends was studied in [19–21]. Zeuch et al. [21] proposed a comprehensive skeletal reaction mechanism of n-heptane, while Tsurushima in [20] presented a skeletal reaction mechanism with 33 species and 38 reactions.

Thus, the paper aims to study numerically the impact of fuel/fuel blends on the rate of heat release, pressure rise, engine performance and pollutant formation at different exhaust gas recirculation rate. The main fuel was n -heptane know as primary reference fuel (PRF) while in the blends the n-heptane is mixed with methane and hydrogen.

2. HCCI combustion mathematical background

HCCI combustion can be divided in three phases, such called: LTF, IF and HTF. The first phase depends on the characteristics of the charge flow; the intermediate phase depends on the kinetics of the chemical behavior of the fluid, and the last phase is influenced by chemical and turbulent mixing conditions.

In order to obtain the rate of heat release in 0D cylinder model following correlation can be used:

$$\frac{\boldsymbol{dQ_F}}{\boldsymbol{d\alpha}} = \sum_{i=1}^{nSpcGas} u_i.MW_i.\dot{\omega}_i \tag{1}$$

where: $nSpcGas$ - number of species in the gas phase u_i - species internal energy [J/kgK]; MW_i - species molecular weight [kg/kmole]; $\dot{\omega}_i$ - species reaction rate [kmole/m^{3}s]

The species mass fractions are calculated as follows:

$$\rho \frac{d\omega_i}{d\alpha} = MW_i . \dot{\omega}_i \tag{2}$$

where: ρ - mixture density [kg/m^3] and ω_i - species mass fraction [-].

The reaction rate of each species $\dot{\omega}_i$ is calculated based on a specified set of chemical reactions that describe the auto-ignition process. In this study a reduced skeletal reaction mechanism on C7H16 (n-heptane) proposed by Barroso [22] was used. This reduced mechanism consists of 26 species and 66 reactions as it based on skeletal mechanism of Newson that involves 67 species and 254 reactions. The analysis reported by Barroso, concerning heat release rate parameters CA10 and CA50 for reduced mechanism revealed maximum deviation of 2°CA degrees compared to the initial mechanism.

The thermodynamic properties of each species is estimated as follows:

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{3}$$

$$\frac{H}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \tag{4}$$

$$\frac{S}{R} = a_1 lnT + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \tag{5}$$

This skeletal reaction mechanism cannot be used to estimate the NOx and soot formation, thus, it was used to predict heat release rate and NO for different fuel blends and EGR rate.

3. Simulation model

The engine that was numerically studied is 2.0 liter four cylinders' direct injection engine, developed for passenger cars. The maximum output power when operating with diesel in conventional compression-ignition mode is 101 kW at 4000 rpm as the maximum torque is 320 Nm at 2000 rpm. The engine is equipped with variable geometry turbocharger. The boost pressure is limited to 1.4 bar. Common rail direct injection fuel system of the engine is delivered by Delphi. The maximum injection pressure is limited to 1600 bar. The engine is equipped with EGR and post treatment system including catalytic converter and diesel particulate filter (DPF). The cylinder head is equipped with four valves per cylinder. The main geometrical parameters of the engine are listed in Table 1.

Table 1. Main engine parameters

Type of engine	Direct injection
Number of cylinders	4
Displacement	2 L
Cylinder bore	85 mm
Cylinder stroke	88 mm
Compression ratio	17,6
Valves per cylinder	4

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This engine was considered suitable to be adapted for HCCI combustion using diesel fuel or fuel blends as it offers direct injection in the cylinder while port injection of high octane or gaseous fuel could be further implemented. The engine model was developed in advanced simulation software AVL Boost (Figure 2). The model is based on 0D cylinder modeling considering uniform thermodynamics parameters in the combustion chamber and 1D unsteady flow modeling into intake and exhaust pipes. The main engine data such as: engine type, operating parameters, friction losses and firing order were

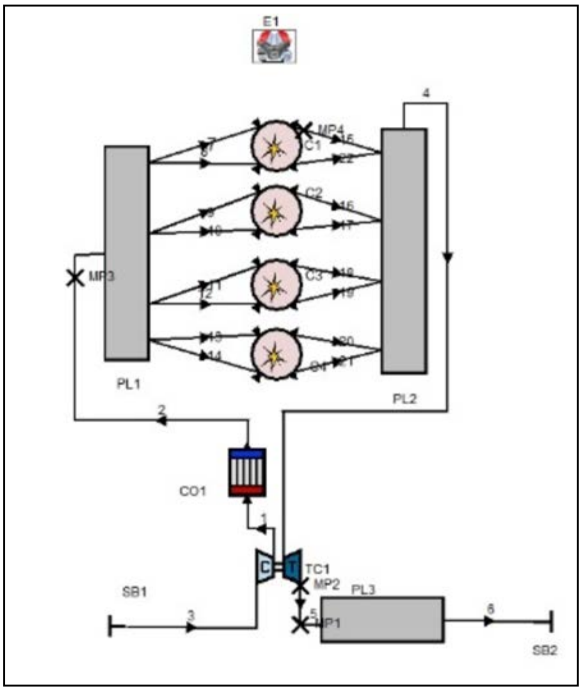

Figure 2. Engine simulation model, built in advanced simulation software AVL Boost

defined in the Engine element - E1. Cylinder geometry was imposed in elements C1 to C4. The single zone HCCI combustion was chosen which required definition of general species transport and detailed reaction mechanism including reaction coefficients. In the element named “Cylinder”, gas to cylinder wall heat transfer was defined as well as the valves lift curves and valves discharge coefficients. The intake and exhaust geometry was presented by pipes and plenums (PL1 and PL2). Moreover, an air intake intercooler was placed after the compressor - CO1. The turbocompressor model (TC1) used simplified modeling with constant pressure ratio and efficiency on the compressor side and equivalent turbine discharge coefficient as well as constant overall efficiency.

Table 2. Simulation constraints

Parameter	Value		
Engine speed	2500 rpm		
Injected fuel	1.5e-005 kg/cycle		
Boost pressure	0.3 bar		
EGR	0%	20%	40%
Fuel mixture	100% C7H16		
	90% C7H16 + 10%CH4		
	80% C7H16 + 20%CH4		
	95% C7H16 + 5%H2		

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In order to establish the EGR rate a simplified approach was used. There was no physical connection between exhaust and intake manifold while the EGR rate was determined by defining the gas composition in intake manifold.

The simulations were carried out at constant engine speed, constant total injected fuel mass and constant intake pressure. In imposed limitations the combustion process, engine performance and NO formation were studied with four fuels at several EGR rate. All limitations and variable simulation parameters are listed in Table 2.

4. Results and discussion

4.1. Study the heat release rate

The heat release rate (HRR) was studied numerically when engine is fueled by: pure n-heptane (C7H16), mixture 90% n-heptane + 10% methane, mixture 80% n-heptane + 20% methane and mixture 95% n-heptane + 5% hydrogen. The results are presented in Figure 3. When no EGR is applied the start of combustion was found to be too early - 25°CA, BTDC. The same value was observed for pure n-heptane and other fuel blends. Increasing the EGR to 20% and 40% leads to late start of combustion as it accounts to 15°CA, BTDC when n-heptane was used. However, when higher EGR rate (40%) is applied the combustion duration is longer for n-heptane due to slight increase in HRR during the LTF. As a result, the maximum HRR for EGR of 40% was at 5°CA, ATDC providing the maximum IMEP. Adding methane and hydrogen in fuel blends reduced the effective EGR rate. In the cases when 10% methane and 5% hydrogen was added to n-heptane the engine IMEP is close to zero when EGR was 40%. Moreover, increasing the methane to 20% in fuel blends leads to effective combustion only without EGR. The maximum HRR is similar for all cases without EGR while 20% EGR leads to reduced maximum HRR value. Here, it was observed the effective combustion with 40% EGR only for pure n-heptane as it significantly reduced maximum HRR to 140 J/deg. When fuel blends were studied, it was observed that the maximum of HRR was close to TDC or after TDC which means higher IMEP and engine thermal efficiency. Using 20% methane in the fuel blend leads to lower intensity of LTF and higher HRR during the HTF as a result maximum HRR occurs at 3°CA, ATDC. However, this fuel blend limited effective EGR range below 20%.

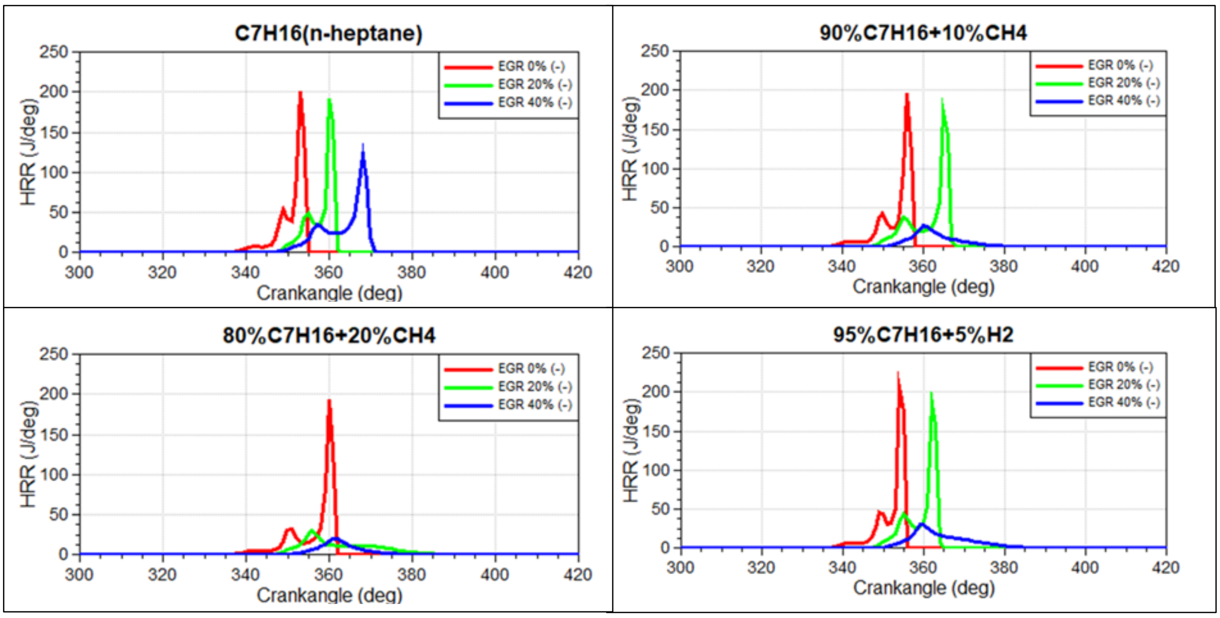

Figure 3. HRR obtained with different fuel/fuel blends and EGR rate

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4.2. Study the in-cylinder pressure

In-cylinder pressure was also studied in order to analyze maximum pressure rise and to evaluate the engine performance. Thus, the impact of fuel/fuel blends and EGR rate within the range of 0% to 40% on in-cylinder pressure was investigated. The results are presented in Figure 4. The maximum in-cylinder pressure was observed for all studied fuel blends to be without EGR. Despite of the fact that start of combustion and CA50 were different for each fuel blend, the maximum pressure was estimated to be within the range of 115 bar to 120 bar. The pressure maximum angular position was affected by fuel blends as it was far before TDC for pure n-heptane while it reached TDC when 20% methane was added. In case of pure n-heptane the maximum pressure had the same value even when 20% EGR was applied. However, the position of maximum pressure was close to TDC. Increasing the EGR to 40% for n-heptane leads to lower in-cylinder pressure as the maximum value was estimated to be 92 bar at 10°CA ATDC. Appling higher EGR rate (40%) for fuel blends leads to very low integral heat release, thus very low IMEP was estimated.

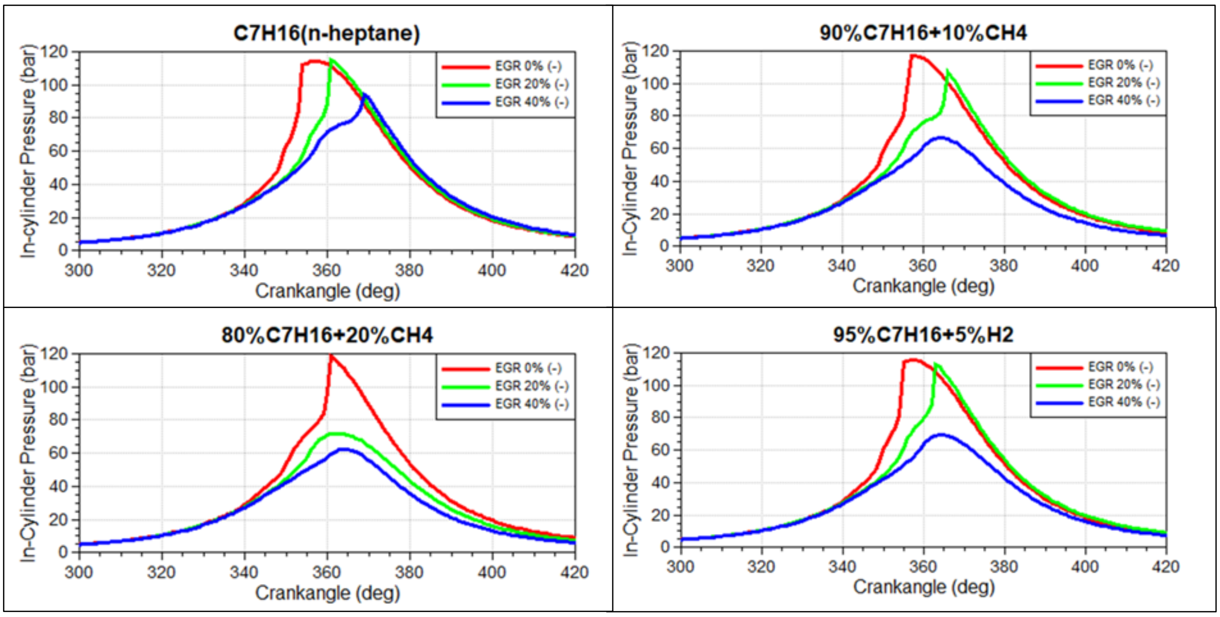

Figure 4. In-cylinder pressure with different fuel/fuel blends and EGR rate

4.3. Engine performance and NO analysis

In HCCI combustion the HRR and in-cylinder pressure curve are very sensitive to fuel reactivity and in-cylinder conditions. Thus, the engine performance is also affected while the start of combustion and CA50 are sensitive to fuel/fuel blends and EGR rate. Estimated engine output performance, maximum pressure rise and NO fraction are summarized in Table 3.

Table 3. Numerical results

Fuel mixture	EGR [%]	Engine torque [Nm]	Engine power [kW]	Pressure rise [bar/deg]	Mass fraction NO [-]
C7H16	0%	30.9	8.1	27.8	5.08e-006
	20%	46.9	12.3	26.8	1.08e-006

	40%	56.3	14.7	7.2	6.94e-008
90%C7H16 10%CH4	0%	36.5	9.6	21.5	4.68e-006
	20%	53.8	14.1	19.8	5.01e-007
80%C7H16 20%CH4	0%	43.9	11.5	22.9	3.22e-006
	20%	14.1	3.7	4.2	5.42e-011
95%C7H16 5%H2	0%	33.4	8.7	32.3	4.88e-006
	20%	50.1	13.1	24.7	8.54e-007

5. Conclusion

The impact of fuel/fuel blends and EGR rate on combustion, performance and NO formation in HCCI combustion was numerically studied. Four fuels were proposed: pure n-heptane (C7H16), 90% n-heptane + 10% methane, 80% n-heptane + 20% methane and 95% n-heptane + 5% hydrogen. For each fuel/fuel blend EGR rate was varied within the range of 0% to 40%. The engine speed was 2500 rpm, total fuel mass was 1.5e-005 kg/cycle and the boost pressure was 0.3 bar. The results revealed that EGR rate has significant impact on start of combustion and CA50 of HRR. The higher range of EGR can be applied when pure n-heptane is used. Adding methane to the n-heptane reduced maximum HRR and retarded start of combustion. It had positive effect to IMEP and engine performance. However, higher concentration of methane limited the effective EGR rate. The engine could not operate with 40% EGR when the fuel blend consists 10% and 20% methane. Moreover, methane concentration more than 10% also reduced EGR rate below 20%. The small quantity of hydrogen has similar effect to 10% methane in the fuel blend. It provided similar engine performance but higher maximum pressure rise with EGR within the range of 0% to 20%. The simulation revealed higher engine performance with pure n-heptane and 40% EGR. Here, the engine torque accounted to 56.3 Nm and output power was 14.7 kW. This case offered lower maximum pressure rise of 7.2 bar/deg and lower NO fraction of 6.94e-008. Similar engine performance was observed with fuel blend of 90% n-heptane and 10% methane. However, the maximum pressure rise is much higher as well as the NO fraction.

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