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SIMULATION OF POLLUANT EMISSION FOR COMPRESSION IGNITION ENGINE FUELED WITH BIOFUELS USING COMPUTER SIMULATION WITH TWO COMBUSTION MODELS

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Abstract**—**This paper presents scientific studies on the development and use of analytical models of the processes occurring during operation of a single cylinder compression ignition engine powered by biofuels. Combustion parameters as cylinder pressure, rate of increased pressure and rate of heat released have been obtained experimentally, and they were studied by simulation. The use of biofuels has been boosted by the severity of current rules on emissions standards and requirements for keeping satisfactory performance in compliance with these rules. The present rules promote the use of biofuels for replacing classic fuels, to help promote use of renewable energy.

Keywords**—**biofuels, simulation, rate of heat released, pollutant emissions, compression ignition engines.

I. INTRODUCTION

CONTINUING increase in the mobility of human society (using massive the means of transport) must relate to direct effects on the environment. Using CI Compression Ignition engines in construction of vehicles cause environmental damage by GHG Greenhouse Gas Emissions. This requires replacing fossil fuels with alternative fuels use currently or technologies that reduce the negative effects of emissions on the environment.

It is now universally accepted that alternative fuels (biofuels) is the immediate solution. To decarbonize the transport domain by gradually substituting fossil fuels. Alternative fuels could replace fossil fuels in Europe by 2050 [1].

Use of biofuels offers some immediate advantages relative to high energy density; power infrastructure consists of filling stations, motor minimum technical changes, etc. [2].

In terms of GHG biofuel is considered that limiting pollutant emissions in the atmosphere from sources characteristic of the life cycle.

Still, besides the above advantages, especially for blended use of biofuels with fossil fuels more than 20% will increase NO_x emissions. NO_x is considered a pollutant that has direct effects on the human body.

Major conclusion was that currently experiences of NO_x size has large discrepancy gaps due to factors involved in the experiments (different engine operating regimes, varying degrees of wear, different number of cylinders, initial operating conditions, type of engine).

This paper presents considerations on the use of a method for determining the optimal operating point of a CI engines, making optimization of the link between experimental model and the models used in computer simulations. Computer simulations offer the advantage of being able to make a minimum number of tests at low cost. Still the confidence in the results must be validated by experimental tests.

Studies and research on the performance of engines that work with biofuels planned the efficiency of opportunities to demonstrate the use of alternative fuels at a moment when Europe is undertaken to reducing pollution and consumption of conventional energy sources and development of alternative energy.

To analyze the processes occurring during operation of a single cylinder compression ignition engine, was created and developed a theoretical model for the simulation engine. After the development of the experimental model for the single cylinder compression ignition engine and after validation of the results, the classical diesel fuel was replaced with various types of biofuels: from pure B100 biodiesel mixtures in various concentrations of diesel and biodiesel (B10, B20 and B50). For all these types of biofuels there were repeated simulations using the theoretical model of engine, then they analyzed results which show the differences that occur between the quantities of heat released from burning the differences that occur between pollutant emissions.

In the CI engines, air fuel mixture is prepared between the beginning of the injection and the start of burning and during the combustion process is obtained a less uniform mixture. CI engines are working continuously with a surplus of air ($\lambda > 1$), and for added air too small increased smoke emissions, carbon monoxide, hydrocarbons and fuel consumption. Injection mixture formation is described by the following parameters: injection pressure, injection time, development of the jet fuel, air movement and air mass. All these quantities have an influence on emissions and fuel consumption of the engine. NO_x formation is favored by the high temperature of combustion and the high oxygen concentration inside of the combustion chamber.

II. Experimental

For research and study of the processes and phenomenon occurring during operation of internal combustion engine with the compression ignition was used single cylinder research diesel engine model AVL 5402 that together with control systems are embedded in the experimental test stand.

AVL 5402 is a research single cylinder in four stroke engine with common rail injection type equipped with a Bosch CR1 injector of 1600 bars with three injections per cycle (pilot injection, main injection and post injection). Electronic injection management system is RPEMS (Rapid Prototype Electronic Management System) system equipped with an electronic control unit ECU 7.1 ETK ETAS whose parameters can be changed via the INCA-PC software and allows full access to the injection parameters: start of injection (SOI), duration of injection (DOI) and pressure of rail (PRAIL) [3].

For the experimental study and simulation of the theoretical model was created and developed single cylinder engine in AVL 5402 in Boost application. For the development of experimental models was used the data from technical books of the engine, together with the diagrams and the experimental data have been extracted from measurements in the laboratory and stored in the post processing software Concerto.

Boost is a software tool which consists in a preprocessing program, used for initial data entry and technical characteristics of the engine to be designed as a model. After forming the engine assembly with annexes systems, mathematical equations and algorithms of the model with the graphical user interface (GUI) will analyze and calculate the processes that are required during simulation [4], [5].

The model for the engine AVL 5402 designed in Boost is shown in Fig. 1.

The main features of the engine AVL 5402 that have been used as initial data to define the cylinder parameters are presented in Table I.

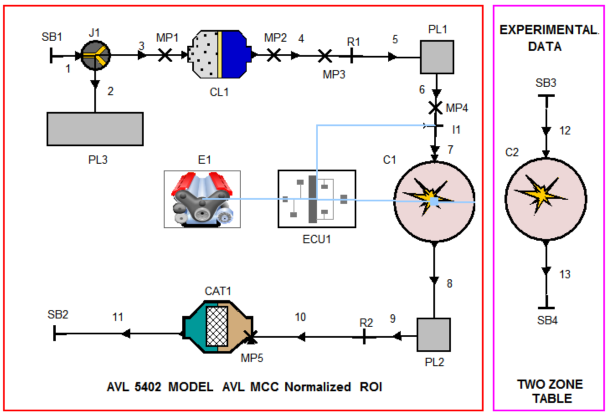

Fig. 1. The simulation model for the engine AVL 5402 in Boost with two combustion models.

TABLE I
THE MAIN TECHNICAL FEATURES OF ENGINE AVL5402

Parts	Value	U.M.
Bore	85	mm
Stroke	90	mm
Con-Rod	138	mm
Ratio	17.5	-
Piston Area	5810	mm^2
Cylinder Area	7500	mm^2
Liner Area	250	mm^2
Intake / Exhaust Inner Seat	24.9 / 24.5	mm
Valve Lift	8.5	mm
Intake / Exhaust Scaling Factor	1.3243 / 1.3319	-

Effective flow area A_{eff} in the cylinder is calculated as:

$$A_{eff} = f_{sc}\alpha\frac{dp_i^2\pi}{4} = \frac{n_v dv_i^2}{dp_i^2}\alpha\frac{dp_i^2\pi}{4} = \pi\alpha\frac{n_v dv_i^2}{4} \qquad (1)$$

where α is the flow coefficient, dp_i is the diameter of attached pipe, f_{sc} is the scaling factor, n_v is the number of valves port, dv_i is the valve seat inner diameter.

Mass flow of fuel is discharged by the injectors by the command sent by the electronic control unit and are calculated using the formula:

$$\dot{m}_{delivery} = \eta_v p_{ref} n V_{disp}\frac{1}{(A/F)_{engine}}\frac{6}{N_{cyl}\Delta\alpha_{inj}} \qquad (2)$$

where $m_{delivery}$ is the rate of spray injector, η_v is volumetric efficiency, n is the engine speed, V_{disp} is engine capacity, $(A/F)_{engine}$ is the air/fuel ratio (A/F Ratio), N_{cyl} is the number of cylinders engine, Δ_{ainj} is during of injection.

Boost application takes in consideration the quantity of fuel that evaporates due to the distillation curve and divided the fuel mass injected into three packages: greater volatility for 0-25% of the evaporated fuel injection, average volatility for 25-75% of evaporated fuel injection and low volatility for 75-100% of the evaporated fuel injection [2].

Ignition delay can be determined experimentally as the time interval between start of injection (SOI) and the beginning of combustion. The start of combustion is the moment when the rate of heat released (ROHR) changes from a negative to a positive value and the start of injection (SOI) is the moment when the injector nozzle needle rises above 5%.

When using the alternative fuels we consider the temperature (K) and the pressure (Pa) at the start of injection:

$$T_{cyl} = T_m \varepsilon_{eff}^{c\ 1} = T_m \varepsilon_{eff}^{\,k^+ - \frac{k^+\ 1}{fn_p + 1} - 1} = T_m \left(\frac{V_{disp}}{V_{soi}}\right)^{k^+ \ \frac{k^+\ 1}{fn_p + 1}\ 1}$$

$$P_{cyl} = P_m \varepsilon_{eff}^{c} = P_m \varepsilon_{eff}^{\,k^+ \ \frac{k^+\ 1}{fn_p + 1}} = P_m \left(\frac{V_{disp}}{V_{soi}}\right)^{k^+ \ \frac{k^+\ 1}{fn_p + 1}} \qquad (3)$$

where P_{cyl} is pressure in the cylinder, T_{cyl} is temperature in the cylinder, P_m is pressure accumulated in the cylinder, T_m is temperature accumulated in the cylinder, c is a constant polytrope, k^+ is the ratio of specific heat, f is constant, n_p is the average of piston speed , ε_{eff} is effective filling ratio, V_{disp} is cylinder volume, V_{soi} is cylinder volume at the beginning of injection [6].

Formation of NO_x emission depending on the characteristics of the injection process is described by:

$$NO_{xcycle} = \frac{\int_{SOC}^{EOC} \sum_{i=1}^{i=n} V_{spray} NO_x \ \frac{N_o}{\rho_f} \ \frac{dm_f}{d\Theta} \ t_{dur}}{V_{cyl}} \qquad (4)$$

where NO_{xcycle} is the average of cycle NO_x, V_{spray} is fuel injected volume, N_o is the number of injection holes, *SOC* is the start of combustion process, *EOC* is the end of combustion process $(dm_f/d\theta)/\rho_f$ is the injection rate, t_{dur} is the duration of combustion process, Σ is the sum of n injected volume [6].

Cylinder of the model in Boost is connected with element Engine, and it defines the type of engine used, operating speeds on it, moments of inertia and break mean effective pressure (BMEP).

First combustion method is chosen for the experimental MCC AVL Model (Mixing Controlled Combustion) model that predicts the rate of heat released (ROHR) and NO_x emissions on the quantity of fuel in the cylinder and the turbulent kinetic energy introduced by the injection of fuel. The law to calculate the injection rate is used for model MCC AVL with Normalized ROI, which determine the fuel injection rate with time [7].

The second combustion method is Two Zone Table that performs an optimum approximation of the actual heat release characteristics of an engine and allows reference points for the rate of heat release over crank angle to be specified. As the specified heat release characteristics will be normalized by the Boost by converting the percent of the total heat input per °CA [8].

For accurate engine simulations the actual heat release characteristic of the engine, which can be obtained by an analysis of the measured cylinder pressure history, should be matched as accurately as possible. To obtain an estimate on the required combustion duration to achieve a certain crank angle interval between 10% and 90% mass fraction burned, the following chart may be used [8].

Initialization conditions for all three methods when setting the cylinder used for start of high pressure (SHP) are defined by the following parameters [8], [9]:

= *start_hp* is the pressure in the cylinder when all valves are closed (Pa);

=*air* is the amount of air (m_{air}) required to burn fuel (m_{fuel}) injected into the cylinder (kg/h);

=*fuel* is fuel injected into the cylinder (kg/h);

=*fuel_cyc* is the quantity of fuel consumed per cycle (kg/h).

To define the law of injection Normalized ROI (Fig. 2), has been introduced the following parameters:

=*phi1*, =*phi2*, =*phi3*, =*phi4* are the values in (°CA) for the injection begins, the duration of injection and the time when the injection are ends, values are calculated:

$$\begin{aligned} phi1 &= inj\_soi \\ phi2 &= inj\_soi + inj\_ramp \\ phi3 &= inj\_soi + inj\_doi \\ phi4 &= inj\_soi + inj\_doi + inj\_ramp \end{aligned} \qquad (5)$$

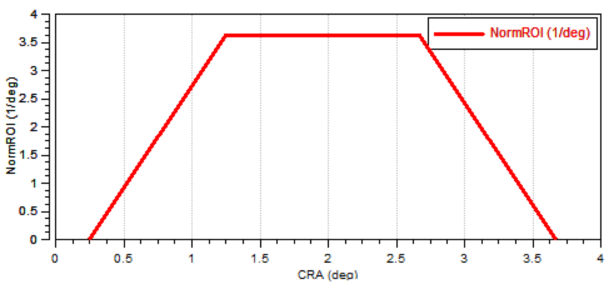

Fig. 2. Theoretical injection law for Normalized ROI.

With the global parameters defined for the time of the start of injection =inj_soi (°CA), and the ramp coefficient of injection =inj_ramp (-) it was calculated the duration of injection (s):

$$= \mathbf{inj\_doi} = \mathbf{fuel\_cyc/inj\_roi} \quad (6)$$

where =inj_roi is the rate of injection (-):

$$= \mathbf{inj\_roi} = \mathbf{inj\_vel} * \mathbf{fuel\_dens} * \mathbf{inj\_area/speed} \quad (7)$$

where =inj_vel is the injection velocity (-):

$$= \mathbf{inj\_vel} = \mathbf{inj\_dc} * (2 * \mathbf{inj\_railp/fuel\_dens})^{2} \quad (8)$$

where =fuel_dens is the density of fuel (kg/m^3), =inj_area is the fuel injection hole area (m^2), =norm_roi is the law of Normalized ROI (1/°CA):

$$= \mathbf{norm\_roi} = \mathbf{inj\_vel} * \mathbf{fuel\_dens} * \mathbf{inj\_area/6/speed} \quad (9)$$

For the simulations with different biodiesel fuel type, engine model created using the Boost program (which has enabled the Classic Species Transport). To generate the types of biodiesel used in Boost Gas Properties Tools were defined the models of biofuel using characteristics from Table II.

TABLE II
THE PROPERTIES OF BIOFUELS

Type of Fuel	Heating Value kJ/kg	A/F Ratio -	Density of Fuel kg/m^3	Carbon Ratio %	Oxygen Ratio %	Molar Mass g/mol
Diesel	44800	14.70	834	86,20	-	226
B10	42270	14.29	848	85.37	1.21	282
B20	38040	14.07	856	82.24	4.47	254
B50	34240	13.40	880	81.33	5.55	271
B100	30620	12.29	884	76.05	11.14	276

Boost Gas Properties Tools allows the user to define the properties of products by combustion for a fuel blend components that can be used later in simulations of Boost. In the fractions that define the components are specified gas mass, gas volume, fluid volume and density of the liquid [10] – [12].

III. RESULTS

After definition of the used biofuels has been run a series of simulations at a speed chosen to 1000 ... 4000 rpm for each model set, and then plot the results in Impress Chart were was analyzed by comparing the curves that define for the rate of heat released (Fig. 3).

A value for the rate of heat released obtained from simulations with biodiesel was present in Table III.

TABLE III
THE VALUES FOR RATE OF HEAT RELEASED

Speed rpm	Diesel	B10	B20	B50	B100
	Maximum Rate Of Heat Released J/°CA				
1000	49.05	48.12	44.74	42.33	41.34
2000	33.66	33.10	30.70	28.96	28.12
3000	39.81	39.32	36.26	33.97	32.47
4000	34.72	34.32	31.62	29.58	28.24
	Rate Of Heat Released J/°CA				
1000	0.449	0.455	0.404	0.364	0.325
2000	0.517	0.523	0.465	0.419	0.375
3000	0.755	0.764	0.680	0.612	0.547
4000	0.785	0.794	0.706	0.636	0.570

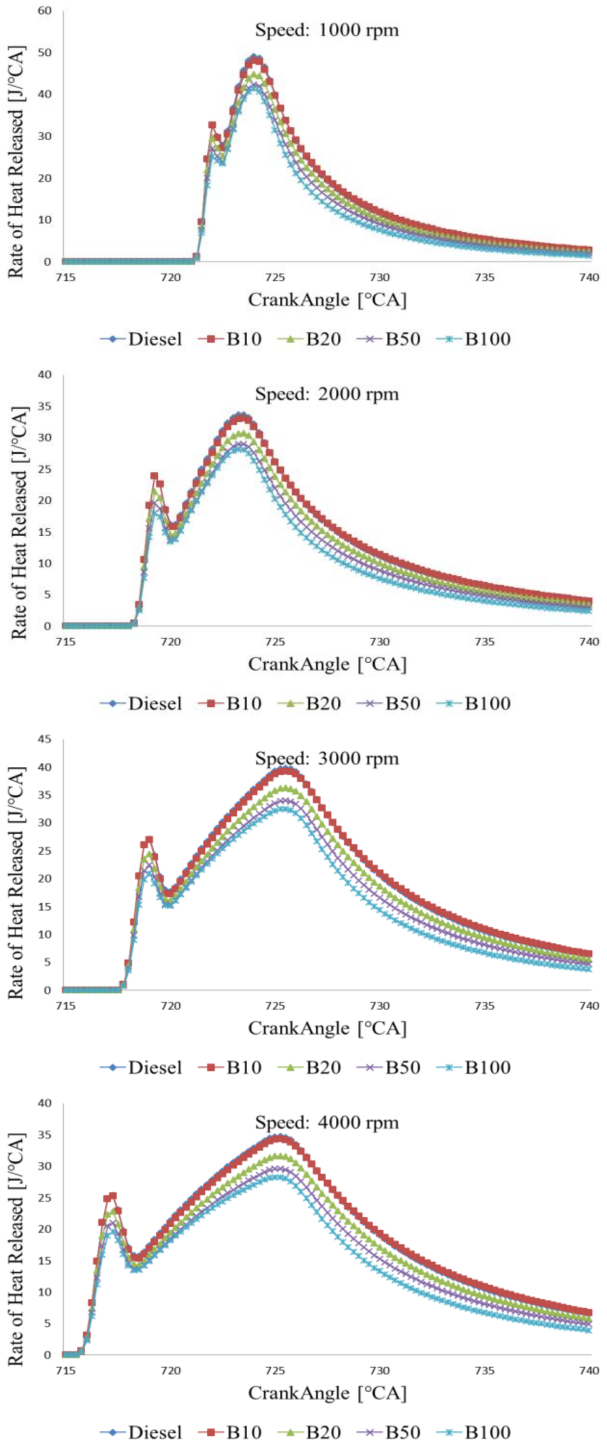

Fig. 3. Simulation results for the rate of heat released ROHR.

Pollutant emissions that have been studied in the simulations with biofuel are nitrogen oxides NO_x and CO carbon monoxide. The results analyze of simulations for NO_x emissions are shown in Fig. 4.

Nitrogen oxides NO_x it is formed by oxidation of nitrogen in the engine at high temperatures. Reduction of NO_x content of exhaust gases can be controlled by setting an optimal point of advance depending on load and engine speed and combustion gas recirculation inlet in place of oxygen for decrease the fuel combustion temperature.

The levels of emissions for nitrogen oxides NO_x increase as the concentration of biodiesel increased due to increased concentration of oxygen in biodiesel.

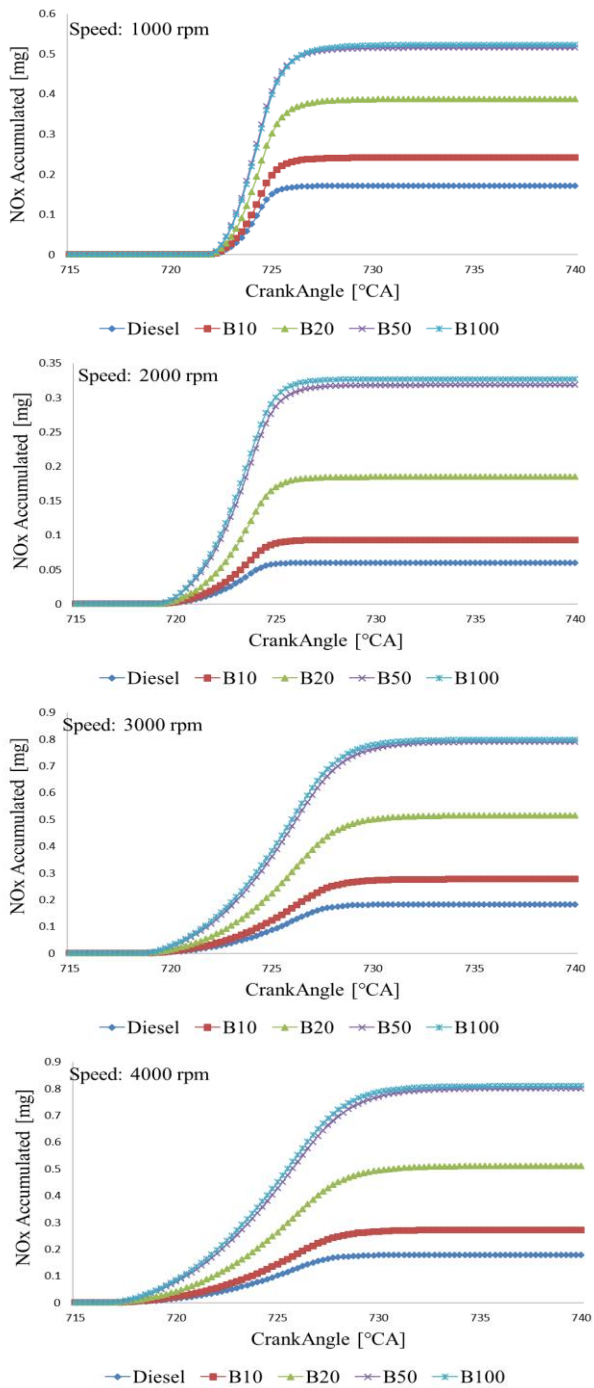

Fig. 4. Emissions of NO_x from biodiesel simulations.

Analyzes of simulations results for CO are presented in Fig. 5.

Carbon monoxide CO is the result of incomplete combustion. Carbon monoxide content of flue gases can be reduced by the catalyst that transforms pollutants into clean gas by optimizing fuel dosage and injection advance [12].

Also due to increased oxygen concentration in biofuel CO concentration values decrease with increasing participation by mixing biodiesel use.

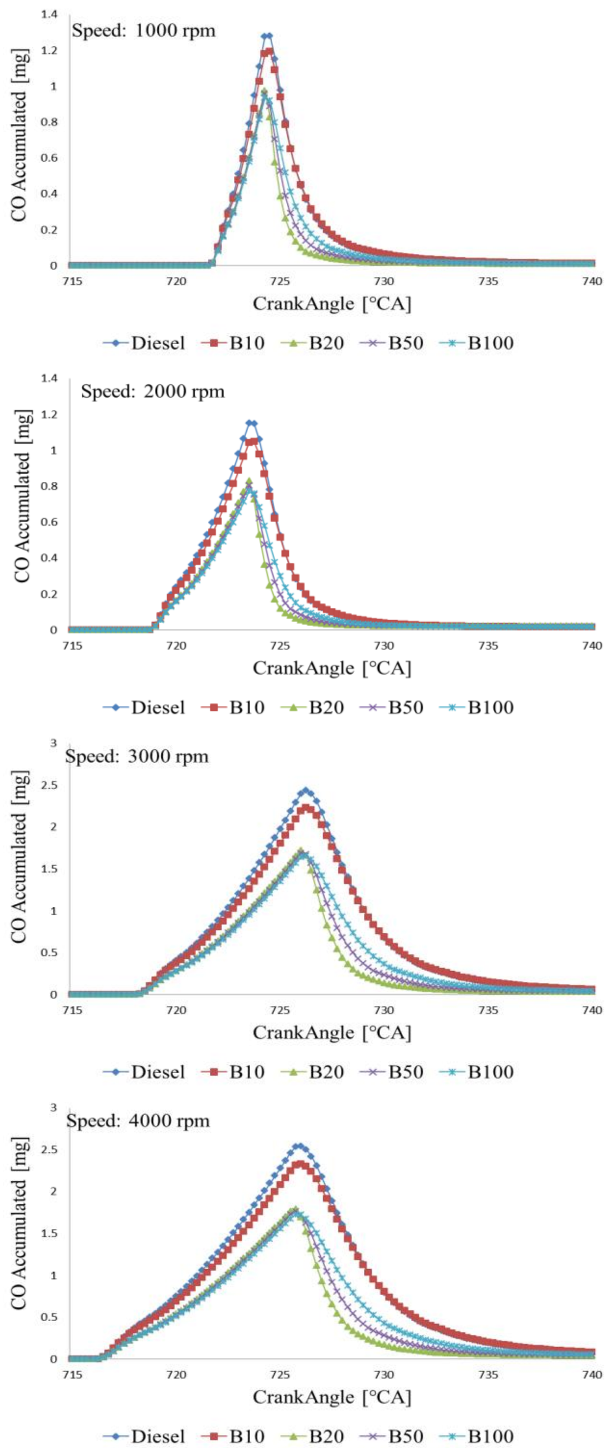

Fig. 5. Emissions of CO in the simulations with biodiesel.

Values for NO_x emissions obtained from simulations with biodiesel are presented in Table IV:

TABLE IV
THE VALUES FOR NO_x EMISSIONS

Speed rpm	Diesel	B10	B20	B50	B100
	Maximum NO_x Emissions mg				
1000	0.171	0.241	0.388	0.515	0.523
2000	0.060	0.093	0.185	0.318	0.327
3000	0.183	0.277	0.515	0.789	0.790
4000	0.179	0.271	0.511	0.800	0.810
Speed	Rate of NO_x Emissions mg/°CA				
1000	0.085	0.119	0.192	0.254	0.258
2000	0.030	0.046	0.092	0.158	0.162
3000	0.090	0.136	0.254	0.393	0.389
4000	0.088	0.134	0.252	0.395	0.400

Values for CO obtained from simulations with biodiesel are presented in Table V:

TABLE V
THE VALUES FOR CO EMISSIONS

Speed rpm	Diesel	B10	B20	B50	B100
	Maximum CO Emissions mg				
1000	1.281	1.194	0.976	0.960	0.936
2000	1.151	1.048	0.830	0.804	0.771
3000	2.438	2.231	1.724	1.690	1.658
4000	2.544	2.333	1.790	1.768	1.725
Speed rpm	Rate of CO Emissions mg/°CA				
	Diesel	B10	B20	B50	B100
1000	0.0096	0.0095	0.0075	0.0073	0.0070
2000	0.0140	0.0135	0.0134	0.0128	0.0120
3000	0.0391	0.0378	0.0277	0.0275	0.0267
4000	0.0492	0.0476	0.0347	0.0338	0.0324

IV. CONCLUSIONS

In the simulations performed it was found that biodiesel is approximately 85% of the energy potential of diesel oil. When biodiesel is blended with diesel oil to more than 20%, the blends behave as conventional diesel. In terms of environmental protection, biodiesel pollutes less than diesel oil, with significant quantities of pollutants, except NO_x levels higher. Biodiesel can be used as fuel in any diesel engines. He has excellent combustion properties leading to a combustion process without sudden increase of pressure and a good running engine has an oxygen content of only 11% which means smaller quantities of soot emitted and has properties good lubrication, is reduced engine wear [12].

In simulations with various models of biodiesel (B10, B20, B50 and B100) showed a decrease of heat released from burning due to low calorific value that is biodiesel. The levels of emissions of nitrogen oxides NO_x emissions increase as the concentration of biodiesel due to increased concentration of oxygen in biodiesel. Also due to increased concentration of oxygen in biodiesel concentration values of CO decreases with increasing participation by mixing biodiesel use.

Main trends in the development of compression ignition engines are reducing emissions and improving fuel economy, namely energy efficiency and environmentally friendly. Main trends in the development of compression ignition engines are reducing emissions and improving fuel economy, namely energy efficiency and environmentally friendly.

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