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Combustion process of direct injected water-coal mixture in diesel engine

The paper describes the problem of coal-water mixture combustion process in heavy duty diesel engines in the energetic sector application. In the future due to depletion of crude oil resources we have to foreseen another fuel for application in power plants. Large deposits of coal and lignite in the world enable to utilize these fuels in different thermal machines, especially in internal combustion engines. A carbon powder containing small molecules about 10–20 micrometers dissolved in water is good fuel for applying in large capacity engines in electrical plants. Aqueous emulsion of coal has possibility of good cooling of injectors cooling and has also good lubricity. Initial experimental tests done in the world indicate a higher thermal efficiency of engine fuelled by water coal emulsion than engine fuelled by diesel oil and also gas turbine driven by gas from coal gasification technology. The increased emission of CO2 can be reduced in the plants simply by chemical reduction. The paper explains thermochemical processes taking place in the engines during combustion process. The work parameters results obtained from calculations were compared with those obtained from CI engine fuelled by diesel oil. The paper is a certain challenge for finding a new fuel sources as a competition for crude oil and allows to get acquainted with new engine fuelling technology.

Key words: *transport, diesel engines, fuelling, water-coal emulsion, combustion*

1. Introduction

Numerous countries in the world are depended on petroleum in energetic sector and in order to be independent in the case of a crude oil crisis many works have been done on heavy duty diesel engines fuelled by coal or water-coal emulsion. The engines are mainly designated for production of electricity working at lower rotational speed (below 1000 rpm). The works done by General Electric on two cylinder test engine fuelled by micronized coal-water-slurry (CWS) with very small diameter of pulverized coal (d < 5 μm) was very successful, but the engine required a new injection system. An application of such engines is possible when a good fuel atomization with good penetration of coal molecules will be assured. The process should enable repeatability and durability of engine parts particularly of injectors. Many problems appear with applying of CWS concerning exploitation and wear of the engine parts. Due to predominant of coal atoms in the fuel such engines emit also higher amount of carbon dioxide to atmosphere in comparison to engines working on diesel oil at the same power. The main benefits is cheaper fuel and high enough caloric value of coal in comparison to gaseous fuels or alcohols. Coal occurring in large quantity in the world enables delivering of energy for centuries. For that reason research works should be done for preparation such engines working with coal-liquid emulsions and applying them in future. Several industrial applications were done in Australia at CSIRO [1, 2]. Also many research and theoretical studies were done with diesel engine fuelled directly by coal or by coal-water mixture [3–5]. Combustion process of CWS was considered by Mochalov et al. [6] and Redkina et al. [7]. The First stage of early work with coal fuel was led by Diesel and then by his co-worker Pawlikowski [8], with engines running for many years on dry solid fuels (dust firing) ranging from lignite to coke. A big study on fuelling of diesel engines with coal fuels was done by Wilson [9] and team for U.S. Department of Energy National Energy Technology Laboratory. By adding the water with fuel by injection into the combustion chamber we can decrease temperature of combustion process and thus decrease nitrogen oxides formation. Water evaporation process contributes to increasing of the charge mass in the cylinder, which influences on the change of indicated pressure.

Figure 1 presents possibility of applying of different sort driving systems in dependence of power and their influence on green gas emission (GGE). Nowadays the DICE are proposed in the range of power 0–200 MW. These heavy duty engines designated for energetic sector work with lower rotational speed. Their CO_2 emission is lower than for the system IGCC (integrated gasification combined cycle).

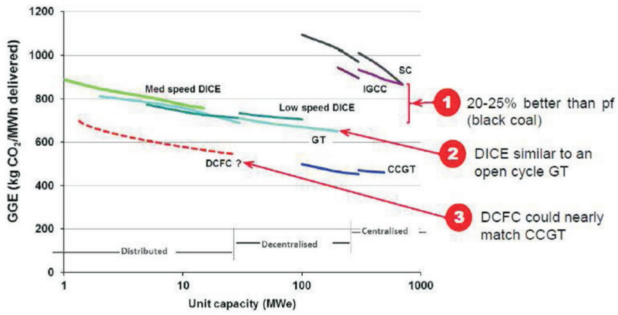

Fig. 1. Application of coal technologies in different thermal machines

The Australian research company CSIRO proposed a whole system of preparing coal-water mixture and injection system for DICE engine with respect to limitation of pollutants coming from combustion process. A proposed technological way for energy plants is shown in Fig. 2.

American company TIAX LLC tested two-cylinder engine with direct coal-water fuel (CWF) and presented many results of their work. In respect to injection system very important is injection timing. Figure 3 shows the period of CWF injection at maximum pressure 75 MPa and at 17% of engine load. The engine was equipped with two injectors (main and pilot). The main injection of CWS begins at 340 deg CA and finished at 376 deg CA.

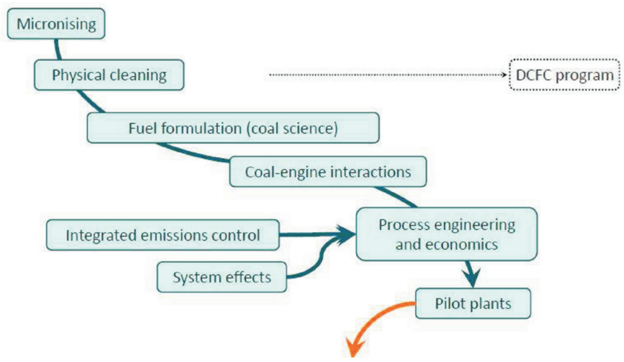

Fig. 2. CSIRO technology for DICEngines [2]

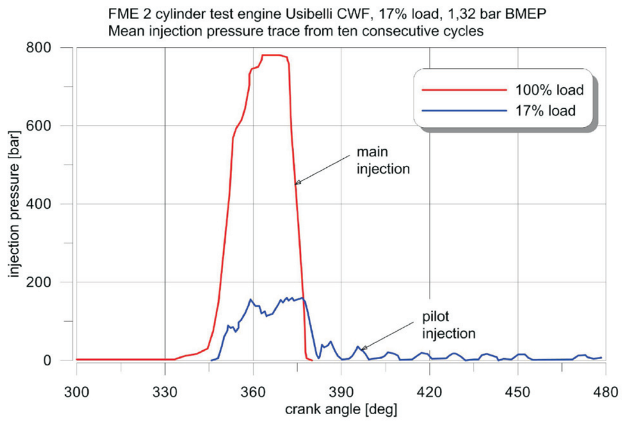

Fig. 3. Injection pressure trace for CWF in test engine [9]

2. Aim and scope of work

There are only few scientific works concerning the problem of coal-water slurry combustion in piston engines, however, many experimental tests were done in the world. Most of them were carried out in Australia and United States. The most important problem is finding dependencies between air fuel ratio and coal water ratio and variations of pressure and temperature of the charge during combustion process. One of the principal problems is determination of beginning of coal-water slurry injection and its duration as in classical diesel engines. The other task is determination of exhaust gas emission in dependence on water ratio in the slurry during injection process. The main task of the work is finding such dependencies and presentation of chosen results obtained from simulation process in CFD program. The work scope is limited to mathematical model of combustion of coal-water slurry and simulation of such process in diesel engine by using of CFD Ansys Fluent program. Naturally simulation of thermodynamic processes in piston engine requires applying of dynamic meshes caused by motion of the piston. The work shows also influences of controlling of water-coal ratio on temperature, pressure and mean indicated pressure in the cylinder. These dependencies were found by using 1-D simulation program written by the author.

3. Coal-water slurry combustion

Combustion of coal in piston engines differs from that in the boilers. The injected pulverized coal with water forms a mixture flowing into the cylinder through the injector nozzles. The nozzles should have higher diameter than for diesel oil. For that reason usually the DICE engines have higher cylinder capacity. The injection of the mixture occurs at high temperature of the compressed air. When a CWS drop gets in a hot combustion chamber there is immediate warm-up of the drop surface and water evaporation from the drop surface. Inside the drop there is gradual warming and as the temperature is increasing the moisture evaporates from the interior of the drop [6]. The process of water evaporation can be described by the following equation:

$$H_2O = \{H_2O\} \quad (1)$$

At high temperature, which still increases there is the process of thermal destruction (pyrolysis) of organic matter on the surface of CWS drop, accompanied by release of volatile substances. The molecules of coal quickly are destroyed and go into volatile as CO, CO_2, CH_4, H_2 and N_2, because bituminous coal and lignite contain those substances. The following equations describe the release of volatile substances:

$$CO + 0.5O_2 \rightarrow CO_2 \quad (2)$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad (3)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (4)$$

Combustion of coal molecules in existence of water occurs in another way due to heat evaporation of water, which decreases gas temperature. Coal undergoes the gasification process and direct oxidation. The processes can be written as follows:

$$C + 0.5O_2 \rightarrow CO \quad (5)$$

$$C + H_2O \rightarrow CO + H_2 \quad (6)$$

$$C + O_2 \rightarrow CO_2 \quad (7)$$

Combustion of surfaces of coal molecules takes place together with water evaporation. The water injection is modelled by different approaches but the most often technique is uses the procedure of Taylor Analogy of Breakup [10] which was used in this work. On the other hand for water evaporation the Spalding model was used, which requires determination of Nusselt and Sherwood numbers. Evaporation is strictly dependent on temperature. Because the injection of water occurs near TDC when the charge temperature reaches value near 900 K and water droplets of small diameter very quick evaporate.

4. Pulverized coal particle combustion

Coal combustion can be calculated by taking into account a particle transport and eddy dissipation calculation for volatile gases contained in the coal particle. Two separate gases are considered in the calculation process: volatiles and char products that form during burning of carbon within the particle. Volatiles can be only either a pure substance or can be a composition of many substances and for each substance a separate chemical reaction is considered. The combustion of the coal particle is a two stage process: the devolatilization of the raw particle of coal and oxidation of the residual char. The devolatilization and char oxidation processes occur very fast. The combustion process of coal-water slurry can be treated as normal combustion process of coal particle as mentioned above with taking into account water evaporation that decreases the charge temperature. Water vapours increase total mass of the gaseous charge. It was assumed that a coal particle consists of mass fraction of raw coal C_O, residual char after devolatilization C_{har} and ash C_A.

Devolatilization was described by Badzioch and Hawksley [11] in a single reaction model:

$$\frac{dC_O}{dt} = -k_v C_O \tag{8}$$

The rate of volatiles production in the gas phase is defined by:

$$\frac{dV}{dt} = Y k_v C_O \tag{9}$$

where: Y – actual yield of volatiles.

The rate of char formation is given by following formula:

$$\frac{dC_{char}}{dt} = (1 - Y) k_v C_O \tag{10}$$

The rate constant in Arrhenius form is obtained from formula:

$$k_v = A_v \exp\left(-\frac{E_v}{R T_p}\right) \tag{11}$$

where: T_p – temperature of coal particles, K, R – gas constant, J/(kmol K), A_v – kinetic reaction constant (from experiment), E_v – activation energy (from experiment), J/kmol.

Coal particle swells due to release of the gas during the devolatilization process. It was assumed that diameter of the coal particle changes in proportion to the volatiles released. After complete devolatilization the particle has increased diameter and this value is an input for burning of the char. The change of the particle diameter during devolatilization is calculated from the relation:

$$\frac{d}{dt} d_p = C_s d_{0,p} \frac{\dot{m}_{ref}}{m_{ref,0}} \tag{12}$$

where: d_p – current particle diameter, m, C_s – swelling coefficient, $d_{0,p}$ – particle diameter at the start of devolitalization, m, $\dot{m}_{ref}$ – rate of mass change of the reference material, $m_{ref,0}$ – mass of the reference material at the start of devolatilization.

5. Simulation of coal-water slurry combustion in diesel engine

Direct injection of coal-water slurry in CFD is defined as multiphase flow, because there is one gaseous phase consisting with many simple gases such as oxygen, nitrogen, carbon dioxide and water vapours. On the other hand the injection of micronized refine coal as a solid fuel (second phase) and water in the liquid form (third phase) determines evaporation of water, diffusion and volatilization of coal. Interaction between three phases can be solved by CFD computer program with taking into account dynamic motion of the piston (dynamic meshing). The author applied Ansys-Fluent program [12] for determination of thermodynamic parameters of the diesel engine with direct coal-water slurry (CWS). In the simulation of combustion process the simple geometry of engine was used. Main engine parameters are given in Table 1.

Table 1. Main geometrical parameters

Parameter	Value
Cylinder diameter	79.5 mm
Stroke	94.2 mm
Compression ratio	15.5
Engine rotational speed speed	1000 rpm

The mesh of engine model contains 85920 hexahedral cells at BDC. The amount of cells decreases during piston motion by applying of layering method in dynamic mesh option. Simulation of injection and combustion processes in naturally aspirated DICE engine with vertical and central position of the injector was carried out at following assumptions:

– start of injection CWS – 330 deg CA,
– duration of injection – 30 deg CA,
– amount of injector nozzles – 4,
– coal mass rate in each nozzle – 0.007 kg/s,
– water mass rate in each nozzle – 0.005 kg/s,
– diameter of pulverized coal – 5 μm.

Heat exchange between gas and cylinder walls was modelled by assumption of real values of walls temperature. Combustion process of coal takes place when it is a volatile form and then the kinetic chemical reaction has the following form:

$$C_{vol} + O_2 \rightarrow CO_2 \tag{13}$$

The precise combustion model will be published in future. Gasification process of coal occurs in high temperature (endothermic reaction between coal and water). The coal with high volatile species described as C_{vol} from Fluent library was taking for calculations. It was assumed the following oxidation reaction of coal with high amount of volatile gases:

$$C_{vol} + 1.598O_2 \rightarrow CO_2 + 1.417H_2O \tag{14}$$

From this equation results that C_{vol} contains 0.654 of C, 0.192 of O_2 and 0.154 of H_2. The rate constant and activation energy in Arrhenius kinetic form was assumed as follows:
– A_v = 2.119e+11
– E_v = 2.027e+8 J/kmol

The charge was treated as ideal gas containing the following species: oxygen, nitrogen, carbon dioxide, water (vapours) and coal volatiles after devolatilization. The calculation model took into account also the injection process of coal-water slurry through the injector with four symmetrical nozzles. It was assumed that the injection of water took place in the same time as injection of the coal at the same nozzle. The injection parameters of the coal-water slurry are presented in Table 2 for engine rotational speed equal 1000 rpm.

Table 2. Injection parameters of coal-water slurry

Parameter	Value
Start of injection BTDC	20 deg CA
End of injection ATDC	5 deg CA
Number of nozzles	4
Coal mass flow rate	0.005 kg/s
Water mass flow rate	0.003 kg/s
Temperature of slurry	310 K
Location of the injector	cylinder centre
Initial slurry velocity	140 m/s

6. Results of simulation

Coal injection parameters determine an excess air ration in the cylinder. During injection process the coal molecules transfer into volatile form due to high temperature and small diameter. Technical problems of CWS were not considered (flow through the nozzles). Engine work is assesses on the base of pressure course in the cylinder. In DICE engine at assumed injection parameters maximum of pressure reaches value 120 bars at 7 deg CA ATDC (Fig. 4). Such high pressure induces also a high mean indicated pressure. Simulation of engine work was carried out at air excess ratio λ = 1.5.

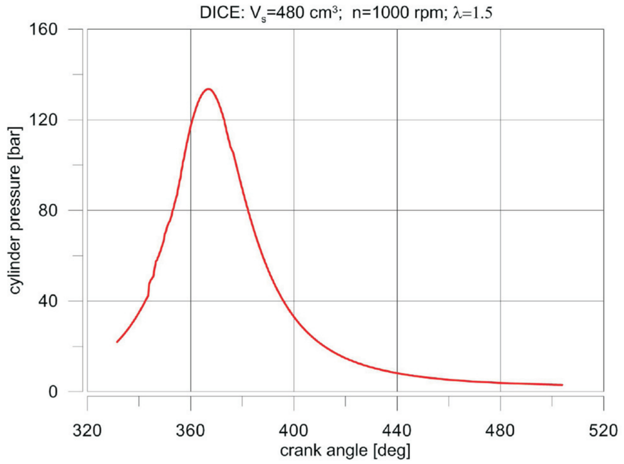

Fig. 4. Cylinder pressure trace

Temperature inside the cylinder is not so high in comparison to engine fuelled by diesel oil. Figure 5 shows course of mean temperature during compression combustion and expansion processes. The initial period of coal combustion characterizes fluctuation of temperature due to coal volatilization and water evaporation, which decreases temperature. Highest mean temperature reaches value 1500 K at 12 deg CA ATDC.

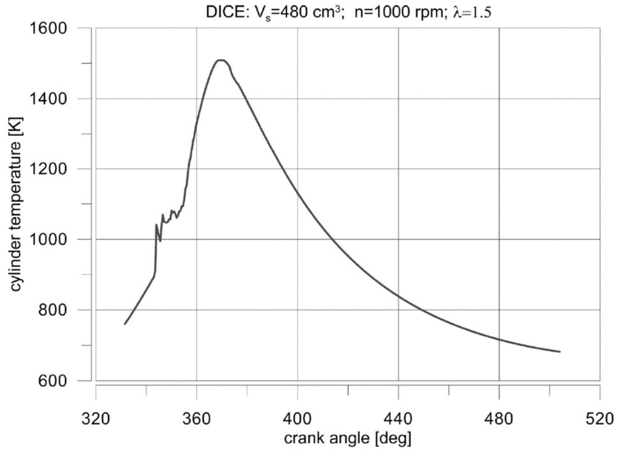

Fig. 5. Course of mean cylinder temperature

Combustion process of the coal injected together with water is observed by an increase of carbon dioxide. Figure 6 presents the change of CO_2 mass fraction. Beginning of fuel combustion occurs already at 13 deg CA BTDC and for assumed air excess ratio λ = 1.5 the maximum of CO_2 mass fraction reaches value about 0.1. It should be indicated that total charge mass of gas increases in respect to water evaporation.

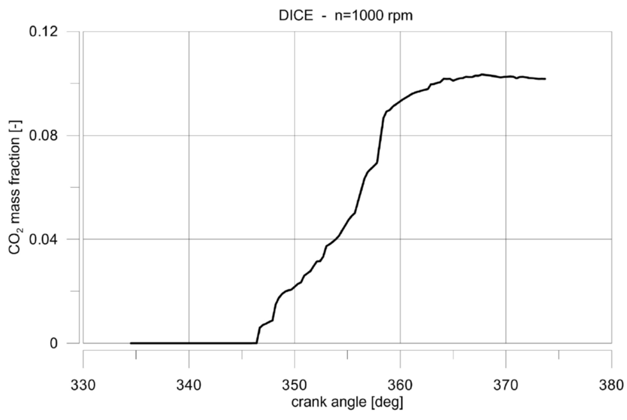

Fig. 6. Variation of mass fraction of carbon dioxide during combustion process

Temperature of the charge during combustion process of water-coal mixture is lower than in the case of burning of diesel oil in the same self-ignition engine. It is caused mainly by water evaporation, when the gas transfers the heat to the water droplets. The lower gas temperature during burning of the coal influences on lower value of mass fraction of nitrogen oxides, particularly on NO. It is confirmed by CFD simulation and Fig. 6 shows very small value of NO mass fraction below 60 ppm, where in classical diesel engine NO_x molar fraction reaches value even 3000 ppm without the catalytic converter.

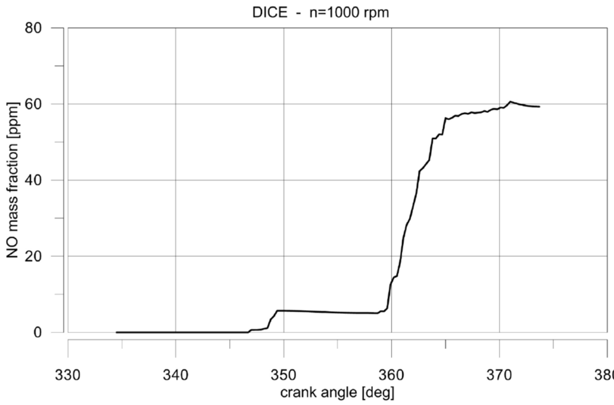

Fig. 7. Variation of mass fraction of nitrogen oxide during combustion process

The simulation of water-coal mixture in diesel engine gives many thermodynamic data, but only a few can be presented in the paper. The most essential factor is start of burning of the fuel, when kinetic reactions occur. In this case only one kinetic reaction of burning of the coal with high amount of volatile components (see eq. 7) was considered. The computer program calculates combustion reaction rate every adaptive calculation step (lower than 0.3 deg CA). The burning of fuel begins on the outer side of the injection streams, where is better contact with oxygen. Figure 8 presents contours of reaction rate (kmol/(m^3 s)) at 13 deg CA BTDC. Maximum of this parameter reaches value 0.0687 kmol/(m^3 s). Unsymmetrical development of the flame is caused by swirl of the charge. Because of evaporation of the injected water droplets the temperature inside the water-coal stream decreases significantly and is about 300 K lower than that on the outside of the slurry stream (Fig. 9). Temperature of the gas amounts about 1000 K and is enough high for beginning of burning of the coal and evaporation of water.

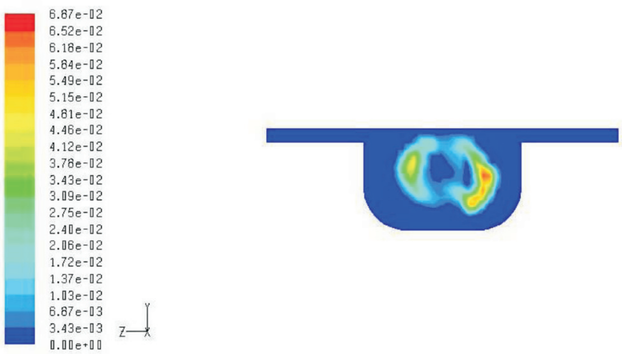

Fig. 8. Contours of combustion reaction rate [kmol/(m^3 s)] at 13 deg CA BTDC

After full injection of water-coal mixture almost whole fuel is burned and temperature of the charge in the piston cavity differs slightly. Contours of temperature at piston position 18 deg CA ATDC are shown in Fig. 10. The highest temperature value is reached on bottom of the piston because there are gathered a lot of carbon particles. Outside of the squish volume temperature of the gas is smallest.

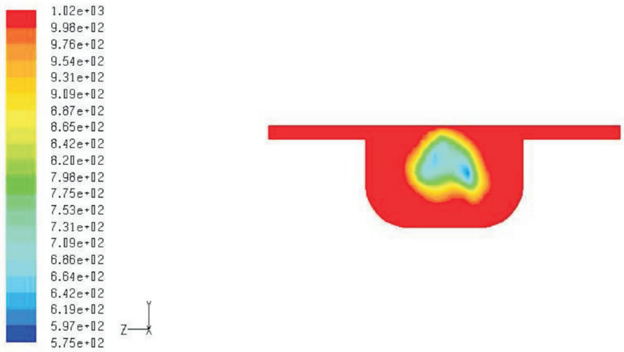

Fig. 9. Contours of temperature [K] at 13 deg CA BTDC

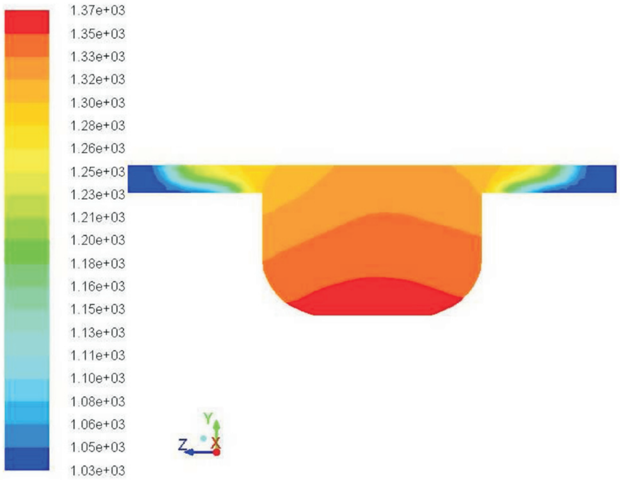

Fig. 10. Contours of temperature [K] at 18 deg CA ATDC

The end of the combustion process has lower activity, which is shown in Fig. 11 at piston position 18 deg CA ATDC. In comparison to reaction rate at piston position 13 deg CA BTDC (Fig. 8) in this case this parameter is many

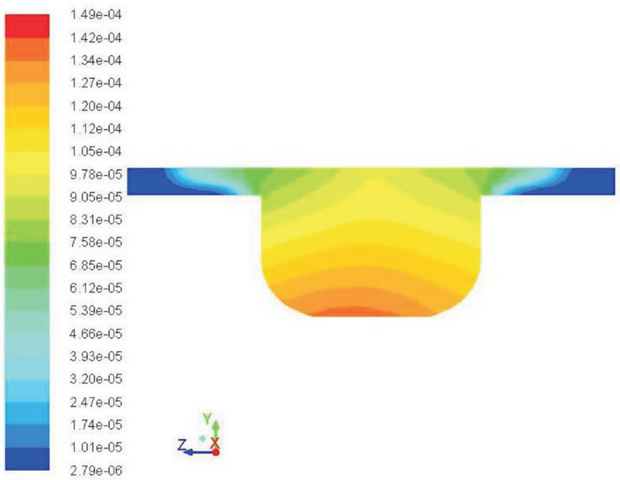

Fig. 11. Kinetic reaction rate [kmol/(m^3 s)] at 18 deg CA ATDC

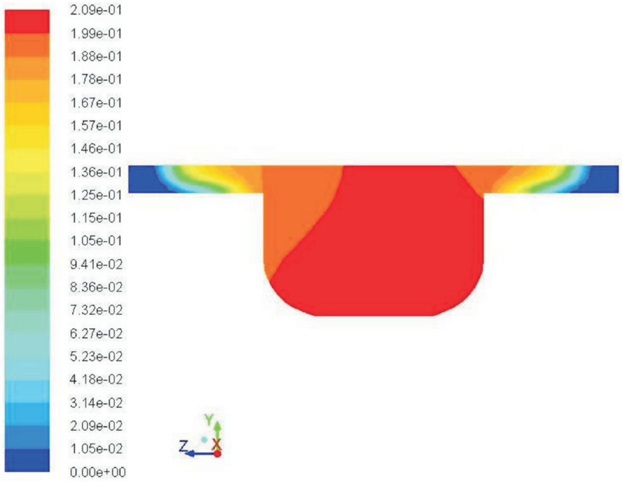

Fig. 12. Contours of mass fraction of CO_2 at 18 deg CA ATDC

times smaller, but still chemical reactions occurred on bottom of the cavity. This phenomenon influences on almost uniform distribution of carbon dioxide in the piston cavity, which was presented in Fig. 12. Mass fraction of CO_2 in the piston cavity reaches value 0.20 which indicates a complete coal oxidation. Like in diesel oil engine the combustion process does not occur in the squish region.

7. Water dose and engine parameters

Injection of coal particles together with water at high pressure influences on pressure and temperature traces in the diesel engine cylinder. It was developed the 0-D mathematical model for calculations of thermodynamic parameters in diesel engine with direct water-coal mixture. The computer simulation program was prepared which was based on this model with taking into account non-steady gas flow in the ducts and pipes. This complex model and computer program are outside of the scope of this paper. After the adoption of different values of water dose in the range of 0 to 0.015 g/cycle for the same engine geometry as in CFD simulation, many thermodynamic parameters were achieved such as pressure, temperature, indicated pressure, fuel consumption, engine efficiency etc. The most important is the change of pressure and temperature in the cylinder. Figure 13 presents the change of pressure in the engine with different water doses per one work cycle. The increase of water dose influences on decreasing of maximum of pressure a few percent, but in particular it should be noted a significant reduction of pressure before TDC. This phenomenon affects on reducing of negative work during compression stroke. Less negative work gives a higher total work and obviously higher engine power. Simulations were carried out for the same rotational speed 1000 rpm.

Evaporation of more water in the cylinder requires delivering of higher amount of heat from the gaseous charge. It was assumed that whole evaporation process takes place during combustion process and specific evaporation heat of water amounts 2263 kJ/kg. For the coal with high volatile species which has to be enriched the caloric value was assumed with value 28 MJ/kg. At such conditions one achieves a variation of temperature of the charge in the range of whole engine working cycle. Figure 14 presents curves of temperature for four different water doses per one cycle. Diesel engine working without adding the water indicates maximum of temperature about 2100 K, but adding small dose of water equal 0.005 g/cycle causes decreasing this parameter to value 1650 K. By increase of water dose to 0.015 g/cycle there is a reduction of temperature to value 1050 K.

By adding higher amount of water in the injected slurry the mass of the charge increases because the water vapours come into the gaseous charge.

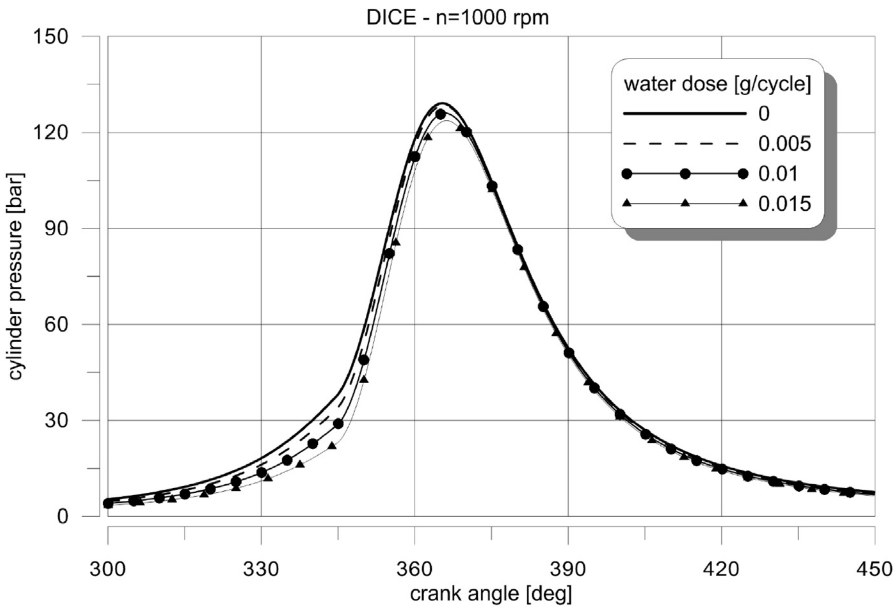

Fig. 13. Variation of cylinder pressure for different water doses at 1000 rpm with constant coal dose

8. Summary

Review of till now designed engine with direct coal-water slurry injection system and own input in a form of simulation results give certain remarks:

1. Heavy duty diesel engines with MRC (Micronised Refined Coal) injection system are designated for energetic plants. They enable efficient work with higher efficiency than diesel engine fuelled by diesel oil.
2. Combustion of coal takes place together with water evaporation and at high temperature a gasification process is observed.

3. Combustion of CWS in diesel engine is more efficient and ecologic (lower GGE) than for other energetic thermal machines (steam and gas turbine).
4. In the era of future fuel crisis replacement of diesel oil by coal fuel is a promising solution due to large coal deposits in the world.
5. The pressure and temperature of the charge in diesel engine fuelled by water-coal slurry is dependent on water dose per cycle. Higher water-coal ratio decreases the negative engine work and thus obtaining a higher value of total work.
6. The CWS diesel engine should be equipped with new resistive on corrosion and friction injection system and valve system.
7. Fuel injection process should be optimized in respect to obtaining maximum of pressure and temperature as in classical diesel engine.
8. Simulation process carried out at rotational speed 1000 rpm and start of injection process at 20 deg CA BTDC indicated that whole injected coal mass is fully burned. Emission of NO_x is quite low in comparison to the classic diesel engine.
9. Combustion process begins in the fuel jet shortly after beginning of fuel injection. From exploitation point of view the proportion of carbon mass to liquid water mass should be higher as possible but enough for lubrication of injector.

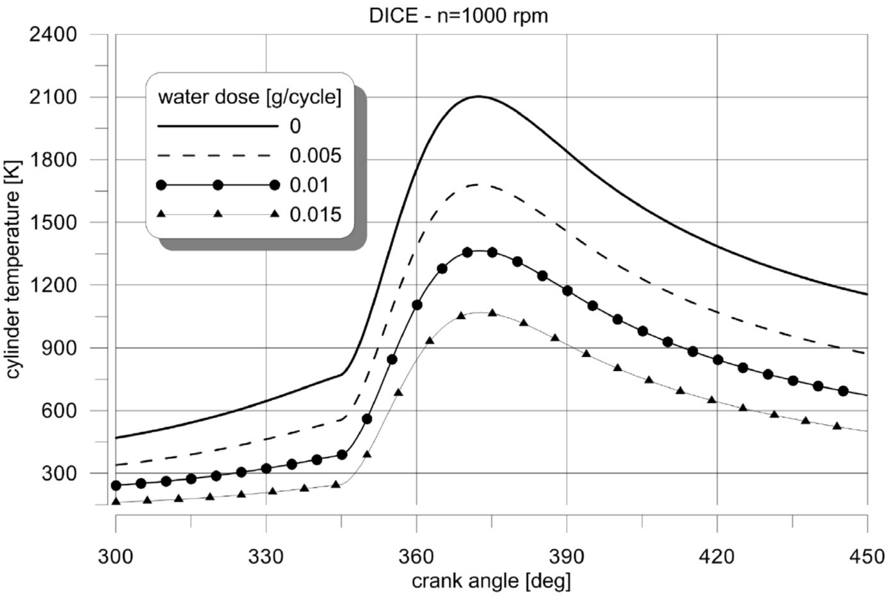

Fig. 14. Variation of cylinder temperature for different water doses at 1000 rpm with constant coal dose

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