INFLUENCE OF FUEL COMPONENTS ON COMBUSTION PROCESS OF HOMOGENEOUS FUEL MIXTURE IN THE HCCI ENGINE

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DOI: 10.17973/MMSJ.2023_10_2023072

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ABSTRACT

Nowadays, the research and development activities performed in the area of internal combustion engines are focused on the LTC technologies, especially on the HCCI technology. It is so because these innovative technologies are characterized by high operational efficiency as well as by low emissions of nitrogen oxides (NO_X) and particulate matter (PM). The combustion process LTC is able to utilize various fuels. The kind of fuel, together with its physical and chemical properties have a major influence on engine power output and gaseous emissions. The presented scientific contribution deals with analysis of an experimental engine operating with the HCCI combustion, specifically it deals with operational influences of several selected fuel mixtures. There is investigated an influence of the fuel mixtures, which consist of different components with various properties, on the engine power output and on the gaseous emissions. These experimentally applied fuels were created as the mixtures of isooctane and n-heptane using different mixing ratios. The obtained results offer a global view on a real effect of the fuel components applied in the fuel mixtures.

KEYWORDS

Alternative fuels, emission, low-temperature combustion

1 INTRODUCTION

During last years, the automotive industry was passing through a breaking period in connection with the prepared industrial policy of EU. The main goal of the future industrial conception is transformation of the European industry to a green, circular and low-carbon economy, reduction of gaseous emissions arising from transport and increasing the share of industrial production in the overall economy within the EU countries. At the same time, the automotive industry faces new challenges such as digitization, electromobility, innovative engine technologies and utilisation of alternative energy sources [Arapatsakos 2008].

The total amount of 53.8 billion EUR is yearly invested into research and development targeted to reduction of the CO_2 emissions. In addition to emissions arising from the passenger and commercial vehicles, a significant attention is also paid to reduction of pollutants generated in the individual industrial branches [Hudak 2021, Kuric 2020].

Nowadays, the term “emission-free driving” means emission-free operation of the motor-car, i.e. just the driving phase. However, an adequate attention must be focused on the whole chain, which includes both production and operation of motor-car that is the complete vehicle life cycle. Therefore, it is necessary to take into consideration all the supply chain groups, namely from production of the car and automotive fuels, through the phase of vehicle utilisation till its final recycling [Ascanio 2008].

In the case of electric cars, generation of the CO_2 emissions occurs in the phase of electric car production and during their recycling. At the same time, it is necessary to say that a possibility for reduction of CO_2 in the phase of electromobile operation is very limited, especially when the charging electric current is not produced from the renewable energy sources [Brezinova 2018, Dragonovska 2018, Krenicky 2018].

Almost 70% of the CO_2 emissions that are arising within the whole motor car life cycle is generated by the piston combustion engine during operation of the vehicle. The remaining 30% is redistributed to the above-mentioned supply chain, which includes vehicle production, final recycling and also production of fuel. A possible solution of such situation offers application of the Low-Temperature Combustion (LTC) technologies. The greatest potential within the LTC technologies has the innovative combustion technology known as the Homogeneous Charge Compression Ignition (HCCI) [Barbouchi 2009, Brennan 2008, Tucki 2021].

The piston combustion engine working on principle of the HCCI technology is a functional combination of the petrol engine and diesel engine, whereby it utilises the best characteristic features of both. It uses gasoline as the fuel while maintaining efficiency of diesel engine. Combustion of homogeneous mixture is running simultaneously in the whole combustion volume of the engine cylinder, so almost the all amount of delivered fuel mixture is burned. Utilisation of the fuel is so efficient that the HCCI technology offers significant fuel savings. In addition, the homogeneous mixing of the fuel with air leads to cleaner emissions and the level of nitrogen oxide emissions is almost negligible. The HCCI combustion technology is characterized by a fact that fuel and air are mixed together before starting of combustion and the fuel/air mixture spontaneously ignites due to increased temperature and pressure in the combustion chamber during the compression stroke. Thus, on one side the working principle of the HCCI engine is similar to the spark ignition engine because both engines use a pre-mixed fuel/air mixture. However, on the other side, functioning of the HCCI engine is similar also to the compression ignition engine with regard to a fact that both these engines rely on self-ignition of mixture in combustion process [Toman 2017, Rodriguez 2022].

The HCCI combustion generates, similarly to diesel fuel, a special two-stage heat release process [Rimar 2022]. The first stage of the heat release curve corresponds to low-temperature kinetic reactions. On the other side, a certain time delay between the first and the second, main heat release phase is caused due to the "Negative Temperature Coefficient” (NTC), which is situated between both these heat release stages. There is no visible any flame propagation during the HCCI combustion [Rodriguez 2023].

In the past, there were commercialized also the internal combustion engines determined for combustion of lean fuel mixture using spark ignition, however they reached only approx. 1.5-times of the stoichiometric air-fuel ratio, so that

the effect of fuel efficiency improving was not relevant in this case.

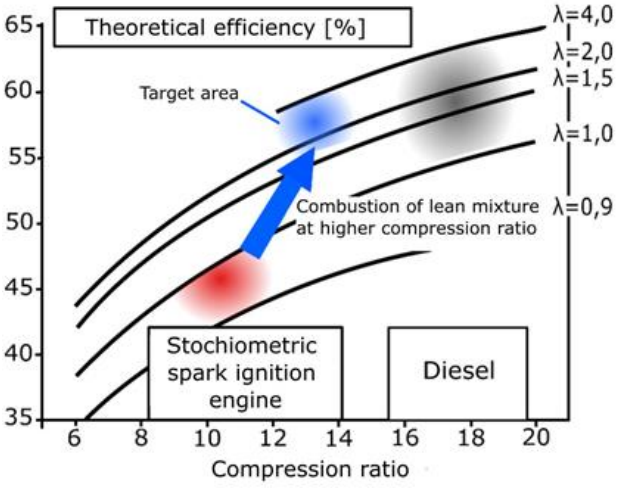

Figure 1. Influence of compression ratio increasing on theoretical efficiency of ab ideal engine

As it is visible in Fig. 1, it is necessary to set up high AFR ratio also for reduction of the NOX emissions. The HCCI concept was originally investigated for the gasoline applications in order to increase combustion stability of two-stroke engines. It was found that it is possible to achieve a significant reduction of gaseous emissions and fuel consumption by creation of such conditions that lead to self-ignition of fuel charge in the engine cylinder. A stable HCCI combustion could be achieved between the limits of low and high load of gasoline engine with the compression ratio of 7.5:1, in the engine speed range from 1,000 to 4,000 rpm. Several researchers investigated the HCCI engine using various fuels, for example the isooctane, ethanol, natural gas, hydrogen, gasoline, diesel, n-heptane, methanol, propane and n-pentane. The above-mentioned studies discovered that the fuels with higher volatility, such as hydrogen and ethanol, are mixing with the air better and create homogeneous fuel mixtures [Birtok-Baneasa 2017].

It was applied a new fuel concept in order to achieve lower emissions as well as wider range of the speed and load of the HCCI engine. This innovative fuel conception is based on mixing of a high octane fuel with a high cetane fuel in real time in order to control the HCCI combustion, specifically using the isooctane and n-heptane. According to the results obtained from the performed tests it is possible to say that the ratio of n-heptane equivalence in the mixtures determines ignition and also controls the HCCI combustion phase. Addition of isooctane slightly extends the limit of detonation combustion. However, occurrence of detonation combustion mainly depends on the total concentration of mixture. Although the operational range in the ratio of equivalence narrows with increasing amount of isooctane, the maximal load of HCCI engine when burning isooctane-heptane fuel mixture controlled in real time, increases approx. about 70% more than in the case of pure n-heptane [Famfulik 2021].

The HCCI engines are working relatively reliably only within the operational range from low to medium load [Bozek 2021]. In the case of high load, the engine needs higher ratios of equivalence, i.e. increased combustion speed, what leads to high rate of pressure increase and consequently to pressure oscillations. This phenomenon causes an unacceptable noise, potential damage of engine and higher NOX emissions. Even in the in-audible cases, these pressure waves can gradually damage the engine. Therefore, it is necessary to take measures in order to avoid hard combustion regimes that cause a rapid increase in pressure. Fig. 2 illustrates course of in-cylinder pressure at operation-al conditions causing abnormal combustion. The pressure fluctuations observed between -1 and 10 CAD are an undesirable physical phenomenon, which is called “knocking”, but due to differences between the HCCI and SI combustion these pressure fluctuations are called "ringing".

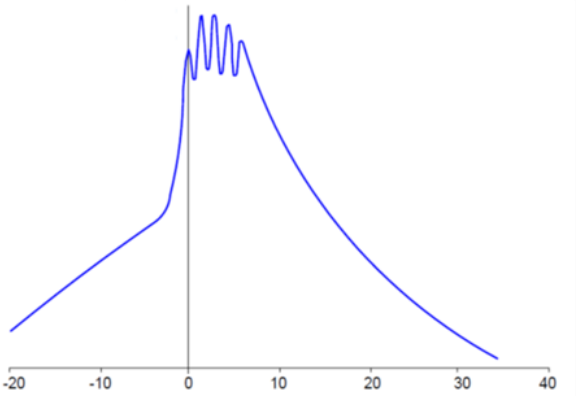

Figure 2. Course of pressure in cylinder depending on crank angle degree during intensive abnormal combustion

The high-frequency pressure oscillations presented in Figure 2 as a result of ab-normal combustion are moving inside the cylinder and reflecting from the cylinder walls, resulting in oscillatory behaviour of the pressure wave. These pressure oscillations create a considerable noise in the engine structure. Calculation of the "ringing intensity", using the equation (6), enables to evaluate noise of the HCCI engine combustion:

$$RI = \frac{\sqrt{\gamma R T_{max}}}{2\gamma P_{max}} \left[\beta \left(\frac{dP}{dt}\right)_{max}\right]^2$$

where (dP/dt)max is the maximal rate of pressure increase, Pmax is the maximal pressure in the engine cylinder and Tmax is the maximal average mass temperature in the cylinder. This temperature is calculated according to the ideal gas law. The value γ is a ratio of the specific heats (Cp/Cv) and R is the gas constant. The value β is a tuning parameter related to the amplitude of pressure pulsations and to the maximal rate of pressure increase. Its typical value is 0.05. Although the HCCI combustion is theoretically idealized as a uniform and homogenous self-ignition process, which is running in the whole volume of the fuel-air mixture at once, in reality the ignition occurs sequentially during a short time and in different locations inside the fuel mixture. These sequential ignitions are caused due to significant differences in local temperatures occurring during the compression stroke [Puskar 2021].

It can be state that the Homogeneous Charge Compression Ignition (HCCI) is dominantly characterised by the chemical kinetics, taking into consideration absence of a flame propagation area. Creation of a complex HCCI combustion model, which is determined for simulation of the combustion process, requires a proper combination of fluid mechanics, thermal analysis and HCCI combustion analysis. The existing simulation software products are applied for analysis of the HCCI combustion in the case of simple fuels. Calculations involving practical fuels are too much demanding. On the other hand, the one-zone HCCI combustion simulation model enables detailed simulation of the chemical kinetics for the practical fuels, assuming that gas in the combustion chamber is homogeneous, with the stable temperature, pressure and gas composition [Kuznetsov 2020]. The one-zone model is able adequately to predict ignition in the HCCI engine if the initial conditions (engine load) are known. However, since this model does not consider the low-temperature areas occurring in the

thermal boundary layers and slots, the one-zone model has a tendency to insufficient prediction of CO and un-burned hydrocarbon (UHC) emissions and at the same time to overestimate the maxi-mal pressures in engine cylinder [Ceviz 2010].

2 EXPERIMENTAL CONDITIONS

A thermodynamic one-zone simulation model with a detailed chemical kinetic mechanism was used as a base for realisation of the experiment. This model assumes that the fuel/air mixture spreads homogeneously in the combustion chamber. The combustion chamber is considered as a one compact zone where the values of pressure, temperature and fuel composition are stable. This mechanism was verified by the obtained experimental results. There are usually used, during the process of mathematical simulation, the physical equations describing the law of mass conservation, energy in gaseous phase, heat release rate, pressure, temperature and indicated work at each time step. Heat transfer through the wall of cylinder is calculated according to the Woschni heat transfer model. In the case of the spark-ignition engine, the main mechanism of heat transfer from gases inside cylinder to the wall of cylinder is convection. Only 5% of heat is transferred by radiation. When applying the Newtonian model, the heat losses on the wall of combustion chamber are given by the relation:

$$Q = hA(T_g - T_W)$$

where:
h = heat transfer coefficient,
A = exposed surface of the combustion chamber,
T_g= gas temperature in cylinder,
T_W = cylinder wall temperature.

In order to determine the relation for heat transfer, it is necessary to take into ac-count heat losses to the walls in cylinder. Thus, the change in pressure depending on the crank angle degree is as follows [Kelemen 2021, Kelemenova 2022]:

$$\frac{dP}{d\theta} = \frac{k-1}{V}\left[Q_{in}\frac{df}{d\theta} - \frac{hA}{\omega}(T_g - T_W)\frac{\pi}{180}\right] - k\frac{P}{V}\frac{dV}{d\theta}$$

where:
ω= angular velocity of crank.

Surface of the cylinder can be determined from a model of the moving crank:

$$A = \frac{\pi}{2}b^2 + \pi b\frac{s}{2}\left[R + 1 - \cos\theta + (R^2 - sin^2\theta)^{1/2}\right]$$

The gas temperature Tg is the average temperature value. This temperature is obtained from the physical equation valid for ideal gas.

$$\bar{T}_g = \frac{PVM}{m\tilde{R}} = \frac{PVM}{\rho V_1 \tilde{R}}$$

where:
M = molar mass of the fuel/air mixture,
m = mass of the fuel/air mixture,
$\tilde{R}$ = universal gas constant.
The following equation is obtained using the relation $r = {}^{V_1}/_{V_1 - V_d}$

$$\bar{T}_g = \left(\frac{r-1}{rV_d}\right)\frac{PVM}{\rho\tilde{R}}$$

There will be discussed two correlations elaborated by the researchers Annand and Woschni in order to determine the heat transfer coefficient. The first of them is created by Annand:

$$Nu = \left(\frac{h_c b}{k}\right) = \alpha\left(\frac{\rho\bar{S}_p b}{\mu}\right)^b$$

where:
h_c = heat transfer coefficient,
b = boring,
k = thermal conductivity,
m = dynamic viscosity,
$\bar{S}_p$= = average piston speed,
a = is a number within interval from 0.35 to 0.8 at normal combustion,
b = 0.7.

Woschni takes into account increase of gas velocity in the cylinder during combustion. Annand assumes a constant characteristic velocity of gas, which equals to the mean piston velocity. The average in-cylinder gas velocity "v" in a four-stroke engine without swirling, determined by Woschni, is:

$$v = c_1\bar{S}_p + c_2\frac{V_d T_r}{P_r V_r}(p - p_m)$$
$$-180 \le \theta \le \theta_0 \rightarrow c_1 = 2{,}28, c_2 = 0$$
$$\theta_b \le \theta \le 180 \rightarrow c_1 = 2{,}28, c_2 = 3{,}24x10^{-3}$$

where:
P_{motor} = pressure in engine cylinder,
T_a = ambient temperature, 298 K,
P_a = atmospheric pressure, 1 atm.

The pressure in engine is defined by the relation:

$$P_{motor} = \frac{\left[\left(\frac{rV_d}{r-1}\right)^\gamma P_a\right]}{V\gamma}$$

The heat transfer coefficient according to Woschni is:

$$h = 3{,}26b^{-0,2}P^{0,8}T^{-0,55}v^{0,8}$$

Technical specification of the piston combustion engine, which was utilised in this experiment, is presented in Tab. 1. The value of compression ratio is in accordance with Fig. 1. There were applied six different fuel mixtures for the analysis. These fuel mixtures are listed in Table 2.

Table 1. Engine specification

Compression ratio	12.2
Bore [mm]	54
Stroke [mm]	54.5
Displacement volume [cm^3]	124.8
Exhaust valve open	130_ATDC
Exhaust valve closed	18_ATDC
Intake valve open	12_ATDC
Intake valve close	142_ATDC

Table 2. Experimental fuel mixtures.

Mixture	% of n-heptane	% of isooctane
N1I0	100	0
N9I1	90	10
N8I2	80	20
N7I3	70	30
N6I4	60	40
N5I5	50	50

3 RESULTS AND DISCUSSION

The results obtained from the performed experiments were compared with the results of simulation for the different fuel mixtures. The simulation results and the experimental results of the pressure values for the N6I4 fuel mixture are presented and mutually compared in Fig. 3. Both sets of the results are in a good agreement each other. The maximal pressure value obtained from the simulation model is slightly higher than the experimentally obtained value because the applied one-zone thermodynamic model predicts overestimated value of the maximal pressure [Saga 2020, Dresler 2018].

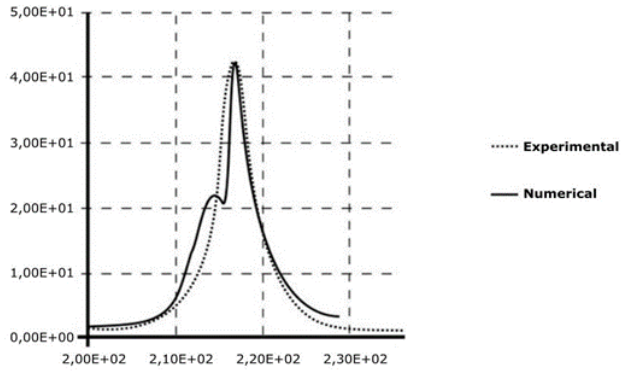

Figure 3. Comparison of the experimental results with the simulation results using the N6I4 mixture

The courses of pressures for the different fuel mixtures are mutually compared in Fig. 4. According to expectation, the N1I0 mixture reached the highest pressures and its combustion started earlier than in the case of other mixtures. The reason is that the octane number of this mixture is lower than others. Since the octane number indicates the resistance of fuel to self-ignition, the fuel with a lower octane number is more self-igniting. Therefore, the N1I0 mixture reaches higher maximum pressure and temperature.

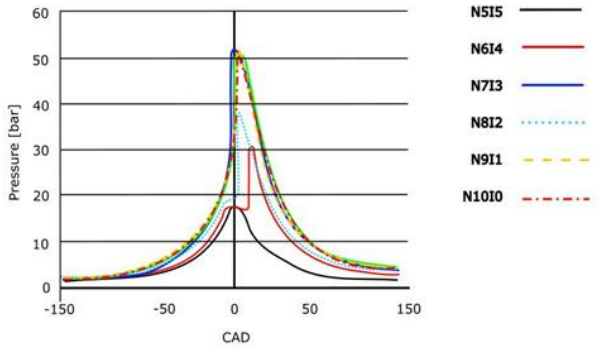

Figure 4. Comparison of pressure courses for different fuel mixtures

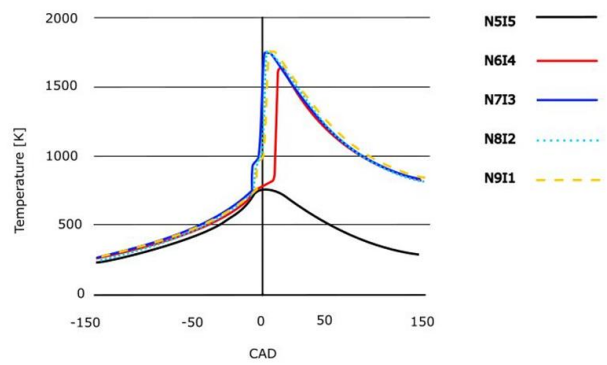

Figure 5. Comparison of temperature courses for different fuel mixtures

If the octane number increases from 0 to 50, the tendency to self-ignition de-creases and consequently decreases the maximal pressure. In the case of the N5I5 mixture the high-temperature combustion does not occur. In this case, the maximal pressure is 51 kPa and it occurs at 1.48 CAD. The courses of temperatures for the different fuel mixtures are compared in Fig. 5. As it was expected, the N5I5 mixture reached the maximum temperature and the N9I1 mixture the minimum temperature. Temperatures of the fuel mixtures are very similar, except of the N9I1 mixture. It is evident, from the pressure diagram that increasing of the octane number from 70 to 100 does not have a significant influence on the combustion performance.

The graph, which illustrates a dependence of the pressure on the volume, is introduced in Fig. 6. The area in this P-V graph corresponds to value of the engine indicated power output. So, the engine reached the maximum indicated power output using the N9I1 mixture. However, the indicated power output is not the most suitable criterion for evaluation of the power output. The most important criterion is the indicated specific fuel consumption. The results of the specific fuel consumption for six different fuels are presented in Fig.7. It is evident that application of the N8I2 mixture offers the minimum specific fuel consumption. Thus, this fuel mixture is the most suitable because it reaches the maximum power output with a given specific amount of fuel [Malakova 2020, Puskar 2022].

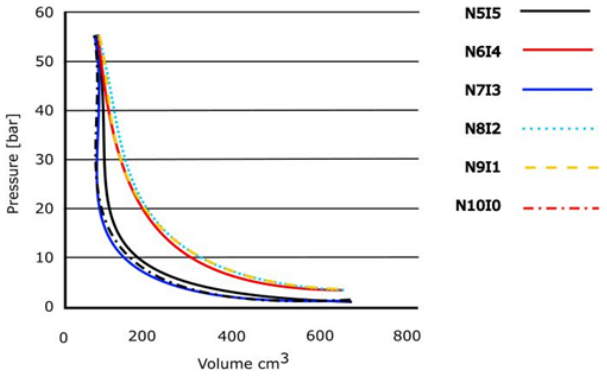

Figure 6. Pressure-volume dependences

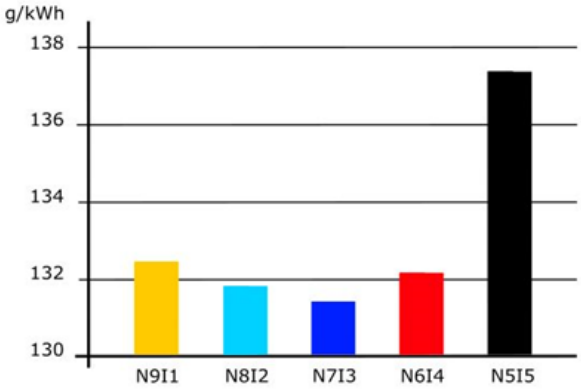

Figure 7. Indicated specific fuel consumption

A comparison of the simulated CO emission concentration with the experimental result is in Figure 8. The numerical, simulation model can predict a trend of CO production, but this model is not able accurately to predict the amount of CO concentration. It was already mentioned that the one-zone thermodynamic model is not suitable for accurate prediction of CO concentration because it is not able to take into account the individual specific areas such as the boundary layers and slots. These areas are sources of CO production. The above-mentioned simulation models consider the combustion chamber as one volume with the stable operational conditions.

The results of CO simulation for different fuel mixtures are in Figure 9. As the temperature in-creases, the concentration of CO emissions decreases because due to high temperature a large amount of the carbon elements is converted directly into CO_2 and the portion of CO is reduced, too. Combustion of the N9I1 fuel mixture achieves the best quality, it is the most complete combustion process, and the immediate concentration of CO is minimal. In the case of the N5I5 mixture, the combustion is not complete, so a large amount of the fuel will not ignite, and the instantaneous concentration of CO is higher than in other cases. The generated CO is not converted to CO_2 and remains in the combustion chamber.

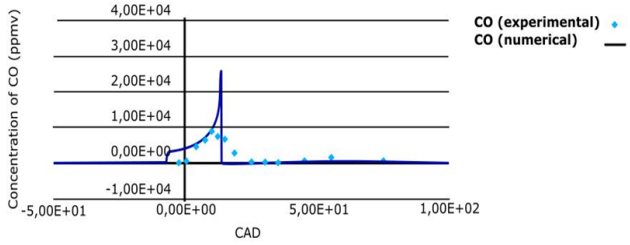

Figure 8. Comparison of simulated and experimentally obtained production of CO emissions

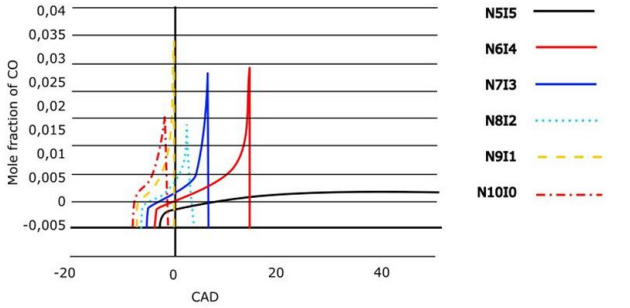

Figure 9. Results of simulated and experimentally obtained production of CO emissions

4 CONCLUSION

Within the framework of this presented scientific-research work, a thermodynamic one-zone simulation model with a detailed chemical kinetic mechanism was used. There were tested various fuel mixtures with different octane and heptane numbers in order to investigate their influence on the engine power output and emissions during the HCCI combustion. The chemical kinetic mechanism, which was used in this work, includes in total 4236 chemical reactions created during the combustion process.

The results obtained from the performed simulations are summarized as follows:

1. If the octane number decreases and the content of heptane increases, the values of maximum pressure and temperature increase because the octane number indicates a resistance to self-ignition. If the octane number decreases, self-ignition occurs earlier, and the fuel ignites more easily, therefore the maximum values of pressure and temperature increase.
2. The area in the P-V diagram characterizes work and power output of the engine. The N10I0 mixture offers the maximum indicated power output because it achieves the maximum self-ignition ability.
3. The indicated specific fuel consumption is the best criterion to assess the engine power output and quality of combustion process in the internal combustion engine. The N8I2 mixture reaches the minimal fuel consumption, therefore it is the most suit-able fuel mixture for application in the tested engine.
4. The thermodynamic one-zone model is not able to predict the exact amount of CO concentration. It can only predict the trend of CO production, which depends on quality of combustion process and on temperature of the products. The N8I2 mixture generates the minimum concentration of CO emissions.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-19-0328. The article was written in the framework of Grant Projects: VEGA 1/0318/21 “Research and development of innovations for more efficient utilization of renewable energy sources and for reduction of the carbon footprint of vehicles” and KEGA 007TUKE-4/2023 “Transfer of innovations and advanced technologies, determined for more ecological and more efficient vehicle drive systems, into the educational process.”

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