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HCCI COMBUSTION MODELING: DEFINING THE EFFECTIVE EGR OPERATING RANGE

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Abstract: *This study focuses on combustion modeling of HCCI combustion by means of single zone model using skeletal reaction mechanism of C_7H_{16}(n-heptane). 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 effective EGR operating range was defined at three engine speeds - 1600, 2000 and 2500 rpm. At each speed the EGR rate was varied within the range of 0% to 60%. It was observed that effective EGR rate highly depends on engine speed. At lower engine speed the optimal EGR rate is higher as the optimal value is 60% at 1600 rpm. Higher engine speed lead to lower effective EGR operating range and lower optimal EGR rate as it accounts to 20% at 2500 rpm.*

Keywords: *HCCI, Combustion, EGR, Modelling*

INTRODUCTION

Modern internal combustion engines (ICEs) implemented in passenger cars offer high performances, moderate thermal efficiency and low pollutant emissions. However, in order to meet the restrictive regulations in EU a complex after treatment system needs to be applied as well as advanced injection strategy has to be used for both gasoline and diesel engines. Moreover, a new homologation procedure for passenger cars Euro 7 is in discussion in EU which aims to further reduction of NOx, particles and limitation of new pollutants such as: ammonia, N_2O, micro particles and etc.

One of the most promising approach to reduce in-cylinder NO_x and soot is the advanced combustion process based on homogeneous charge compression ignition (HCCI) and also known as low temperature combustion (LTC) (Krishnamoorthi et al., 2019). HCCI is recognized by long ignition delay period due to the fact that the whole fuel is injected early before the compression stroke and fully premixed combustion occurs (Gan et al., 2011). Depending on ignition delay period and reactivity control several LTC were determined such as: premixed charge compression ignition (PCCI), partially premixed charge compression ignition (pPCCI), reactivity controlled compression ignition (RCCI) and etc. In terms of ignition delay period PCCI and pPCCI are placed between HCCI and conventional CI engines. RCCI is a combustion process where two fuels with different reactivity are used (Reitz and Duraisamy, 2015).

HCCI is very sensitive to a number of factors such as: fuel reactivity, injection timing, injector characteristics, injection pressure, piston geometry, intake charge temperature, exhaust gas recirculation (EGR), turbocharging, compression ratio and etc. (Bendu and Murugan, 2014; Mathivanan et al., 2016; Thangaraja and Kannan, 2016). The influence of EGR rate on combustion characteristics was widely studied in the literature (Lü et al., 2005a, 2005b; Putrasari et al., 2017; Thangaraja and Kannan, 2016). Lü et al. in (Lü et al., 2005b) presented an experimental study of cooled EGR when n-heptane and RON75 were used. The results revealed that EGR up to 45% could be applied as the higher value led to retard start of combustion for both fuels. However, a wide variation in EGR effective range was reported in the literature.

Thus, this paper aims to determine the effective EGR rate in terms of engine performances and NO emissions in case of HCCI operation while the fuel was n-heptane known as primary reference fuel (PRF).

EXPOSITION

Mathematical background

HCCI combustion is usually two or three stage combustion with low temperature phase (LTF), intermediate phase (IF) and high temperature phase (HTF) (Blomberg et al., 2018; Pachiannan et al., 2019) that cannot be expressed with conventional diesel combustion mechanism. 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 related chemical and turbulent mixing conditions. 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 (Tsurushima, 2009; Xu et al., 2012; Zeuch et al., 2008). Zeuch et al. (Zeuch et al., 2008) proposed a comprehensive skeletal reaction mechanism of n-heptane, while In this study a reduced skeletal reaction mechanism on C_7H_{16} (n-heptane) proposed by Barroso (Raya, 2006) was used. This reduced mechanism consists of 26 species and 66 reactions.

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. The thermodynamic properties of each species is estimated as follows:

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

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

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

Engine modelling

The engine that was numerically studied is 2.0 litre four cylinders' direct injection engine, developed for passenger cars. The maximum output power when operating on diesel fuel 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 developed by Delphi. The engine is equipped with water cooled EGR. The cylinder head is equipped with four valves per cylinder.

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 (Fig. 1). The model is based on 0D cylinder modelling considering uniform thermodynamics parameters in the combustion chamber and 1D unsteady flow into intake and exhaust pipes. The main engine data such as: engine type, operating parameters, friction losses and firing order were defined in the Engine element - E1. Cylinder geometry was imposed in elements C1 to C4. The single zone HCCI combustion was chosen which required determination 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). An air intake intercooler was downstream the compressor - CO1. The turbocompressor (TC1) used simplified modelling approach with constant pressure ratio and efficiency on the compressor side as well as equivalent turbine discharge coefficient.

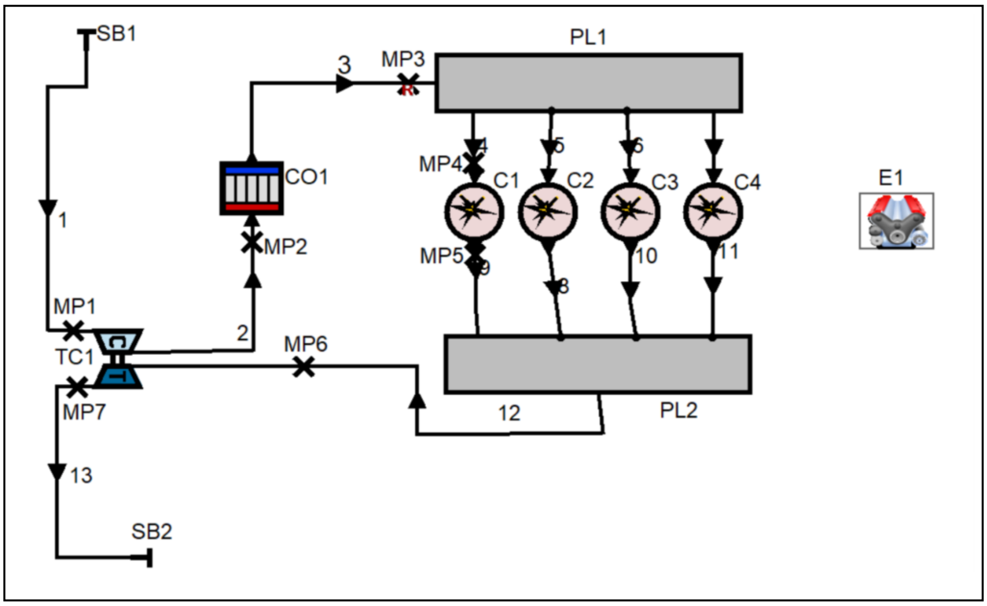

Fig. 1. Engine simulation model, developed in simulation software AVL Boost

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 the intake manifold.

Table 1. Simulation parameters

PARAMETER	**VALUE**			
Engine speed	1600 rpm	2000 rpm	2500 rpm	
Injected fuel	1.5e-005 kg/cycle			
Boost pressure	0.3 bar			
EGR	0%	20%	40%	60%
Fuel	C_7H_{16} (n-heptane)			

The simulations were carried out with constant total injected fuel mass and constant intake pressure. For each engine speed the EGR rate was varied within the range from 0% to 60%. In imposed limitations, the combustion process, engine performance and NO formation were studied. All simulation constrains and parameters are listed in Table 1.

Numerical results

The first study was carried out at 1600 rpm when EGR was varied within the range mentioned above. The engine combustion process was studied as well as the engine performance. The main results are presented in Fig. 2.

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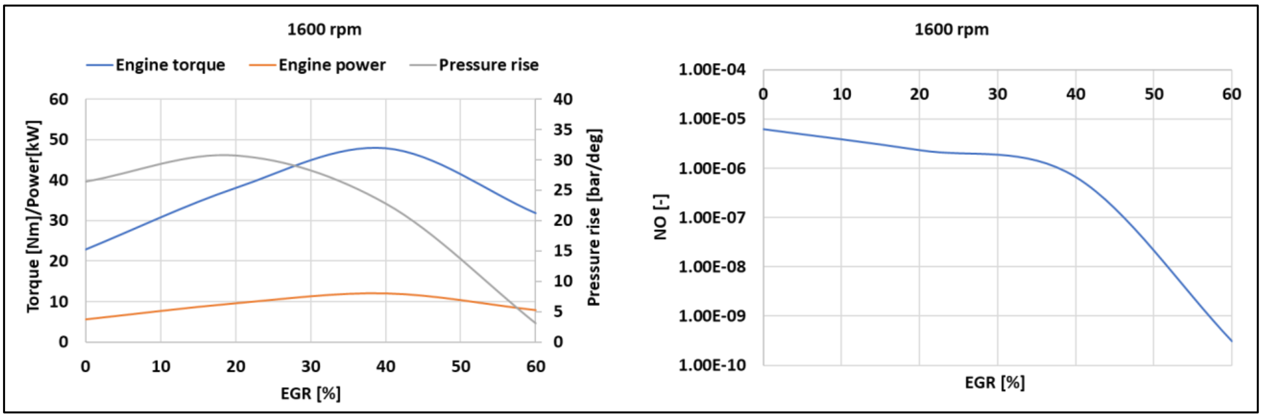

Fig. 2. Engine performance and NO fraction vs EGR rate at 1600 rpm

At 1600 rpm, increasing the EGR rate from 0% to 40% led to higher output torque and power. In terms of engine performance, the optimal EGR rate was 40%. It offers engine torque of 47.8 Nm and output power of 8 kW. However, in terms of pressure rise the optimal EGR rate is 60% as it led to much lower pressure rise of 3.1 bar/deg. At this high EGR value the engine performance is lower than maximum values but similar to operating at 20% EGR. NO fraction slightly decreased as a function of EGR rate. The lowest in-cylinder NO was estimated at 60% EGR.

Similar trend was observed at 2000 rpm - Fig. 3. The optimal engine performance was estimated when EGR rate is 40%. In this case, the engine power had maximum value of 11.1 kW, while the engine torque accounted to 52.9 Nm. Lower EGR led to very high pressure rise which reached 27.9 bar/deg when EGR is 0%. Increasing the EGR rate to 40 % reduced pressure rise to 20.2 bar/deg. Although the EGR of 60% offered significantly lower pressure rise - 1.76 bar/deg, it led to reduced performance by 85%. NO fraction values were very similar to those obtained at 1600 rpm as the minimum was estimated at 60% of EGR.

The third studied engine speed was 2500 rpm. The results are shown in Fig. 4. In this case the operating range of EGR was reduced as the engine cannot operate with EGR rate higher than 40%. Even at 40% the engine performance was very low. The optimal EGR rate in terms of performance was 20%. It offered to the engine 116.5 Nm brake torque and brake power of 30.5 kW. Also, it led to pressure rise of 6.2 bar/deg, which is acceptable even for conventional combustion process in diesel engines. This EGR rate of 20% offered lower NO fraction compared to other studied speeds and 40% EGR rate. The estimated engine torque, power, pressure rise and NO fraction are summarized in Table 2.

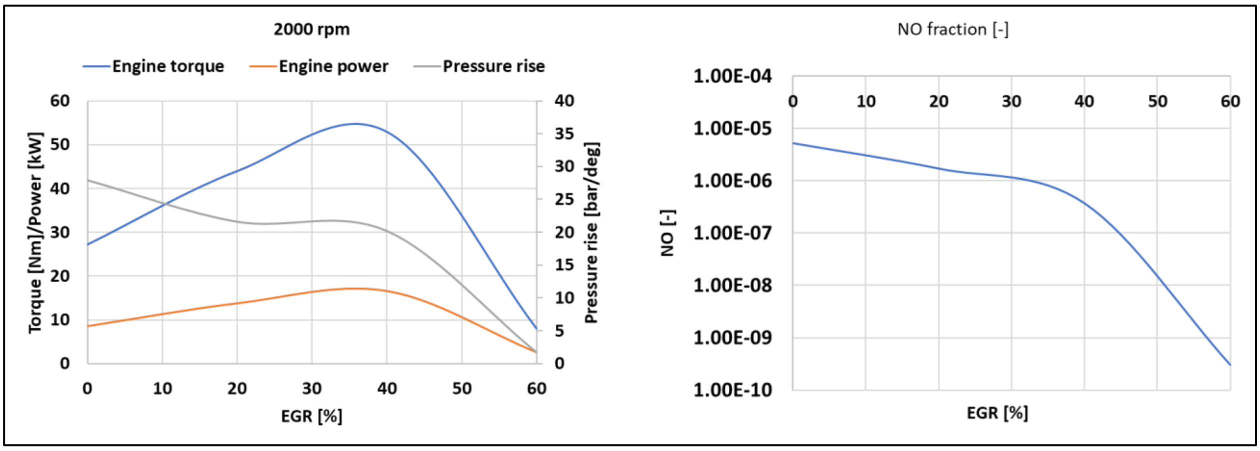

Fig. 3. Engine performance and NO fraction vs EGR rate at 2000 rpm

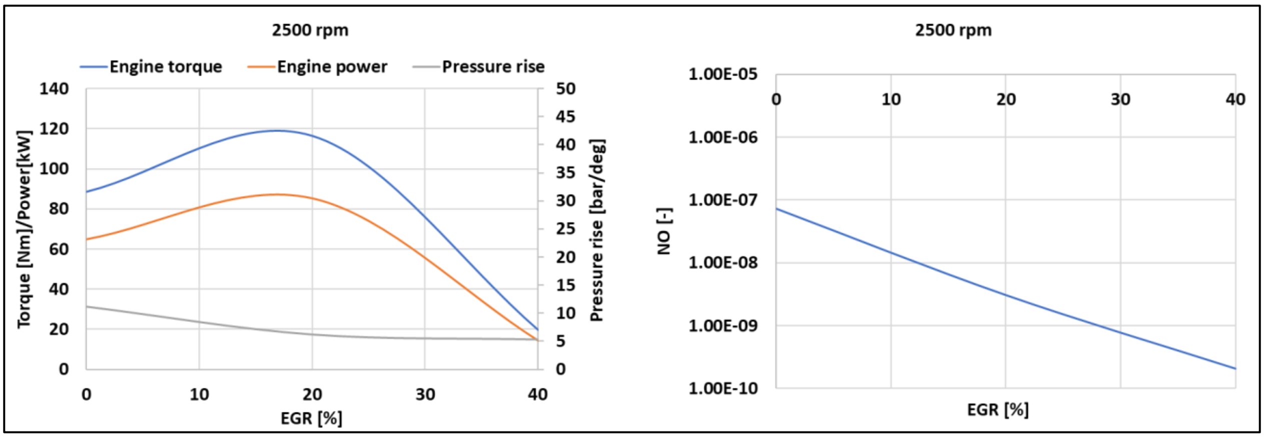

Fig. 4. Engine performance and NO fraction vs EGR rate at 2500 rpm

Table 2. Engine performance and NO fraction

Engine speed	EGR [%]	Engine torque [Nm]	Engine power [kW]	Pressure rise [bar/deg]	Mass fraction NO [-]
1600 rpm	0%	22.84	3.8	26.4	6.32E-06
	20%	38	6.4	30.7	2.37E-06
	40%	47.8	8	22.8	6.70E-07
	60%	31.8	5.3	3.1	3.06E-10
2000 rpm	0%	27.2	5.7	27.9	5.18E-06
	20%	43.9	9.2	21.6	1.70E-06
	40%	52.9	11.1	20.2	3.70E-07
	60%	8	1.7	1.76	3.06E-10
2500 rpm	0%	88.6	23.2	11.2	7.29e-008
	20%	116.5	30.5	6.2	3.05e-009
	40%	19.6	5.1	5.3	2.06e-010

CONCLUSION

The effective EGR range was determined in case of HCCI combustion for three engine speeds when injected fuel was constant. The study was carried out by means of numerical simulation. Advanced software for 0D-1D simulation AVL Boost was used. The engine that was studied is a direct injection, four cylinders, equipped with turbocharger. In order to evaluate the EGR effect on the engine performances, a single zone HCCI combustion model was implemented based on skeletal reaction mechanism of C_7H_{16}(n-heptane) that uses 26 species and 66 chemical reactions. The EGR rate was varied within the range of 0% to 60% at each studied engine speed - 1600, 2000 and 2500 rpm. The engine performance was evaluated based on engine output power and torque, maximum pressure rise in the cylinder and in-cylinder NO fraction.

On the basis of the results, it can be stated that EGR ratio has significant impact on engine performances. It is due to the impact on start of combustion and heat release rate. For 1600 rpm and 2000 rpm, EGR rate that offered engine operation was the whole studied range - 0% to 60%. However, very difference engine performance was observed. For both engine speeds, the optimal EGR rate was 40% in terms of brake torque and power but it was achieved with high maximum pressure rise that accounted to 22.8 bar/deg and 21.6 bar/deg, respectively. In terms of maximum pressure rise, the optimal EGR rate is higher than 40%. At 1600 rpm it was close to 60% but at 2000 rpm it would be close to 40% due to significant reduction at brake power.

At 2500 rpm, we founded that effective EGR rate was smaller than other speeds. It was within the range of 0% to 40%. Moreover, the impact of EGR rate on the engine performance was higher. The optimal value in terms of brake power was EGR of 20% while increasing the EGR to 40% led to significant reduction of engine performances. In this speed 20% EGR offered moderate

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maximum pressure rise of 6.2 bar/deg. As a conclusion it can be stated that EGR rate needs to be precisely controlled in case of HCCI combustion. Lower engine speed offers wider EGR operating range in terms of engine performance while the higher engine speed needs lower EGR rate which offers optimal performance and NO formation.

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