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THE EFFECT OF METHANOL-DIESEL COMBUSTION ON PERFORMANCE AND EMISSIONS OF A DIRECT INJECTION DIESEL ENGINE

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Abstract

The results of CFD modelling a dual fuel diesel engine powered with both methanol and diesel fuel is presented in the paper. Modelling was performed with 20 and a 50% energetic share of methanol in the entire dose. The analysis was conducted on both the thermodynamic parameters and exhaust toxicity of dual fuel engine. It was found that the various share of methanol influences the ignition delay of the combustion process and after start of main phase of combustion, the process occurs faster than in case of the diesel engine. It was found that the time of 10-90% burn of the fuel is much shorter than it is in the diesel engine. The dual fuel engine was characterized by higher indicated mean pressure in the whole range of diesel fuel injection timings. While analysing toxic exhaust emission from the dual fuel engine powered with methanol, it was found that the rate of NO formation was significantly higher than from the diesel engine. The combustion process in the dual fuel engine occurs more rapidly than in the conventional diesel engine, which contributes to form areas with high temperature, and in combination with presence of oxygen from the air and oxygen bonded in the methanol, promotes the NO formation. In the case of the dual fuel engine, it was found that soot emission was reduced. The engine running with diesel injection start at 8.5 deg before TDC, the soot emissions were more than twice lower in the dual fuel engine, while the emission of NO was much higher.

Keywords: *dual fuel engine, exhaust emission, modelling, diesel*

1. Introduction

In the available literature, there are many works devoted to dual-fuel engines. As a dual-fuel engines customers usually prefer compression-ignition engines. Dual fuel technology usually is realized in two ways of co-combustion of alcohol and diesel fuel. The first way is to produce a blend of diesel fuel with alcohol and then bring the mixture to the engine, using a typical supply system for a diesel engine. The greatest difficulties are the alcohol and diesel fuel cannot be mixed perfectly at large percentage of alcohol, hence use of diesel-alcohol blends is not feasible. In addition, the blends are not stable and separate in the presence of trace amounts of water. In such a power, system cannot change the ratio of diesel/alcohol. The second way is fumigation system, which injects an alcohol fuel into the intake port of an internal combustion engine. Into the engine cylinder is delivered air–fuel mixture, nearly homogeneous. The ignition process is controlled by the injected dose of diesel fuel. This requires the addition of an injector, along with a separate fuel tank, lines and controls [21].

The use of methanol for diesel engines has been investigated in several studies [19] because of its advantages over traditional fuels. It has better lean combustion characteristics than hydrocarbon fuels. Chemically synthesized methanol was used as a diesel engine fuel in Germany during World War II.

In the paper [28] authors was conducted research to investigate the operating range and combustion characteristics in a methanol-fumigated diesel engine. The experimental results showed that the viable diesel methanol dual fuel (DMDF) operating range in terms of load and methanol substitution percent (MSP) was achieved. The lower bound of the operating range is limited by partial burn, which occurs at 20% load conditions with high MSP. At the partial burn bound, the combustion process is highly deteriorated due to the cooling effect of premixed methanol in the intake process and compression stroke. The decrease of the pilot diesel injection and extremely low intake temperature cause the fuel/air mixture unable to ignite or reach HCCI-like knock in some cycles [28]. In the paper [16], the authors present results of methanol-diesel and ethanol-diesel fuel blends combustion on the performance and exhaust emissions of diesel engine. The results showed that brake specific fuel consumption and emissions of nitrogen oxides increased while brake thermal efficiency, smoke opacity, emissions of carbon monoxide and total hydrocarbon decreased with methanol-diesel and ethanol-diesel fuel blends [16, 20]. Some authors have investigated ethanol fumigation on combustion, smoke and nitrogen oxides (NO_x) emission and performance parameters of a turbocharged IDI automotive diesel engine [14]. Experimental results showed that smoke emission reduces for up to 4-8% ethanol ratios but then it begins to increase. Tests results showed that NO_x emission takes lower values than that of neat diesel fuel. In heat release, rate diagram two distinct peaks are observed for high ethanol additions [14, 21, 24]. The first peak occurs before top dead centre (TDC) and the second peak takes place after TDC [14]. On the other hand, the first peak becomes larger, but the second peak diminishes as ethanol percentage increases [14, 15]. That is, premixed combustion of ethanol–air improves engine performance and also it increases in-cylinder pressure. The dual fuel engines emit less soot than diesel engines [21, 24, 25]. Nowadays the emphasis is put on emissions of particulate matter. It was found that dual-fuel engines are characterized by low emission of soot particles [10]. The fumigation method results in a significant decrease in particulate mass and number concentrations from medium to high engine loads, due to the increase of fuel burned in the premixed mode and a reduction of diesel fuel involved. Fumigation methanol also slightly decreases the fraction of accumulation mode particles and thus the particulate geometric mean diameter [29]. As the fuel to dual fuel diesel engine was also used LPG [13]. Authors stated that value of maximum torque of a dual-fuel engine fuelled with LPG is limited by the occurrence of knocking combustion. Engine powered by LPG was characterized lower CO, CO_2 and NO_x emission, HC at a similar level and clearly reduced opacity [11]. There are some works on the use of natural gas as a fuel to dual fuel diesel engines [19]. Studies report shown that dual-fuel combustion of premixed natural gas has advantages of increased efficiency and decreased smoke and nitrogen oxides (NO_x) emissions. Dual fuel engines are also used for the combustion of generator gas [23] or other fuels of vegetable origin [9]. One of the effective way to reduce nitrogen oxides emission is dual fuel engine with two-stage combustion system using engine prechamber [5-7]. This system allows to burn very lean air-fuel mixtures.

Modelling dual fuel engine is an issue rarely presented in the literature [7, 25]. There are some works where author used KIVA code to model dual fuel engine [8, 17, 18]. Authors stated that the modified KIVA model was found to predict combustion and emissions at low diesel pilot quantities reasonably well. In recent years, more and more studies are carried out using a CFD software [2, 6, 7, 25]. The paper presents the results of CFD modelling of diesel engine operating as a dual fuel engine.

2. Object of investigation

Modelling the thermal cycle of a dual fuel CI internal combustion engine was carried out within the study. As the research object was taken an internal combustion engine, operated at constant rotational speed equalled 1500 rpm. The displacement volume of one cylinder of the engine was equal 0.97 dm^3. Engine power from one cylinder was 8 kW. The boundary conditions such as temperature of combustion chamber parts, valves and ports were taken from literature. The initial conditions of flow field were taken on the basis of author research [22]. The three cases were modelling: the first as a classic diesel engine powered by the diesel fuel (D-1.0, methanol-0.0), the second as dual fuel engine with 20% of energy supplied in methanol (D-0.8, methanol-0.2) and the last with 50% share of methanol (D-0.5, methanol-0.5).

The positive effects of the dual fuel engine are the following:

- improvement in the engine indicated efficiency,
- carrying out the combustion process in a shorter time and in the optimal position of the crankshaft from the point of view of obtaining a high indicated work of engine,
- the ability to control of the start of combustion by the diesel injection timing,
- engine start using only diesel fuel,
- the ability to improve exhaust emissions,

The negative effects of dual fuel engine:

- the possibility of uncontrolled auto-ignition mixture at the end of the compression stroke,
- the possibility of knock due to the rapid pressure increase after the start of combustion.

Methanol (CH_3OH) known as wood alcohol, is considered as an alternative fuel for internal combustion engines. Methanol has physical and chemical properties similar to ethanol. It is generally produced by steam-reforming natural gas to create a synthesis gas. Feeding this synthesis gas into a reactor with a catalyst produces methanol and water vapour [3]. The main benefits of methanol [3] are presented in the table 1:

- cheap to produce relative to other alternative fuels,
- lower risk of flammability compared to gasoline,
- manufactured from a variety of carbon-based feedstocks, such as natural gas and coal.

Methanol can also be produced from CO_2 and water (H_2O) using sunlight, which may help to control the global warming and serve as a renewable source of energy [12].

Because of its higher octane rating and oxygen content, the utilization of methanol in compression ignition engines yields better results than gasoline [4].

Lower heating value (LHV) of methanol is lower in comparison to diesel fuel, hence, to obtain the same engine performance, higher amounts of methanol should be provided. Its relatively low air–fuel (A/F) stoichiometric ratio, high oxygen content and high H/C ratio may be beneficial at improving the combustion process and reducing both soot and smoke [24].

Tab. 1. Comparison of various physicochemical properties of methanol and diesel fuel

Parametr	Diesel	Methanol
Chemical formula	$C_{10}H_{22} – C_{15}H_{32}$	CH_3OH
Molecular weight	190-220	32
Cetane number	51	<5
The calorific value (MJ/m^3)	42.5	20.5
Density at 20°C (kg/m^3)	840	790
Viscosity at 20°C (mPa·s)	2,8	0.59
Heat of vaporization (kJ/kg)	260	1178
Stoichiometric air fuel ratio $(A/F)_{st}$	14.7	6.45
Ignition temperature (°C)	316	464
The flame temperature (°C)	2054	1890

Methanol has higher heat of vaporization than diesel fuel, therefore it absorbs heat from surroundings when it vaporizes hence, its cools the cylinder charge and therefore can reduce NO_x emissions from combustion. Oxygenated fuels contain additional oxygen that participates in combustion, enhances the premixed combustion phase and improves the diffusive combustion phase [24, 26]. Fig. 1 shows three computational domains, which were used to CFD modelling. The first domain is used during the calculation of the intake stroke, the second during the compression and work stroke and the third, during the exhaust stroke.

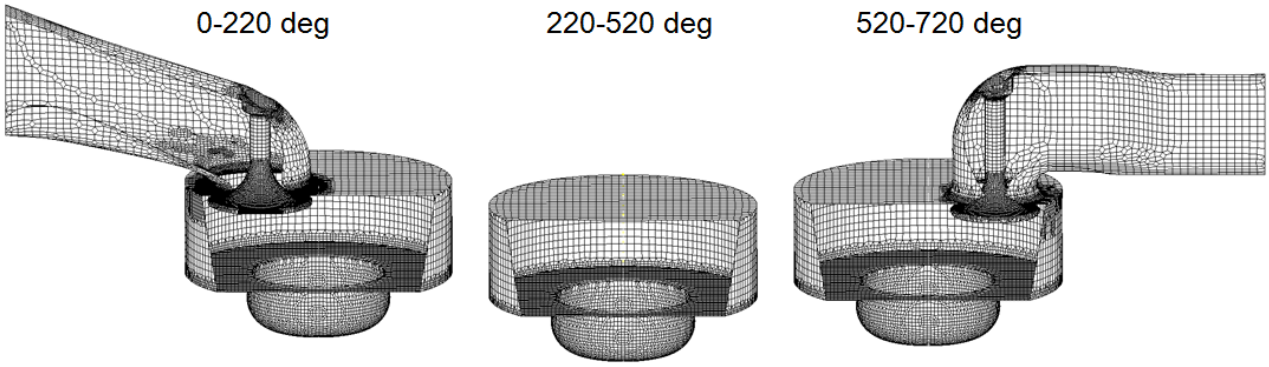

Fig. 1. The computational mesh of engine

Mesh density was selected on the basis of a series of simulations. The turbulence was modelled with the k-zeta-f model and the combustion was represented by the Extended Coherent Lame Model (ECFM-3Z) model [1]. The required initial and boundary conditions adopted on the basis of experimental research [21, 22, 24].

3. Results

In the first stage of the research was carried out modelling studies of CI engine powered by diesel, and methanol with 20 m and 50% share of energy. The engine operated with injection timing equal 8.5 deg before TDC.

3.1. Thermodynamic parameters

In Fig. 2, the pressure courses of the dual fuel CI engine are presented. It is also a validation of the model.

The dual fuel engine model assumes that the engine cylinder is filled with a homogeneous mixture of methanol-air. Combustion process is initiated by injection of diesel fuel into the engine cylinder 8.5 deg before TDC. In the first step of modelling the classical CI engine powered by diesel was performed. Such calibrated model was used to model the dual fuel engine. In the dual fuel engine, diesel fuel is injected into methanol-air lean mixture, also more appropriately due to increased temperature ranging compression. This mixture is also heated by compression to a sufficiently high temperature, but still below the auto-ignition temperature of the mixture. The reaction of the combustion of diesel fuel in an environment with methanol-air runs in another rate than in the air. To determine combustion model parameters results of experimental researches dual fuel engine were used. In Fig. 2 is also showed courses of heat release rate of diesel and dual fuel engine. The shape of these curves shows the diversity of the combustion process, its stages and variable dynamics. Engine powered by diesel fuel a classical division can be seen on the stage of the kinetics and diffusion combustion. With the increase in the share of methanol, it can be seen that the greatest intensification of the combustion process takes place in the final stage of combustion. One reason for such combustion is the difference in the rate of combustion of fuels. Therefore, where a greater proportion of the fuel is methanol, after ignition the combustion occurs much faster as compared to the classical CI engine.

In Fig. 3, the heat release rate and the heat released are presented, in conditions of injection timing 8.5 deg before TDC. It can be stated that engine operated on 20% of energetic share of methanol the course of heat release rate is similar to course of the classical diesel engine. There is visible both characteristic phases of combustion process, the premixed and diffusion phase. In case of the engine operated at 50% energetic share of methanol, the combustion process occurs faster but it still occurs in two stages.

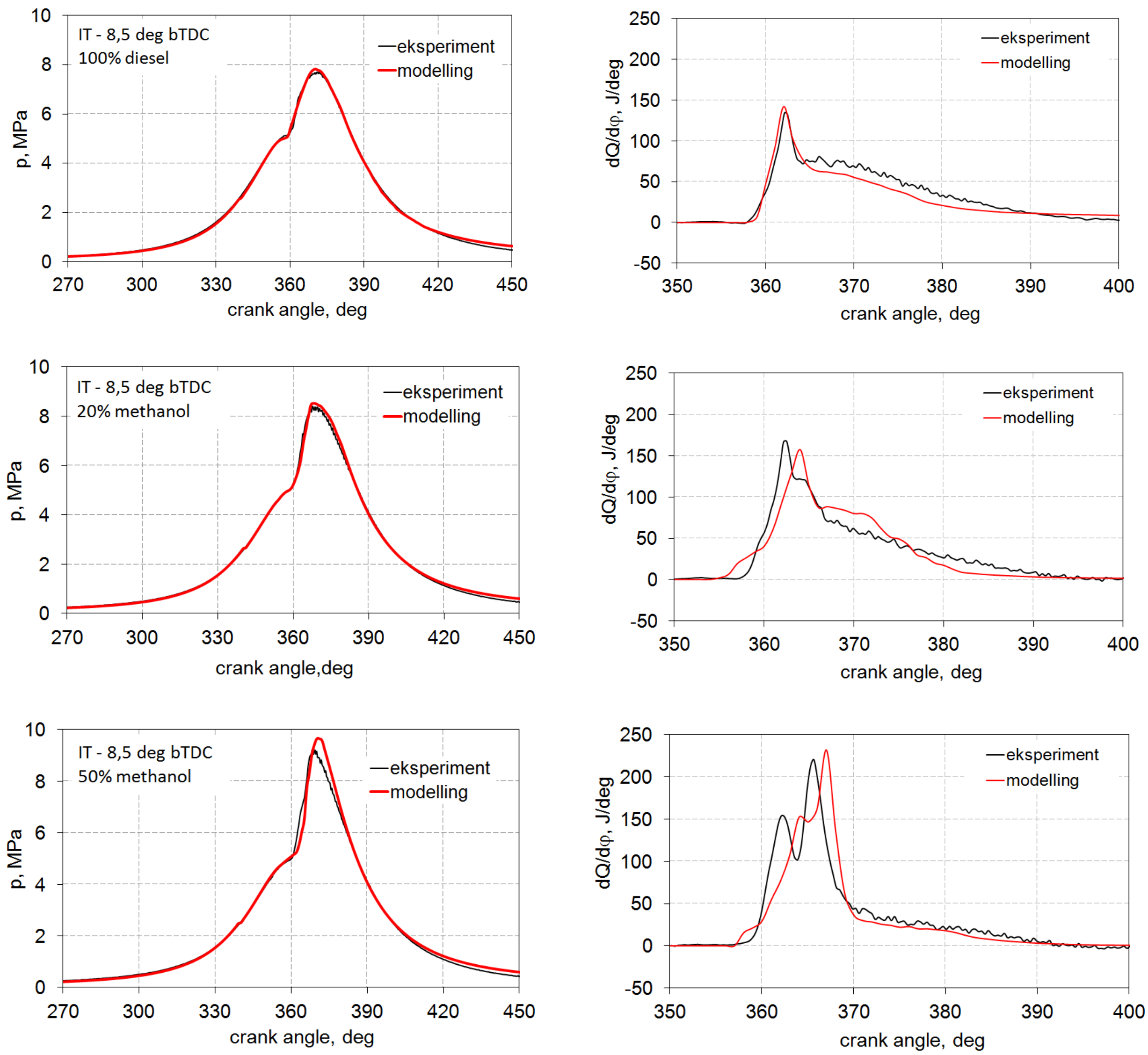

Fig. 2. Results of model validation of diesel and dual fuel engine

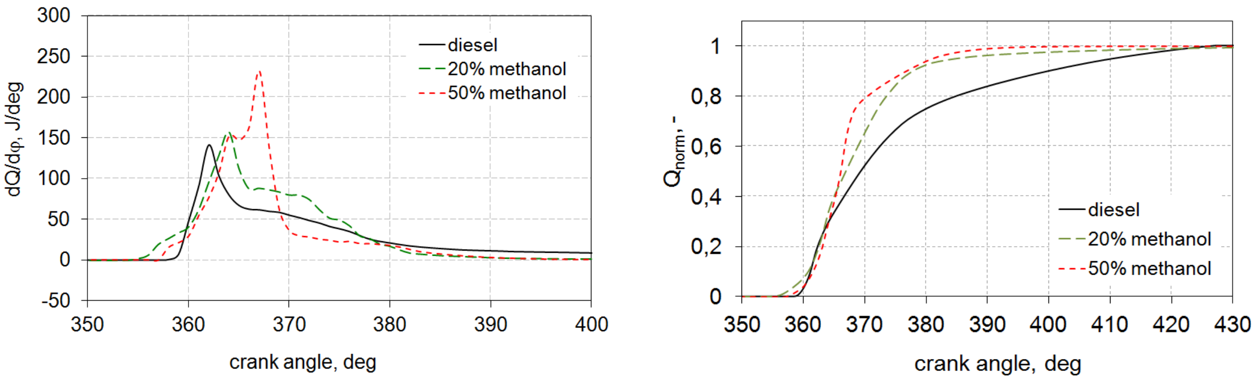

Fig. 3. Heat release rate (dQ/dφ) and accumulative heat release (Q), (injection timing: 8.5 deg before TDC)

In Fig. 4, the pressure courses are presented for various energetic shares of methanol for ignition timing in range of 3.5-18.5 deg before TDC. It is visible that the methanol participation in combustion process causes an increase in peak pressure value. It is also visible that the combustion process occurs in shorter time. As it is known along with the shortening of combustion process the engine efficiency increases.

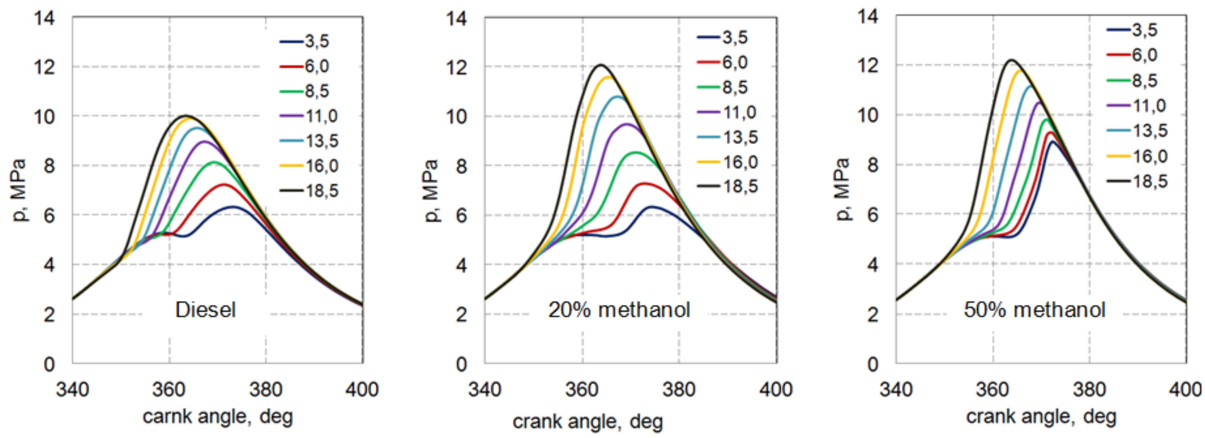

Fig. 4. The courses of the combustion pressure in a diesel and dual fuel engine

3.2. Exhaust emissions

Nitrogen oxides are one of the main pollutants emitted by the IC engines. The nitrogen pollutants are formed from the molecular nitrogen (N_2) carried with the air and the organic nitrogen bound in fuels [27]. The main components of NO_x are nitric oxide (NO) and nitrogen dioxide (NO_2). Generally, the two mechanisms are responsible for nitric oxides production. First, it is thermal NO_x mechanism and second prompt NO_x. The thermal mechanism of NO formation is strongly dependent on temperature, oxygen concentration and residence time. To destroy the stable bond of the molecular air-nitrogen the high value of activation energy is necessary, that is a high temperature is required therefore, it is a thermal mechanism. The thermal NO formation in burnt gases is faster than in the flame front and represents the main source of nitric oxides in the IC engine [13]. The thermal mechanism of NO_x formation is described by a many of highly temperature-dependent chemical reactions well known as the extended Zeldovich mechanism. The prompt mechanism of NO_x formation is most prevalent in rich flames [13]. For NO_x production during combustion process are responsible many reactions and many possible intermediate species. The prompt mechanism of NO formation is important at low temperatures (below 1000 K) and at reach mixtures. This mechanism is initiated during hydrocarbon combustion at the flame front where there is a recombination of CH radical and N_2 into HCN [1, 27].

In Fig. 5, the nitric oxide (NO) and soot emission of diesel and dual fuel engine are presented. It can be stated that in all cases of the engine with the increase in the angle of the start of diesel fuel injection increases the emissions of NO in the exhaust. In a dual fuel engine powered by methanol the rate of NO formation is significantly higher than in diesel engine. The increase in injection start angle causes an increase in pressure and thus increases temperature in the combustion chamber, and this with the presence of oxygen favours the formation of NO. In all causes with an increase of injection start, the soot formation decreased. Engine operated with fuel injection start equal 8.5 deg before TDC the soot emission was 2-times lower in case of dual fuel engine but NO emission was near 3-times higher. Already a 20 percent share of methanol significantly reduced soot emissions.

It can be concluded that in a diesel engine, an increase of the angle of the diesel fuel injection causes a drop in soot emissions by a relatively small increase in emissions of NO. In the case of dual fuel engine, an increase of the angle of the diesel fuel injection causes results in a decrease in soot emissions, and causes increases in emissions of NO.

4. Conclusion

The paper presents results of CFD modelling of dual fuel diesel engine powered by methanol of various energetic shares to diesel fuel.

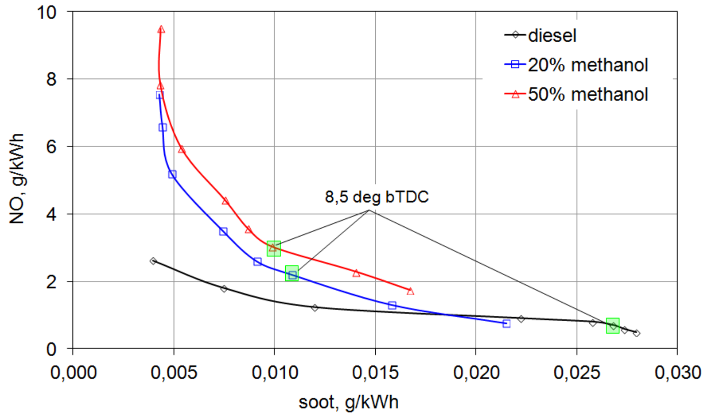

Fig. 5. The interdependence of NO and soot emission in a dual fuel engine

- The methanol participation in combustion process causes an increase in peak pressure value. It is also visible that the combustion process occurs in shorter time.
- It can be stated that engine operated on 20% of energetic share of methanol the course of heat release rate is similar to course of classical diesel engine. There is visible both characteristic phases of combustion process, the premixed and diffusion phase. In case of engine operated on 50% energetic share of methanol, the combustion process occurs faster but it still occurs in two stages.
- In all analysed causes with an increase of injection start, the soot formation decreased. Engine operated with fuel injection start equal 8.5 deg before TDC the soot emission was 2-times lower in case of dual fuel engine but NO emission was near 3-times higher. The 20% share of methanol significantly reduced soot emissions.

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