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CFD modelling of combustion in HCCI engine using avl fire software

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Abstract. HCCI (Homogenous Charge Compression Ignition) combustion system is now one of the most promising solutions used in piston engines. The paper presents the results of three-dimensional modeling of combustion in the single-cylinder HCCI engine powered with Diesel fuel. 3D modeling was performed in AVL Fire code. The basic combustion parameters including start of the ignition (SOI), burn duration (BD), indicated pressure (pi) and nitric oxide (NO) and soot (Soot) emissions were analyzed. The modeling results show that combustion process in HCCI engine compared to a conventional engine with compression ignition is characterized by an earlier ignition (SOI) and shorter burn duration (BD). The impossibility of controlling HCCI combustion process leads to deterioration of engine performance and increased emissions of harmful exhaust gas components. Calculations showed that for the same equivalence ratio of burn mixture, uncontrolled HCCI combustion compared to a controlled combustion in engine with fuel injection operated is characterized by higher NO emission and reduced Soot emission.

Key words: homogenous charge compression ignition (HCCI), exhaust gas recirculation (EGR), heat release rate (HRR), start of the ignition (SOI), burn duration (BD), injection timing (IT), conventional compression ignition engine (CI), indicated pressure (pi), nitric oxide (NO).

INTRODUCTION

HCCI (Homogenous Charge Compression Ignition) combustion system is now one of the most promising solutions used in piston engines. It combines the best features of spark ignition engines and compression ignition engines, and is characterized by low NO_x and PM emissions and high efficiency. So far conducted research on HCCI engine not solved the problem of control of moment of autoignition of homogeneous mixture supplied to engine and duration of the combustion process. The presented work concerns the numerical study of the combustion process of homogeneous mixtures in HCCI engine. The basic combustion parameters including start of the ignition (SOI), burn duration (BD), indicated pressure (p_i) and nitric oxide (NO) and soot (Soot) emissions were analyzed. Modelling in the AVL Fire was carried out. The aim of modelling was to get acquainted with the course of HCCI combustion process and compare the basic parameters of the uncontrolled HCCI combustion with controlled combustion in a conventional engine with compression ignition.

THE EXISTING STATE OF RESEARCH

Development works on combustion, emissions of harmful exhaust gas components and controlled autoignition in HCCI system s well as application of the system in a real engine are conducted in many research centers and universities around the world. The work [1] briefly describes the history of origin, worldwide research work results, advantages and problems following from specific combustion process, typical for HCCI engines which are so different from the well known and widely used spark and diesel engines. More than twenty years left since the HCCI concept was first proposed and demonstrated and steady progress has been made in developing the technology. Previous and current research works in the world have indicated that the engine working in HCCI mode can be supplied by means of different fuels at extremely low emissions and high efficiencies. Homogeneous charge compression ignition (HCCI) engine technology has received increasing attention in recent years due to its intrinsic benefits in terms of high efficiency and low NO_x and Soot emissions [2]. However, unresolved issues include combustion phasing (i.e., the control of the start and duration of combustion), high carbon monoxide and unburnt hydrocarbon emissions, limited load-speed operating window, and transition to spark-ignited combustion at high loads. Several strategies for mixture control have been devised and are currently being considered to help overcome these difficulties. These include diverse fuel injection schemes such as port fuel injection and single or multistage direct injection (DI or MDI), as well as external exhaust gas recirculation (EGR), variable valve timing, and variable compression ratio. Homogeneous charge compression ignitron (HCCI) is nowadays a leading trend in the development of gasoline internal combustion engines. The application of this novel combustion system will allow for compliance with future legislations concerning the exhaust emissions including carbon dioxide. The paper [3] presents a design and implementation of a research engine with a direct fuel injection and the capability of HCCI combustion via an internal gas recirculation and negative valves overlap (NVO). The technical approach used in the engine allowed and autonomous HCCI operation at variable loads and engine speed without the need of a spark discharge. Experiments were conducted at a wide range of valve timings providing data which allowed as assessment of a volumetric efficiency and exhaust gas recirculation (EGR) rate. Permissible range of air excess coefficient, providing stable and repeatable operation has also been identified. The use of direct gasoline injection benefited in the improvement of the start of the combustion (SOC) and heat release rate control via the injection timing. The objectives of the study [4] is to clarify ignition characteristics, the combustion process, the knock limit and the misfire limit of natural gas mixed with a small amount of dimethyl ether (DME) in a HCCI engine. In the combustion test, natural gas and small amount of DME were charged into the suction air homogeneously. The equivalence ratio of natural gas was increased to find the knock limit or the misfire limit of the HCCI test engine under a constant DME amount. The effect of the natural gas addition on suppression of the low temperature reaction of DME, and the effects of the DME amount and the intake temperature on the reaction rates, the knock limit of the DME/natural gas mixture, and the operation load range of the HCCI engine were investigated experimentally. The paper [5] presents results of the research carried out on the impact of initial temperature and combustible mixture composition on work of engine based on the HCCI principle. The researchers found that there is a specific value of the mixture initial temperature (approximately 200°C). When it is reached, further temperature rise does not cause any distinct increase of combustion process maximum pressure, pressure buildup rate and self-ignition delay. This initial temperature value slightly depends on combustible mixture composition. Work [6] investigates the basic combustion parameters including start of the ignition, burn duration, cycle-to-cycle variation, and carbon monoxide (CO), unburned hydrocarbon (UHC), and nitric oxide (NO_x) emissions of homogeneous charge compression ignition engines fueled with primary reference fuels and their mixtures. Two primary reference fuels, n-heptane and iso-octane, and their blends were evaluated. The experimental results show that, in the first-stage combustion, the start of ignition retards, the maximum heat release rate decreases, and the pressure rising and the temperature rising during the first-stage combustion decrease with the increase of the research octane number. Furthermore, the cumulative heat release in the first-stage combustion is strongly dependent on the concentration of n-heptane in the mixture. The start of ignition of the second-stage combustion is linear with the start of ignition of the first-stage. The combustion duration of the second-stage combustion decreases with the increase of the equivalence ration (inverse of the excess air factors) and the decrease of the octane number. The cycle-to-cycle variation improved with the decrease of the octane number. In [7], which is a continuation of [6], the influence of exhaust gas recirculation (EGR) rate, intake charge temperature, coolant temperature, and engine speed on the HCCI combustion characteristics and its emissions were evaluated. The experimental results indicate that the ignition timing of the first-stage combustion and second-stage combustion retard, and the combustion duration prolongs with the introduction of cooled EGR. At the same time, the HCCI combustion using high cetane number fuels can tolerate with a higher EGR rate, but only 45% EGR rate at 1800 rpm. Furthermore, there is a moderate effect of EGR rate on CO and UHC emissions for HCCI combustion engines fueled with n-heptane, but a distinct effect on emissions for higher octane number fuels. Moreover, the combustion phase advances, and the combustion duration shorten with the increase of intake charge temperature and the coolant out temperature, and the decrease of the engine speed. At last, it can be found that the intake charge temperature gives the most sensitive influence on the HCCI combustion characteristics.

In this paper, by using the advanced combustion simulation package AVL Fire, HCCI combustion process in test engine were investigated and analyzed numerically. The basic combustion parameters including start of the ignition timing (SOI), burn duration (BD), indicated pressure (p_i) and nitric oxide (NO) and soot emissions (Soot) of a single-cylinder (HCCI) engine powered with diesel fuel were analyzed.

In recent years the numerical modelling investigations using more and more advanced mathematical models have been intensively developing. The development of numerical modelling is reinforced with increasing computational power that allows modelling of not only flow processes but also combustion in 3D [8, 13]. One of more advanced numerical models used for combustion process in piston engines modelling is AVL Fire [14]. In 2009 Institute of Thermal Machinery of Czestochowa University of Technology began University Partnership Program with AVL List GmbH Company and to modelling thermal cycle of IC engines using AVL Fire software [15, 21]. The Fire software belongs to contemporary programs which are used for modelling of thermal cycles of internal combustion engines. AVL Fire allows modelling of a flow and thermal processes that occur in the intake manifold, the combustion chamber of IC engine and the exhaust pipe with a catalyst and a particulate filter. This programme enables the calculation of transport phenomena, mixing, ignition and turbulent combustion in internal combustion engine. Homogeneous and inhomogeneous combustion mixtures in spark ignition and compression ignition engines can be modeled using this software as well. The kinetics of the chemical reactions phenomena is described by combustion models that take into account the oxidation processes in high temperatures. Several models apply to auto ignition processes including HCCI combustion. AVL Fire allows modelling of knock processes that occurs in the combustion chamber of IC engine. This program allows building three-dimensional computational grids, characterizes the boundary conditions of surfaces and initial conditions of simulation. The postprocessor gives a possibility to visualize the results.

TEST ENGINE AND MODEL ASSUMPTIONS

Modelling of the thermal cycle of the HCCI engine in the AVL Fire program was carried out. The object of the investigations was a modernized diesel engine 1hc102 Andoria fueled with diesel fuel. As a result of the modernization the shape of the combustion chamber was modified. The compression ratio has not changed and was equal to 17.5. The engine was operated at a constant speed of 1800 rpm. The engine is a stationary, two-valve unit with a horizontal cylinder configuration. The cooling system of engine is the evaporation of the water jacket. Table 1 presents the main engine parameters, initial conditions and Fire sub-models.

Table 1. Modelling parameter

Engine parameters	
Type	Water-cooled, 4 stroke
Number of cylinder	1
Displacement volume	918 cm^3
Engine speed	1800 rpm
Bore×stroke	100×120 mm
Connecting-rod length	216 mm
Squish	2.5 mm
Compression ratio	17.5:1
Injection timing (conventional engine)	14,12,10, 8, 6 deg BTDC
Initial conditions	
Initial pressure for 180 deg BTDC	0.9 MPa
Initial temperature for 180 deg BTDC	340 K
Equivalence ratio	0.5
Fuel	Diesel
AVL Fire sub-models	
Turbulence model	k-zeta-f
Combustion models	Eddy Breakup Model
Ignition models	Diesel (conventional engine CI) HCCI Shell Model (HCCI engine)
NO formation model	Extended Zeldovich Model
Soot formation model	Frolov Kinetic Model

On the basis of the real dimensions of the experimental engine a three-dimensional mesh of engine combustion chamber was built (Figure 1). The mesh of the modeled combustion chamber of the 1hc102 modernized test engine consisted of nearly 32000 computation cells. Two-layered wall boundary layer was considered.

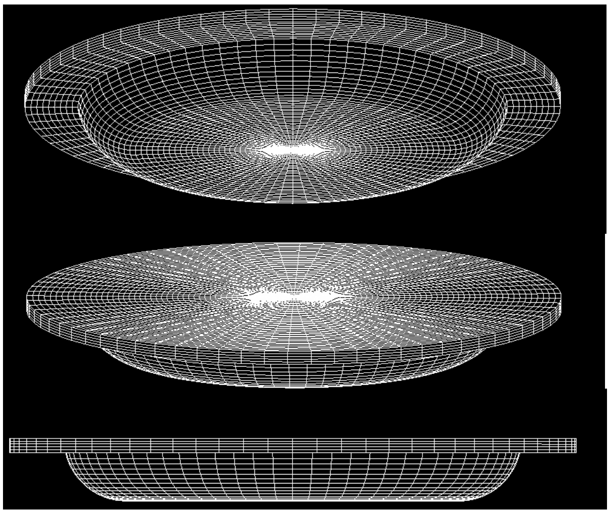

Fig. 1. The computational mesh for combustion chamber of the test engine

Computations were conducted for the angle range from 180 deg before top dead centre (BTDC) to 180 deg after top dead centre (ATDC). Calculations included the study of a HCCI engine and conventional compression ignition engine CI. HCCI engine and conventional engine was fueled with a mixture of diesel-air equivalence ratio of 0.5. The modelling of a conventional combustion process was conducted for five of injection timing: 14, 12, 10, 8 and 6 deg before top dead center for which there was no knock combustion [22, 26]. HCCI combustion process was not controlled and preceded spontaneously. On the basis of the pressure data obtained from modeling indicated pressure p_i was calculated. The indicated pressure is one of the parameters determining the performance of a combustion engine. The calculated indicated pressures do not include certain losses both in the combustion process as well as the flow losses and blow-bys.

RESULTS OF CALCULATION

Figure 2 shows a comparison history of diesel fuel combustion between the HCCI engine and conventional compression ignition engine CI. Some basic combustion parameters of the combustion process in HCCI and conventional engine CI are also shown in this figure. HRR_{max} is defined as the maximum value of heat release rate in combustion process. The timing of SOI (start of ignition) is defined as that point on the HRR graph at which the rate of heat release rate exceeds 0.5 J/deg, as shown in Figure 2 [27]. The BD (burn duration) is defined as the combustion duration, which is the distance between the crank angle of SOI and crank angle corresponding to

20% of the magnitude of peak of heat release rate on the falling side of the curve [6]. Characteristics show a large difference between the HCCI engine and a conventional engine in the ignition timing, maximum heat release rate, maximum pressure and temperature. In the case of the conventional engine, the ignition occurs near TDC because the ignition timing can be controlled by the fuel injection timing, while, in the case of the HCCI engine which does not have a mechanism to control combustion, the ignition occurs earlier than in the case of the conventional compression ignition engine.

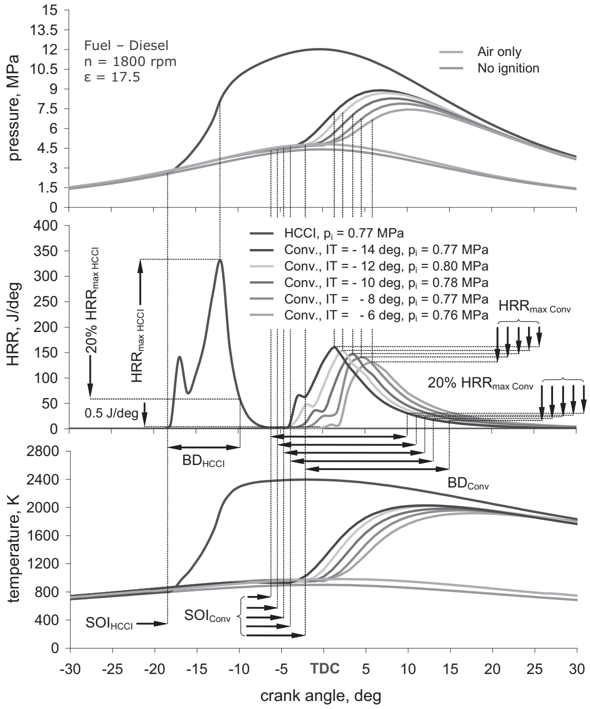

Fig. 2. Comparison of the history of the diesel fuel combustion between HCCI and conventional compression ignition engine CI

As shown in the heat release curves, diesel fuel in HCCI clearly shows two-stage combustion phenomena, that is, the low-temperature reaction and high-temperature reaction. The two-stage combustion mechanism is typical of diesel fuel and also occurs with lighter fuels, such as kerosene. In the case of this type of combustion, at 760 - 880K, about (5-15) deg CA before principal and fast heat release, cold blue flames appear and preliminary heat release occurs [29]. The results of modelling show that for a conventional engine powered by mixture of er = 0.5, the most optimal of injection timing angle (IT) is angle equal to 10 deg before TDC. For this injection angle the maximum indicated pressure achieved equals to 0.78 MPa. In the HCCI engine, with er = 0.5, the maximum indicated pressure achieved similar value equals to 0.77 MPa. Figure 2 and Table 2 shows, that combustion process in HCCI engine compared to a conventional engine is characterized by an earlier ignition (SOI) and shorter burn duration (BD).

Table 2. Selected results of the modeled combustion process

	IT deg	p_i MPa	SOI deg	BD deg	NO_x ppm	Soot mg/m^3
Conv.	-14	0.77	-7	17	425	1.25
Conv.	-12	0.80	-6	17	380	4.28
Conv.	-10	0.78	-5	18	358	6.45
Conv.	-8	0.77	-4	19	327	9.63
Conv.	-6	0.76	-2	19	285	16.58
HCCI	-	0.77	-18	9	1067	1.5e-06

Temperature distribution in the working area of conventional CI engine and HCCI engine for er = 0.5 is depicted in Figure 3. At 8 deg before TDC in conventional engine is realized ignition of diesel fuel injected. At the same time, in HCCI engine, the combustion process is already taking place in the entire volume of the combustion chamber.

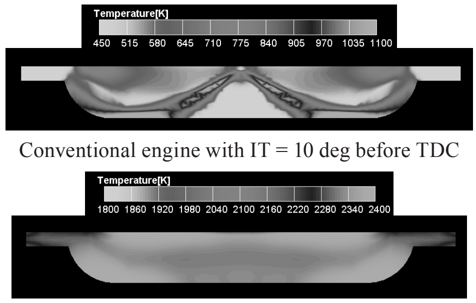

Fig. 3. Temperature distribution in combustion chamber of the conventional CI engine and HCCI engine for er = 0.5 at 8 deg before TDC

HCCI engine characterized by a higher NO emissions and lower Soot emissions compared to conventional engine CI (Table 2, Figure 4 and 5). Uncontrolled HCCI combustion is characterized by higher emission of the nitric oxide and lower emissions of the soot than it is in the case of a controlled combustion in a fuel injected engine.

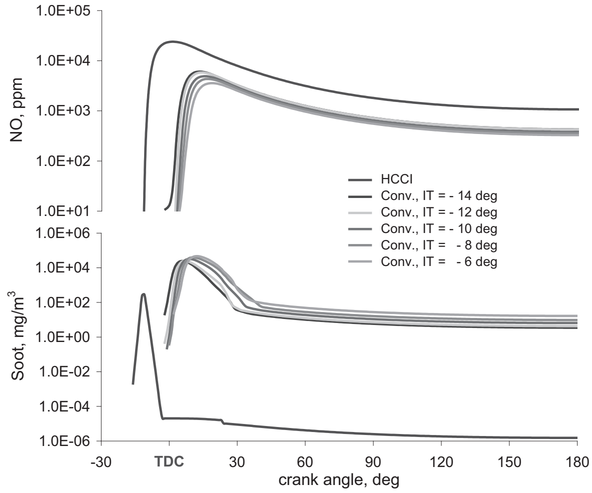

Fig. 4. Nitric oxide and Soot emission of conventional CI engine in comparison with emission of HCCI engine

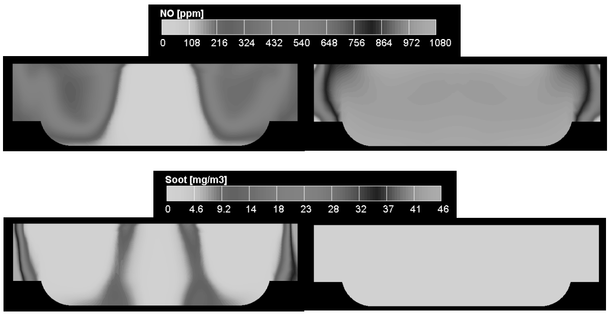

Fig. 5. NO and Soot concentration in combustion chamber of conventional CI engine and HCCI engine for er = 0.5 at 40 deg after TDC

CONCLUSIONS

This paper discussed the effect of EGR rate on HCCI combustion parameters and NO emissions. Based on these discussions, some conclusions may be drawn.

1. HCCI combustion process compared to a conventional compression ignition engine is characterized by an earlier ignition (SOI) and shorter burn duration (BD).
2. Compared to the CI engine, too early ignition of uncontrolled HCCI combustion leads to an increase in the maximum values of pressure, temperature and heat release rate in the cylinder. Higher pressures, however, cause no increase in indicated pressure (p_i), which is the utility parameter and shows the engine performance.
3. Uncontrolled HCCI combustion is characterized by higher emission of the nitrogen oxide (NO) and lower emission of the soot (Soot) than it is in the case of a controlled combustion in fuel injected engine.
4. Control of ignition and combustion process in HCCI engine can be an effective method of reducing emissions of NO [30]. The most commonly used systems of HCCI process control include Variable Valve Timing (VVT), external and internal EGR, Variable Compression Ratio (VCR) and a system of cooling and heating of inlet charge.

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REFERENCES

1. **Motyl K., Rychter T. 2003.** *HCCI engine – a preliminary analysis*. „Journal of Kones", vol. 10, p. 3–4.
2. **Fabrizio Bisetti, J.-Y. Chenb, Evatt R. Hawkes, Jacqueline H. Chen. 2008.** *Probability density function treatment of turbulence/chemistry interactions during the ignition of a temperature-stratified mixture for application to HCCI engine modeling*. „Combustion and Flame", vol. 155, p. 571–584.
3. **Hunicz J., Niewczas A., Kordos P. 2010.** *A reseaech into a gasoline HCCI engine*. „Combustion engines", No. 1/2010 (140), p. 3–13.
4. **Ishida M., Jung S., Ukei H., Sakaguchi D. 2005.** *Combustion of premixed DME and natural gas in a HCCI engine*. „Combustion engines", No. 2/2005 (121), p. 20-29.
5. **Motyl K., Lisowski A. 2008.** *Wpływ temperatury początkowej i składu mieszaniny palnej na pracę silnika HCCI zasilanego biogazem*. „Inżynieria Rolnicza" 1(99)/2008, p. 311–317.
6. **Lu X.C., Chen W., Huang Z. 2005.** *A fundamental study on the control of the HCCI combustion and emissions by fuel design concept combined with controllable EGR. Part 1. The basic characteristics of HCCI combustion*. „Fuel", 84, p. 1074–1083.
7. **Lu X.C., Chen W., Huang Z. 2005.** A fundamental study on the control of the HCCI combustion and emissions by fuel design concept combined with controllable EGR. Part 2. Effect of operating conditions and EGR on HCCI combustion. „Fuel" ,84, p. 1084–1092 .
8. **Jamrozik A., Kociszewski A., Sosnowski M., Tutak W. 2006.** Simulation of combustion in SI engine with prechamber. „CADMD'2006", Ukraine, p. 66–69.
9. **Jamrozik A., Tutak W., Kociszewski A., Sosnowski M. 2006.** *Numerical Analysis of Influence of Prechamber Geometry in IC Engine with Two-Stage Combustion System on Engine Work Cycle Parameters*. „Journal of Kones". Vol 13, No 2, p. 133–142.
10. **Tutak W., Jamrozik A., Kociszewski A., Sosnowski M. 2007.** *Numerical analysis of initial swirl profile influence on modeled piston engine work cycle parameters*. „Combustion engines", 2007-SC2, p. 401–407.
11. **Kociszewski A., Jamrozik A., Sosnowski M., Tutak W. 2007.** *Simulation of combustion in multi spark plug engine in KIVA-3V*. „Combustion engines". 2007-SC2, p. 212–219.
12. **Tutak W. 2009.** *Modelling of Flow Processes in the Combustion Chamber of IC Engine*. „MEMSTECH'2009", Ukraine. p. 45–48.
13. **Tutak W. 2008.** *Thermal Cycle of Engine Modeling with Initial Swirl Process into Consideration*. „Combustion Engines", 1/2008 (132), p. 56–61.
14. AVL Fire version 2009, *ICE Physics & Chemistry, Combustion, Emission, Spray, Wallfilm*. „AVL LIST GmbH".
15. **Jamrozik A., Tutak W. 2010.** *Modelling of combustion process in the gas test engine*. „MEMSTECH 2010". p. 14–17.
16. **Tutak W., Jamrozik A. 2010.** *Numerical analysis of some parameters of gas engine*. „Teka Polish Academy of Science Branch Commission of Motorization and Power Industry in Agriculture", Volume X, p. 491–502.
17. **Tutak W., Jamrozik A. 2010.** *Modelling of the thermal cycle of gas engine using AVL Fire Software*. „Combustion engines", No. 2/2010 (141), p. 105–113.
18. **Tutak W. 2011.** *Possibility to reduce knock combustion by EGR in the SI test engine*. „Journal of Kones", No 3, p. 485–492.
19. **Tutak W. 2011.** *Numerical analysis of the impact of EGR on the knock limit in SI test engine*. „Teka Polish Academy of Science Branch Commission of Motorization and Power Industry in Agriculture", T11, p. 397–406.
20. **Tutak W. 2011.** *Numerical analysis of some parameters of SI internal combustion engine with exhaust gas re-*

circulation. „Teka Polish Academy of Science Branch Commission of Motorization and Power Industry in Agriculture, T11, p. 407–414.

21. **Cupiał K., Tutak W., Jamrozik A., Kociszewski A. 2011.** *The accuracy of modelling of the thermal cycle of a self-ignition engine*. „Combustion engines", No. 1/2011 (144), p. 37–48.
22. **Naber J.D., Szwaja S. 2007.** *Statistical approach to characterize combustion knock in the hydrogen fuelled SI engine*, „Journal of Kones", vol. 14, No. 3, p. 443–450.
23. **Szwaja S. 2009.** *Hydrogen rich gases combustion in the IC engine*. „Journal of Kones", vol. 16, No.4, p. 447–455.
24. **Szwaja S. 2009.** *Time-frequency representation of combustion knock in an internal combustion engine*, „Combustion Engines", PTNSS-2009-SC-132, p. 306–315.
25. **Szwaja S. 2009.** *Combustion Knock - Heat Release Rate Correlation of a Hydrogen Fueled IC Engine Work Cycles*, „9th International Conference on Heat Engines and Environmental Protection. Proceedings", Hungary.
26. **Cupiał K., Szwaja S. 2010.** *Producer gas combustion in the internal combustion engine*, „Combustion Engines", No. 2/2010, p. 27–32.
27. **Inagaki K., Fuyuto T., Nishikawa K., Nakakita. 2006.** *Combustion system with premixture – controlled compression ignition*. „R&D Review of Toyota" Vol. 41, No. 3, p. 35–46.
28. **Ishida M., Jung S., Ukei H., Sakaguchi D. 2005.** *Combustion of premixed DME and natural gas in a HCCI engine*. „Combustion engines", No. 2/2005 (121), p. 20–29.
29. **Hunicz J., Niewczas A., Kordos P. 2010.** *A research into a gasoline HCCI engine*. „Combustion engines", No. 1/2010 (140), p. 3–13.
30. **Jamrozik A. 2011.** *Numerical study of EGR effects on the combustion process parameters in HCCI engines*. „Combustion engines", No. 4/2011 (147), p. 50–61.