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INVESTIGATIONS OF ENGINE EXHAUST GAS EMISSION WITH OXYGEN ENRICHED MIXTURE AND HIGH EXHAUST GAS RECIRCULATION

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Abstract

The paper presents an explanation of the formation process of toxic exhaust gas components during combustion process of oxygen-enriched mixtures in SI engine. In order to explain this phenomenon the simulation process was carried out, in which the experimental data from dynamometer tests of the 4-stroke SI engine were used. The tests were done at different oxygen volumetric ratios and at increased exhaust gas recirculation ratios until the mixture of oxygen and exhaust gases has not contained any nitrogen. The EGR system was applied in order to decrease gas temperature in the cylinder. Simulation of engine combustion process with oxygen-enriched mixture and with different EGR ratios was carried out by using the program Kiva3v for calculation of full engine phenomena with simple combustion model. This combustion model took into account 10 kinetic and equilibrium chemical reactions. Both experimental and simulation test indicated nonlinear variation of mole fractions of carbon monoxide and carbon dioxide with increasing of oxygen amount in the charge from 21% to 32% by volume. The engine has higher emission of carbon monoxide and carbon dioxide in comparison to the emission of the engine filling with air-fuel mixture in normal conditions. The paper explains from chemical reactions point of view a non-linear change of CO and CO2 emission in a function of the charge oxygen mass ratio at constant oxygen excess ratio. The paper presents the graphs showing variations of emission and volumetric concentration of chosen chemical species in the charge in a function of crank angles and variation of the engine parameters at different EGR and oxygen ratios in the engine charge.

Keywords: *transport, combustion engine, EGR, oxygen enriched mixtures, emission*

1. Enriched mixtures in IC engines

Kuznetsov [6] already considered applying of oxygen-enriched mixture in internal combustion engines (ICE) 50 years ago. The new technology called "downsizing" forces to find new fuelling systems in order to increase amount of charge in the cylinder and then to deliver higher dose of fuel. The other way of increasing of engine power is filling of the SI four-stroke engine only by oxygen and fuel and thus forming the mixture close to stoichiometric value [9]. Adding higher amount of O_2 than in the air it gives the same effect as a charging system. However, the burning of such mixture causes significantly higher combustion temperature and also higher NOx emission. Decreasing of combustion temperature and NO_x is possible by applying the exhaust gas recirculation system (EGR). Improvement of engine performance by using oxygen enriched air charge was partly considered by Zvirin and Tarkovski [18], by Maxwell *et al* [7] with taking into account emission of toxic components. Applying of an oxygen-enriched charge creates opportunity of better engine work during "cold start" and it was investigated by Li Gong *et al* [4].

The diesel engine with higher oxygen volumetric ratio (x_{O2}) tested by Xiao *et al* [15] was designed to obtain better start ability. Simulation of SI engine work fuelled by oxygen-enriched charge was carried out by Caton [2] and partly by authors [12]. Some experiments were carried out at partial loads of SI engine with such mixtures for example by Shuici and Kajitani [10]. The tests have indicated the ability of the engine filled by oxygen-enriched mixture to work in knocking range.

2. Aims and goals

The target of the authors was to find dependencies between increased amount of oxygen in the charge delivered to the combustion chamber and emission of toxic components in exhaust gases. In order to reduce amount of NOx and maximal temperature during combustion process, the EGR system was applied. Both the experimental and simulation tests were carried out only for the case when the engine was filled by fresh charge containing oxygen, gasoline in stoichiometric value in relation to oxygen. The exhaust gases in EGR system were deprived of water vapour by condensation. The main objective of the study was to verify the tests with results from simulation. Explanation uneven change of CO_2 and CO mass ratios in exhaust gases gas at different mass ratios of oxygen in the fresh charge has been the one of the most important tasks in the work.

One of the main tasks of the research tests of the combustion process of the oxygen-enriched charges was the determination of dependencies between oxygen excess ratio λ_{O_2}, EGR ratio and mole fractions of the main compounds in gas products at constant λ_{O2}. The paper introduces results of calculation of combustion process of the mixture containing only O_2, fuel at stoichiometric value and exhaust gases as rest of the charge. Such mixture was determined as the charge with 100% EGR, because of existence of maximum exhaust gases in whole charge.

3. Experimental test

The experimental work was done on the liquid cooled 2-cylinder 4-stroke spark ignition SPI engine Honda GX360 (S/D=58/68) with cylinder capacity 180 cm^3 at constant speed of 3000 rev/min. The initial results of experimental tests were presented in the paper [11]. Operating engine parameters are as follows: maximum power 9.2 kW/3600 rpm and maximum torque 26 Nm/3000 rpm. The simplified diagram of the experimental stand is shown in Fig. 1.

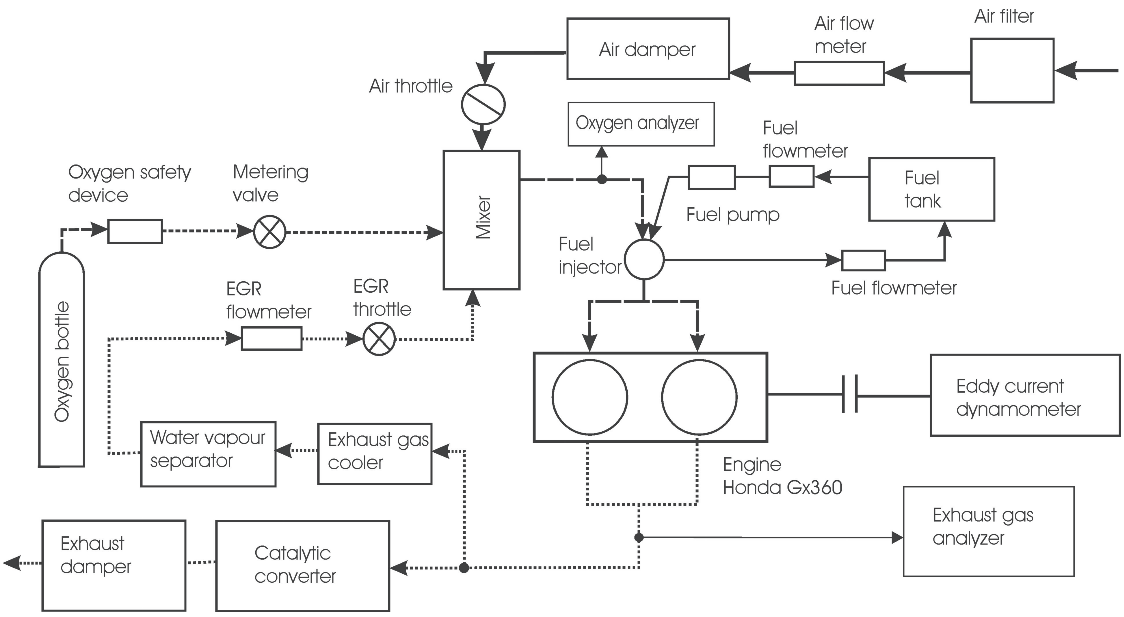

Fig. 1. Scheme of laboratory stand without electronic control system

The exhaust gases in the system passed through the drainage system in order to remove water vapours from EGR and their concentrations have been measured by Horiba analyser. The mass flow rate of exhaust gases was measured by a special measuring system including the volume fraction of exhaust gas components CO, CO_2, HC and NOx. The defined oxygen volumetric ratio x_{O2} in the charge was set in the range of 21 to 32%. The EGR ratio in the tests was determined as follows:

$$EGR = \frac{m_{exh}}{m_c - m_{O_2} - m_f}, \tag{1}$$

where m_{exh} is the mass of exhaust gases from EGR system, m_c is the total mass of the fresh charge entering into the cylinder, m_{O2} is the oxygen mass and m_f is the fuel mass. The charge consisting O_2 and changeable portion of the added exhaust gases from previous working cycles and N_2 indicated an increment of CO_2, CO and HC volumetric fractions and decreasing of NO_x content with increasing of EGR ratio, which is presented in Fig. 2. It is caused due to the fact of decreasing of the engine power with increasing of EGR ratio despite of the same amount of the supplied fuel.

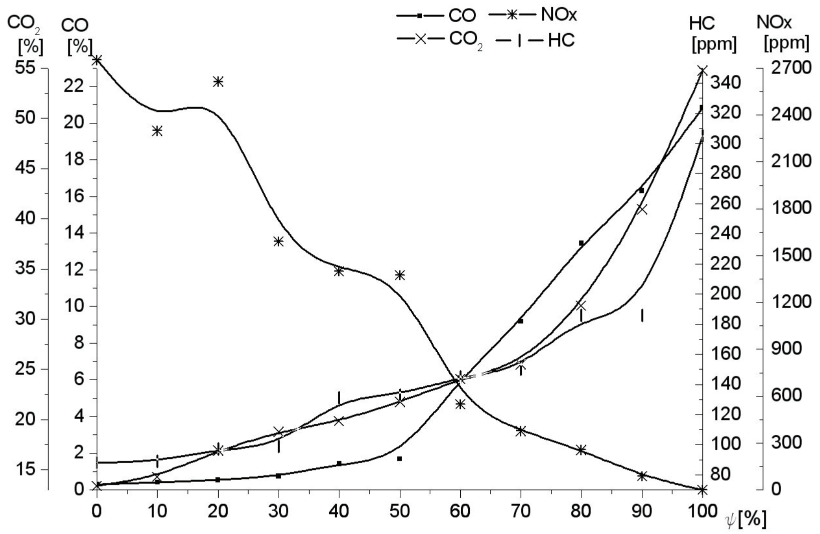

Fig. 2. Volumetric fractions of CO_2, CO and HC in function of changeable EGR ratio at constant x_{O2} = 21% for λ=1.0 at constant engine speed 3000 rpm and constant G_h = 1.5 kg/h

The bigger amount of O_2 in the fresh charge is not utilized during the combustion process. It results on decreasing of CO and HC contents in exhaust gases and on the other hand higher content of CO_2 results from the oxidation of CO (Fig. 3).

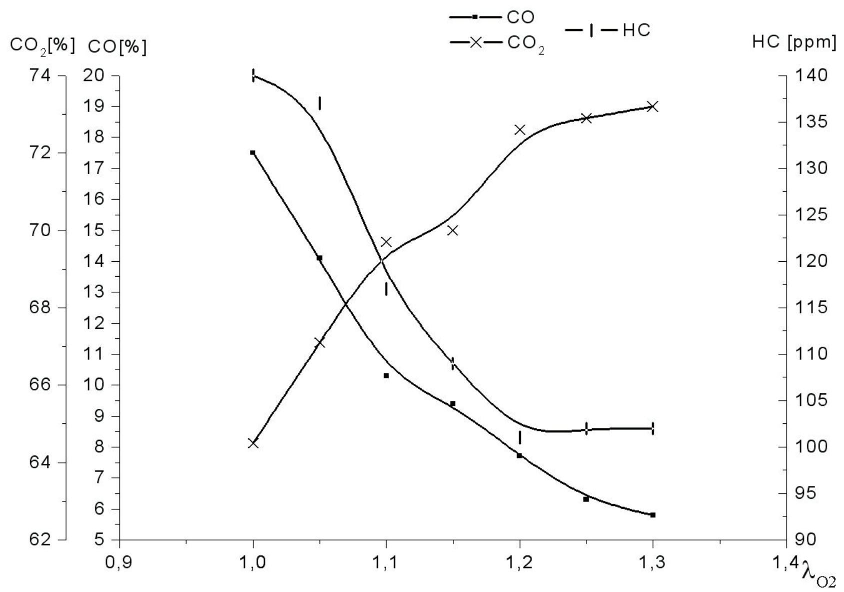

Fig. 3. Volumetric fractions of CO_2, CO and HC in dependence of λ_{O2} at 100% EGR and n=3000 rpm

The increase of λ_{O2} by 30% results in a reduction of mean effective pressure (*mep*) and reduction of useful work by 43% at simultaneous reduction of the *bsfc* (Fig. 4). The increment of amount of O_2 in the charge takes effect also on growing of exhaust gases temperature at the same advance ignition angle 40° CA BTDC.

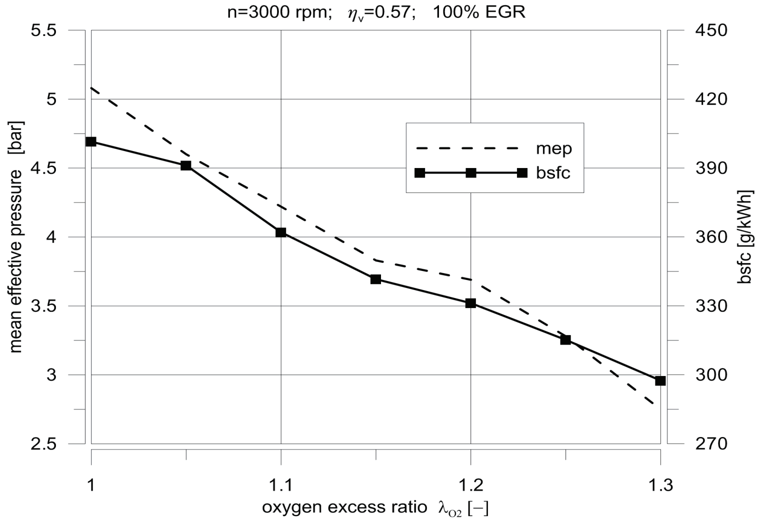

Fig. 4. Influence of λ_{O2} on engine mep and bsfc at n=3000 rpm, η_v =0.57 and 100% EGR

Combustion process in SI engine fed by the charge with the increased O_2 mass ratio in the range 21-31% at constant λ_{O_2} =1.0, where the rest were exhaust gases, indicated irregular variation of CO_2 and CO volumetric fractions (Fig. 5). Despite of proportional increment of the delivered fuel mass and oxygen, the HC volumetric fraction decreases at the same λ_{O2}.

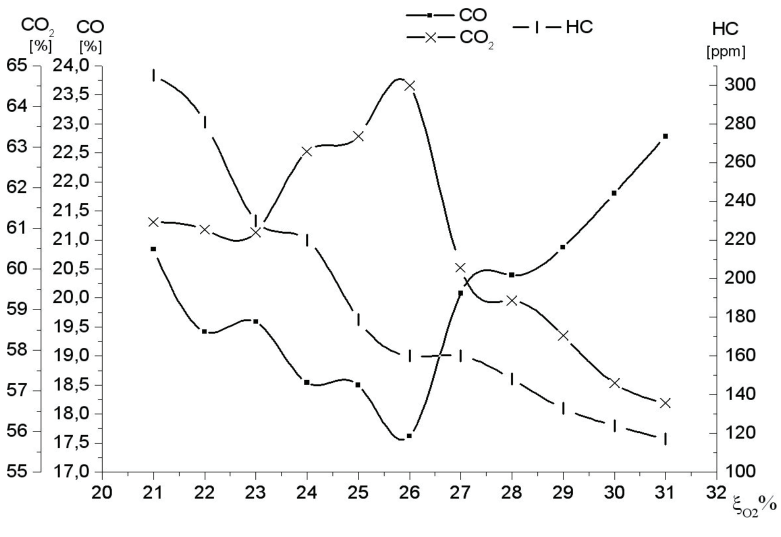

Fig. 5. Volumetric fraction of CO_2, CO and HC at changeable x_{O2} and 100% EGR for λ_{O2}=1.0 at 3000 rpm

It was found the increment of volumetric concentration of CO_2 (about 12%) in the exhaust gases at O_2 volumetric ratio equal 26% in the fresh charge. On the other hand, emission of CO decreases by 15%. Further increasing of oxygen mass ratio causes bigger increment of CO emission and decreasing of CO_2 emission. Volumetric ratio of O_2 in the charge amounting to 26% is a critical value, while at the end of the combustion process the chemical equilibrium reactions between CO_2 and CO take place ($CO + O_2 <-> CO_2$).

4. Simple chemical combustion model

Generally, in 0-dimensional or 2-zones models of combustion process in the piston engines the kinetic reactions are not taken into account. Generally, in the popular KIVA program [1] applied in calculation of combustion processes of ICE four kinetic reactions are assumed in simulation of gasoline burning according to the general chemical formula C_8H_{17}:

1. equation of gasoline combustion:

$$4\ C_8H_{17} + 49\ O_2 \Leftrightarrow 32\ CO_2 + 34\ H_2O, \tag{2}$$

2. equation of NO formation according to Zeldovich mechanism:

The elementary reversible and irreversible reactions were considered with adequate Arrhenius coefficients for calculations of burning of the gasoline and they were included in Kiva3v program. Besides the kinetic reaction in the program Kiva3v, also the dissociation reactions were taken into account, which occur during the expansion stroke at high temperature above 2000 K. The mesh was created internally by program and the model contained 54500 hexagonal cells. The simulation was carried out after closing of inlet valve. The standard Arrhenius constants were adopted in the kinetic reactions.

5. CFD simulation of combustion process

The analysis of combustion process in Kiva3v program was carried out for three oxygen mass ratios at rotational speed 3000 rpm as in the experimental tests. The premixed combustion model was taken into account for different oxygen mass ratios. Heat transfer with changeable thermal conductivity dependent on charge temperature and with constant temperature of the walls was applied. The kinetic reactions take place in the moving flame as a result of diffusion. Simulation process began after closing of the inlet valve at 50 deg ABDC with initial cylinder pressure 0.096 MPa and temperature 495 K. Mass fractions of chemical compounds in the charge delivered to the cylinder are presented in Tab. 1.

Tab. 1. Mass fractions of chemical compounds in fresh charge

Volumetric ratio of O_2 [%]	Mass ratio				
	O_2 [-]	fuel [-]	CO_2 [-]	CO [-]	H_2O [-]
21	0.233	0.0671	0.500	0.121	0.0789
26	0.288	0.0832	0.508	0.09	0.0308
31	0.341	0.098	0.45	0.108	0.003

Figure 6 presents variation of cylinder pressure in a function of crank angle (CA) for three values of the volumetric ratio of oxygen. For higher mass ratio of oxygen in the charge, the higher maximum of pressure is reached in the cylinder. The higher oxygen mass ratio in the charge influences also on the increase of combustion temperature in the cylinder. Simulation was carried out at the same ignition parameters (energy and ignition point).

Variation of CO volume fraction in the cylinder during combustion process as shown in Fig. 7a is depended on amount of exhaust recirculation gases and x_{O2}. Big mass fraction of CO, delivered to the cylinder by EGR system, is very fast consumed during first stage of the combustion process after ignition. The oxidation of CO is faster than oxidation of the fuel. For that case the amount of oxygen should be higher in order to oxidation both the fuel and CO. The water is formed during combustion process and thus CO volume fraction in the charge is decreased after this process in comparison to the initial stage. Participation of the water in the charge after burning of the fuel influences also on volume fraction of another exhaust gas components. At highest temperature a maximum of mass ratio of CO is reached. Later the oxidation of CO occurs. Formation of CO is connected with the equilibrium reactions where CO_2 decomposes on CO and O. Like in the

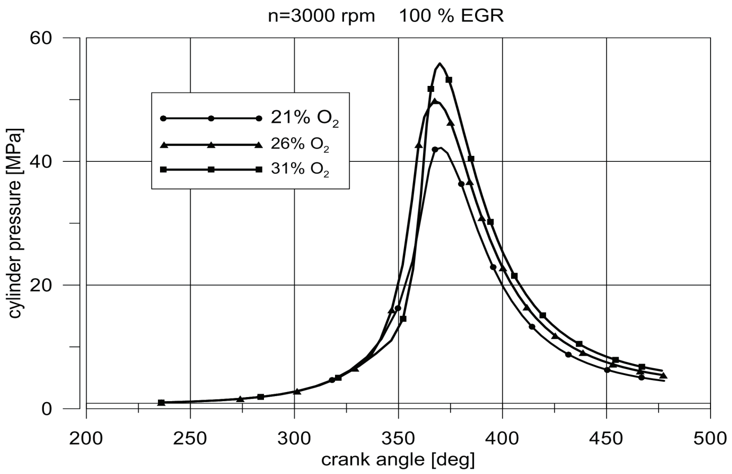

Fig. 6. Pressure traces in cylinder at different mass oxygen ratios and 100% EGR

experiment at x_{O2} = 26% the simulation indicated lower emission of CO, where mass fraction of CO_2 in EGR system amounted 64.51%. For this case, lower amount of O_2 was needed for oxidation of CO. The decomposition of CO_2 runs significantly slower during the expansion stroke. For middle range of the oxygen mass fraction in the fresh charge the lower values of volumetric fraction of CO are obtained. On the other hand, the volumetric fraction of CO_2 is higher for middle range of the oxygen mass fraction in the fresh charge as shown in Fig. 7b. Because the fuel is consumed fully while the combustion process, therefore, the change of volumetric fraction CO and partly CO_2 is caused by the dissociation process. Volumetric fraction of CO_2 reaches maximum values close before opening of the exhaust valve.

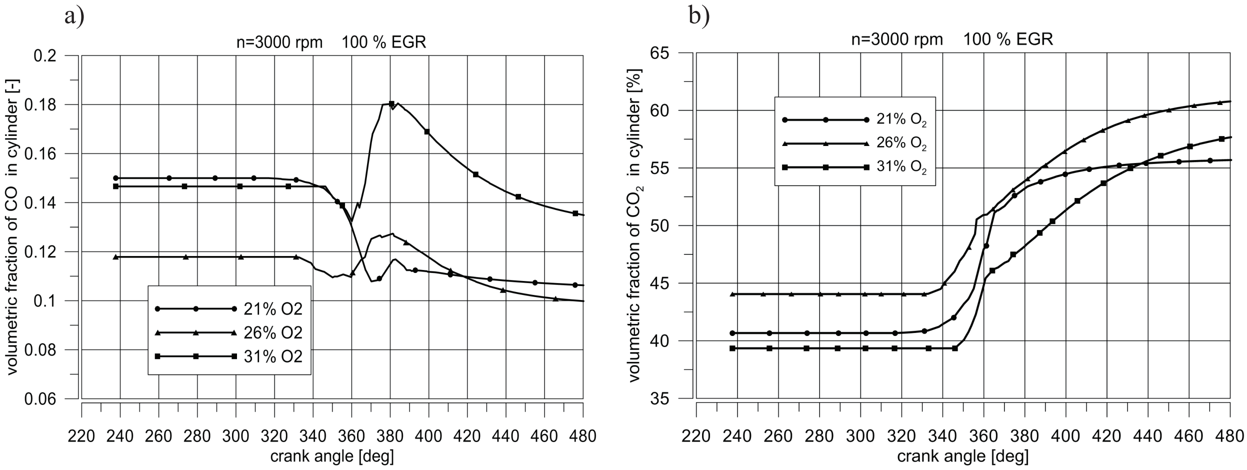

Fig. 7. Volumetric fraction of a) CO and b) CO_2 in cylinder at different volumetric oxygen ratios and 100% EGR

6. Detailed kinetic reactions

Combustion of the typical engine fuels should be modelled by participation of about 600 chemical compounds and several thousand kinetic reactions. The authors used academic version of the program Kintecus ver. 3.95 [5], which takes into account 0-D model. Thermochemical properties and the extended chemical mechanism were given by Curran *et al* [3], Westbrook [13] and Ranzi *et al* [9]. The chemical mechanism was adapted for this work by reduction of number of reactions. However, this model was extended by adding the additional model of nitrogen oxides formation, which was taken from GRIMECH [16] with 858 species and 3627 chemical reactions.

The program enables the change of volume and heat transfer in a function of time and calculates every time step the volumetric molar concentration of the individual species in unit of mole/cm^3. The fuel was treated as a mixture of two hydrocarbons: C_8H_{18} and n-heptane in proportion to octane number of gasoline (RON=95) and its initial molar concentration was given for every case like as for the other species: O_2, CO, CO_2 and water. Initial values of mole fractions of the chemical compounds entering to the cylinder as EGR (such as CO, CO_2 and H_2O), fuel and O_2 were assumed according to the experimental data achieved for different volumetric ratios of O_2. The calculation program assumed the combustion process beginning in the whole volume. At higher volumetric fraction of O_2 in the inlet charge, the higher maximal gas temperature occurs and this higher value takes place during expansion process. The increase of temperature is almost proportional to the volumetric fraction of O_2 in the inlet mixture. It is caused by bigger amount of fuel in the mixture at the same $\lambda_{O2} = 1.0$. The radical of 1-atom H have been formed as a result of reaction $CO+OH \Leftrightarrow CO_2+H$ and by chemical reactions $OH+H_2 \Leftrightarrow H+H_2O$ and $O+H_2 \Leftrightarrow H+OH$. The simulation of combustion of the enriched oxygen mixtures with 100% EGR indicated a certain increase of H_2 after combustion process. The decomposition of CO_2 in the charge (EGR) into CO and O in the reaction $CO_2 \Leftrightarrow CO + O$ takes place for an early stage of combustion process. At highest combustion temperature, the mole fraction of CO_2 decreases (Fig. 8) and mole fraction of CO rapidly increases (Fig. 9).

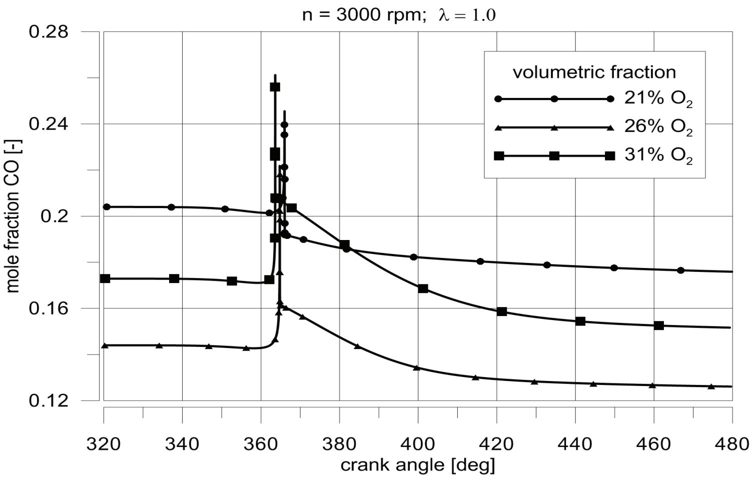

Fig. 8. Mole fraction ratio of CO in the cylinder at x_{O2} = 21, 26 and 31%, 100% EGR, λ_{O2}=1.0, n=3000 rpm

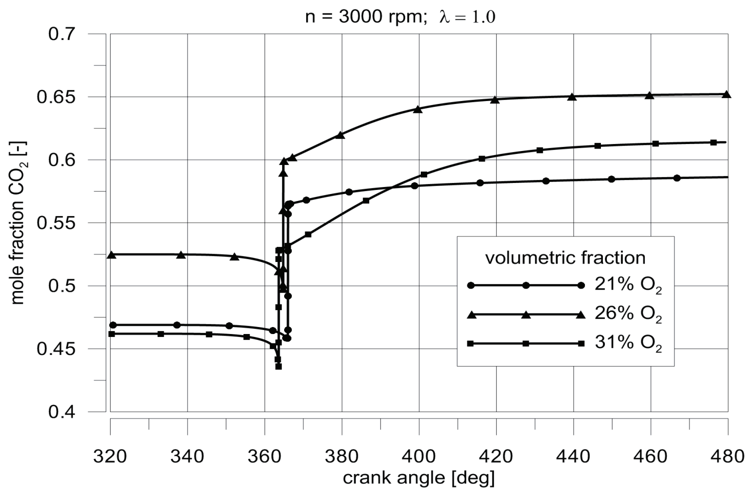

Fig. 9. Mole fraction ratio of CO_2 in the cylinder at x_{O2}=21, 26 and 31%, 100% EGR, λ_{O2}=1.0, n=3000 rpm

The amount of CO decreases slightly during expansion process and amount of CO_2 increases. Lowest mole fraction of CO (0.128) and highest mole fraction of CO_2 (0.65) was obtained for the fresh charge containing 21% O_2 and the rest was constituted by EGR. The charge with 31% O_2

after the combustion process gives the medium values of CO and CO_2 mole fraction in the exhaust gases. For the three mixtures, the mole fractions of CO have lower values than in the fresh charge. On the other hand, mole fractions of CO_2 in the burned charge are higher than in the fresh charge. Such combustion process influences on formation of the free oxygen O and other radicals.

7. Conclusions

The presented work concerns only to the charge deprived of nitrogen, however with the high EGR ratio and at stoichiometric conditions in relation to oxygen. The advance ignition angle was extended at lower value of oxygen mass ratio in the fresh charge.

1. The engine filled with the high EGR ratio emits also high amount of hydrocarbons (Fig. 2).
2. The change of molar concentration of CO and CO_2 during combustion process is dependent on the running of dissociation process (forward and reverse reaction) and diffusion process.
3. Higher initial volumetric fraction of oxygen at constant λ_{O2} causes higher cylinder pressure and also higher internal work and such way of fuelling substitutes the charging system.
4. The test showed the necessity of increasing of advance ignition angle at higher EGR ratio and lower oxygen mass fraction in the fresh charge.
5. Rapid variation of the pressure and temperature occurs during kinetic reactions, where a sudden change of CO molar concentration occurs.
6. Simulation of kinetic chemical reactions has indicated that after combustion of the assumed mixtures a big amount of hydrogen exists in the gas products, which has not been measured during the experimental tests.
7. For the mixtures with x_{O2} = 26% the lower mole fraction of CO and higher mole fraction of CO_2 has occurred in the charge after combustion process than in other two considered cases.

Simulation models were designed to explain the results of experimental studies and validation will be published in next paper and cannot be given here in respect to limitation of this paper.

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