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Experimental and numerical assessment of ignition delay period for pure diesel and biodiesel B20

Mohanad Aldhaidhawi *,1,2, Marek Brabec 4,5, Miron Lucian¹, Radu Chiriac 1,3, Viorel Bădescu¹

¹ University Politehnica of Bucharest, Faculty of Mechanical Engineering, Spl. Independentei 313, Sector 6, 060042, Bucharest, Romania

²Al-Furat Al-Awsat Technical University, Technical Institute of Kufa, Iraq

³ Associated Member to EA7341 CMGPCE of Conservatoire National des Arts et Metiers, Paris, France

⁴ Institute of Computer Science of the ASCR, Pod Vodarenskou vezi 2, 182 07 Prague 8, Czech Republic

⁵ Czech Institute of Informatics, Robotics, and Cybernetics, Czech Technical University in Prague, Zikova 4, 166 36 Prague 6, Czech Republic

Abstract. The ignition delay period for a compression ignition engine fueled alternatively with pure diesel and with biodiesel B20 has been experimentally and numerically investigated. The engine was operated under full load conditions for two speeds, 1400 rpm speed for maximum brake torque and 2400 rpm speed for maximum brake power. Different parameters suggested as important to define the start of combustion have been considered before the acceptance of a certain evaluation technique of ignition delay. Correlations between these parameters were analyzed and concluded about the best method to identify the start of combustion. The experimental results were further compared with the ignition delay predicted by some correlations. The results showed that the determined ignition delays are in good agreement with those of the Arrhenius type expressions for pure diesel fuel, while for biodiesel B20 the correlation results are significantly different than the experimental results.

Keyword: Ignition delay, biodiesel B20, diesel engine

1. Introduction

Presently, there is an increasing interest in biodiesel behavior as fuel in compression ignition engines due to many environmental and economic benefits. Biodiesel is composed of fatty acids produced from vegetable oil or animal fat via chemical processes called transesterification. Biodiesel has higher cetane number, higher oxygen content, lower aromatics and is free of sulphur content. It is contributing as an improver of the combustion process and reduce the exhaust gas emissions [2-3]. Biodiesel is safe to store and handle due to its high flash point and lower volatility with respect to diesel fuel. Since biodiesel has a higher bulk modulus and higher density, these characteristics lead to an advance in the start of fuel injection [4-8]. The higher cetane number of biodiesel is expected to reduce the ignition delay period resulting in emissions reductions [9,10]. Ignition delay is the period between the start of fuel injection (SOI) and the start of combustion (SOC) [11]. The start of fuel injection is easy to identify because is related to the time when the injector needle lifts off while the start of combustion is more difficult to be defined. There are several methods currently used for the measurement of the start of combustion such as an abrupt change in the cylinder pressure gradient, the combustion of a certain mass of fuel, the change of

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slope in the heat release profile, light emission detected by a photocell diode and cylinder temperature rise due to combustion [11]. An abrupt change in the cylinder pressure gradient and change of slope in the heat release profile methods are widely used to determine the start of combustion in the diesel engines. However, selecting the suitable technique to identify the start of combustion is still an important question in the ignition delay studies. In previous studies, such as that of Alkhulaifi and Hamdalla [12] the start of combustion was determined based on the change of gradient in the heat release rate is determined by the minimum value on the curve. Rodriguez et al. [13] used the maximum value of the first derivative of incylinder pressure as a technique to identify the start of combustion. Assanis et al. [14] concluded that the second derivative of in-cylinder pressure is a suitable method for determining the start of combustion in compression ignition engines compared to the other techniques. Katrasnik et al. [15] determination the start of combustion (SOC) based on the maximum of the third order derivative of the cylinder pressure with respect to the crank angle. Thoo et al. [16] proposed the point at which the net heat-release rate first reaches 2 J/degree, this value was set above the maximum heat-release rate of the motored engine cycles with respect to the crank angle as the appropriate criterion for SOC detection. In Theobald [17] and Dhole et al. [18] the point at which the heat release rate is zero was considered as the initiation of combustion.

The main objectives of this study are to test different parameters suggested as important to define the start of combustion in diesel engine and to choose the best assessment evaluation technique. The experimentally determination of ignition delay period by conducting a series of test runs on a tractor diesel engine under full load operating conditions and engine speeds 1400 rpm and 2400 rpm fueled with pure diesel and biodiesel B20 and comparing it with those obtained from different correlations suggested in previous studies represent the work developed by the research team. This work emphasis some experimental techniques used for ignition delay determination and the differences which occur by comparison with different theoretical correlations.

2. Experimental setup

A tractor diesel engine, four- cylinder, four-stroke, naturally-aspirated, DI was used. Several types of equipment were installed on the test engine to measure the engine performance and combustion characteristic as shown in figure 1. The main engine specifications were listed in table 1. Two AVL GM 12 D pressure transducers with a sensitivity of 15.76 pC/bar were used to measures the in-cylinder pressure rate, and one AVL QL21D pressure transducer with a sensitivity of 2.5 pC /bar was used to measures the high-pressure line values. The pressure transducers measurements will be used later to identify the start of injection and the start of combustion. The fuel system was adapted for multiple fuels operation, allowing the engine to be alternatively fueled with pure diesel and biodiesel B20. The experiment was conducted under full load operating conditions at engine speeds 1400 rpm (speed of maximum brake torque) and 2400 rpm (speed of maximum effective power). The properties of the test fuels pure diesel, biodiesel B20 and B100 (as a reference) were measured in two different places. The cetane number and cold filter plugging point were tested in the laboratories of Rompetrol oil company, located in Constanta city, Romania. The fuels density, viscosity, flash point, pour point and cloud point were tested in the chemical laboratory (LAMC), Bucharest, Romania. The test fuels properties with the test method are listed in table 2.



Figure 1. Schematic layout of the test bench.

Tractor Diesel engine	4-stroke
No. of cylinders	4 in line, vertical
Bore x stroke (mm)	102 x 115
Displacement (cm ³)	3759
Fueling system	Direct injection (DI)
Maximum brake torque (Nm) at 1400 rpm	228
Rated power (kW) at 2400 rpm	50
Compression ratio	17.5:1

Table 1. The main engine specifications.
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Properties	Pure diesel	B20	B100	Test method		
Density (g/cm ³) @ 20°C	0.820	0.8565	0.886	SR EN ASO 3675		
Viscosity (cSt)@ 20°C	2.53	5.12	8.06	SR EN ASO 3104		
Flash point (°C)	58.5	85	184	SR 5489		
Cetane Number	51.1	55.5	-	EN ISO 516598		
Cold filter plugging point (°C)	-24	-18	-	SR EN 116 2016		
Cloud point (°C)	-16	-10	-4	SR EN 23015		
Pour point (°C)	0	-7	-18	SR 13552		
Lower Heating Value (MJ/kg)	41.87	40.59	37.4	ASTM D 240		

Table 2. The test fuel properties.

3. Simulation Procedures

Due to advances in computational hardware, AVL Workspace has become an option to studies the engine performance, combustion process and emissions formation in a wide variety of engines at different operating conditions fueled with different standard fuels such as diesel, gasoline, hydrogen... etc. However, the biodiesel B20 properties were obtained as optional fuel in the AVL Boost program by the authors using the AVL procedures and data bases. Two models were created to understand the combustion process, one in AVL Boost and the other in AVL Fire.

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3.1. AVL Boost Simulation Model

The engine model was built by using the AVL Boost 2016 simulation code to estimate the performance, combustion characteristic, and emissions. The model calibration for the combustion chamber process initially was selected based on documentation (AVL Boost theory and AVL Boost users guide v2016) [19]. The calibration parameters were adjusted according to the model results to reach a good agreement with experimental data. All engine components, such as the intake manifolds, air filter, cylinder geometry, system boundaries, exhaust pipe, and catalyst geometry were based on the real values taken from the test engine and linked together by pipes and implemented in the Boost interface as shown figure 2. The start and the rate of fuel injection, the air mass flow, and the fuel mass flow rate were experimentally measured at specified operating conditions to implement them in the AVL Boost before running the program. The AVL- MCC combustion model and the Woschni 1990 heat transfer model were chosen.

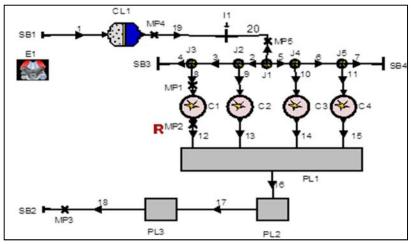
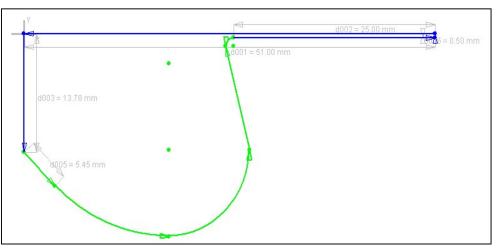
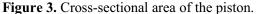


Figure 2. Schematic of the engine symbolic model.

3.2. AVL Fire Model

The simulation model was created by using the AVL Fire 2016 simulation. The 2D Sketcher software from AVL Fire was used to draw the piston bowl shape, and ESED was used for injector shape, block structure, and selections. The importance of the piston shape is due to the need for controlling the flow of fuel and air inside the cylinder together with injector characteristics. Piston bowl dimensions were considered according to the official work drawing of the part obtaining thus a cross-sectional area of the piston, as it is presented in figure 3. The injector characteristics were considered as five holes with 0.000239 m nozzle diameter with a spray angle of 160 degrees. Computational meshes were created by using the parameters entered in the block structure section. An average cell size of 0.001m was chosen in order to reduce the computational time. A compensation volume was adopted to take into account the pressure losses alongside the piston rings, thus obtaining a dynamic compression ratio equal to 16.4. The resulted mesh is seen in figure 4. AVL Fire ESED uses complex mathematical models with the aim of simulating the fuel spray development, vaporization, combustion and pollutant emissions formation specific to the direct injection diesel engine. The calculations were made within a range of -80/+80 crank angle degree (°CA) specific to top dead center (TDC) using initial values as cylinder pressure measured data and calculated bulk temperature obtained from AVL Boost. The ECFM-3 combustion model was used as it is specific to the diesel combustion process because it best correlates with our experimental data. The autoignition was controlled using the table autoignition model which utilizes detailed chemical kinetics. The Wave Break-up model was used for fuel jet spray dispersion as it increases the accuracy of the calculation. These models were selected and implemented in the ESED software with the aim of obtaining good accuracy while minimizing computational time.





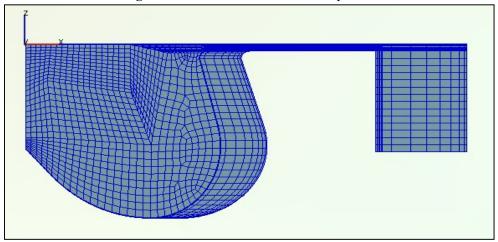


Figure 4. Meshes generated of a piston.

4. Theoretical Approach

The mean value of the cylinder pressure at all operating conditions for both test fuels was obtained from the experimental work. The mean cylinder gas temperature was obtained from the numerical simulation using AVL Boost 2016 code. The mean cylinder pressure and mean gas temperature during the ignition delay period were taken and implemented in several correlations collected from previous studies in order to evaluate the ignition delay period. The correlations were used to estimate the ignition delay for pure diesel fuel as following and to perform comparisons with ignition delays experimentally determined:

• Correlation proposed by Assanis [14]

$$\tau_{D10} = 2.4 \frac{\exp(\frac{2100}{T})}{p^{1.02} \cdot \varphi^{0.2}} \tag{1}$$

• Correlation proposed by Watson [20]

$$\tau_{D100} = 3.45 \frac{\exp(\frac{2100}{T})}{p^{1.02}} \tag{2}$$

• Correlation proposed by Rodriguez et al. [13]

$$\tau_{D100} = \frac{\exp\left(\frac{950}{T}\right)}{p^{0.24} \cdot \varphi^{0.04}}$$
(3)
Correlation proposed by El-Kasaby et al. [21]
$$\tau_{D100} = 26.06 \frac{\exp(\frac{1038}{T})}{p^{1.21} \cdot \varphi^{1.36}}$$
(4)

Only one correlation proposed in [21] was used to estimate the ignition delay period for biodiesel B20. The results obtained from this equation were compared with experimental data at both engine speeds under full load conditions:

$$\tau_{B20} = 74.32 \ p^{-1.32} \ \varphi^{-1.39} \exp(\frac{1022}{T}) \tag{5}$$

Here: τ -ignition delay period (ms), T-temperature (K), p- pressure (bar), φ -equivalence ratio.

5. Results and Discussions

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In this part of the study, the results from the simulation study are first compared to the experimental results to examine the usefulness of the models. In the second part, the start of combustion is estimated by using different methods. In the third one, the effect of diesel and biodiesel blend B20 on the ignition delay period is presented.

5.1. Cylinder Pressure

The variations of cylinder pressure with respect to the crank angle position, experimental and simulation (obtained from AVL Boost and AVL Fire) for diesel fuel at different engine speeds and full load operation conditions are given in figure 5. From this figure, a good agreement between experimental trace as average over 200 consecutive cycles and the simulations results can be observed. The relative deviation between the experimental and numerical for maximum cylinder pressure obtained from AVL Boost and AVL Fire for diesel fuel at engine speed of 2400 rpm is 1.108% and 0.95%, respectively. Similar good agreements between simulation and experiments have been obtained for all operating conditions specified in this study.

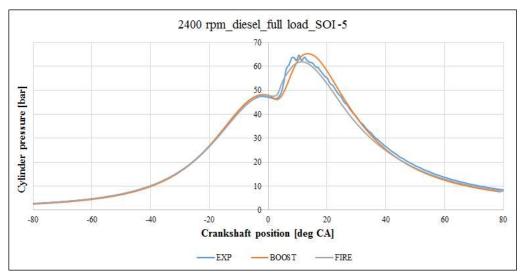


Figure 5. Comparison between experimental and simulation pressure traces for full load, 2400 rpm speed, diesel fuel.

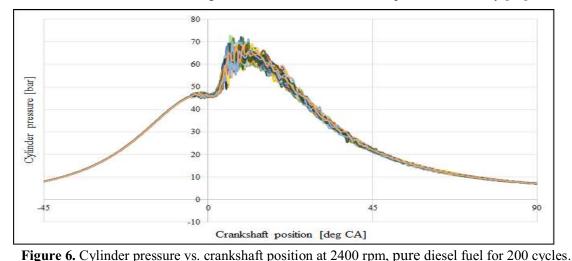
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5.2. Estimate the Start of Combustion (SOC)

There are several technical methods in the literature that were used to identify the start of combustion in compression ignition engines. The start of combustion was determined from the cylinder pressure and rate of heat release curves by using several evaluation techniques before the acceptance of a certain evaluation that was used to estimate the ignition delay period. The needle lift, the rate of heat release and the cylinder pressure results were used based on the average of 200 successive cycles. The large number of cycles was necessary to avoid the random deviations in measurements. To explore the SOC from the cylinder pressure trace and rate of heat release curve, a model for smoothing data was needed. Therefore, the raw data were smoothed via penalized spline GAM model (mgcv library in R), the fitted curve differentiated numerically via Deriv function from Pracma library (with step size 0.1). The raw cylinder pressure of diesel engine at 2400 rpm under full load conditions fueled with pure diesel fuel for 200 successive cycles is given in figure 6. The first and second derivatives result of smoothed cylinder pressure for all cycles were determined by this model and it is shown in figure 7. Figure 8 presents the start of combustion identified from the maximum value of the first, second, third and fourth order derivative (D1f, D2f, D3f, and D4f, respectively) of the cylinder pressure (as an example for one cycle). As shown in this figure, there is some deviation in SOC estimated from different derivatives. However, the second order derivative was more sensitive to identification of the start of combustion in comparison with the other derivatives. This finding is consistent with the results reported in the study [14].



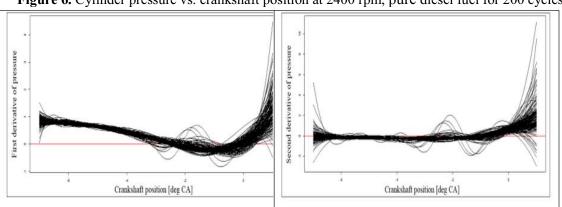


Figure 7. First and second order derivative of smoothed cylinder pressure at 2400 rpm, pure diesel fuel for 200 cycles.

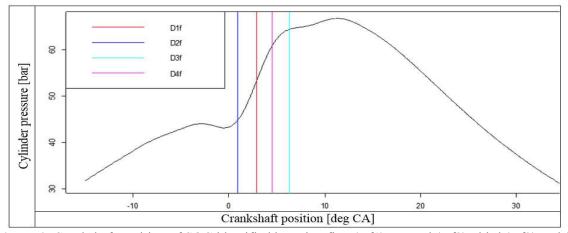


Figure 8. Crankshaft position of SOC identified by using first (Df1), second (Df2), third (Df3) and fourth (Df4) order derivative of cylinder pressure at 2400 rpm under full load fueled with pure diesel fuel for 200 cycles.

There is another method that was covered in this study to identify the start of combustion from the rate of heat release curves. The rate of heat release curves for 200 cycles for engine fueled with diesel fuel and running in the same conditions (full load and engine speed 2400 rpm) is given in figure 9. Figure 10 presents the smoothed of the rate of heat release. Here, the start of combustion SOC was considered as the root of the rate of heat release ($dQ_f/d\varphi = 0$) (see figure 11). Figure 12 presents the distributions of the start of combustion that were determined from the second order derivative of the cylinder pressure (the most sensitive way to identify the SOC compared to other derivatives according to our findings) and from the root of the rate of heat release. As shown in this figure, the root of the rate of heat release method appeared more sensitive for identification of the SOC than the second order derivative method, due to normal distributions of SOC with this method. However, the same steps listed above were followed to determine the SOC inside the cylinders when using pure diesel and biodiesel B20 at different engine speeds under full operating conditions. The same conclusion was obtained, that the root of the rate of heat release method ($dQ_f/d\varphi = 0$) is the proper technique to be used to identify the SOC. Therefore, this method will be considered in the determination of SOC in our calculation to predict the ignition delay period.

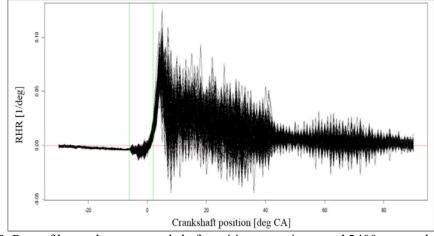


Figure 9. Rate of heat release vs crankshaft position at engine speed 2400 rpm under full load fueled with pure diesel fuel for 200 cycles raw data.

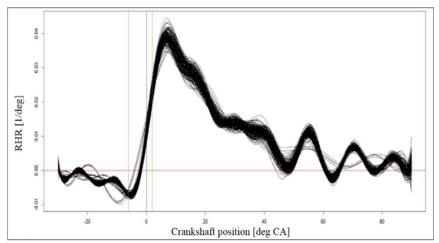


Figure 10. Rate of heat release smoothed curves vs at engine speed 2400 rpm at full load fueled with pure diesel fuel for 200 cycles.

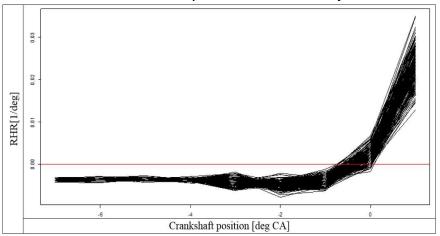


Figure 11. Crankshaft position of SOC estimated by using zero root of rate of heat release at 2400 rpm, full load fueled with pure diesel fuel for 200 cycles.

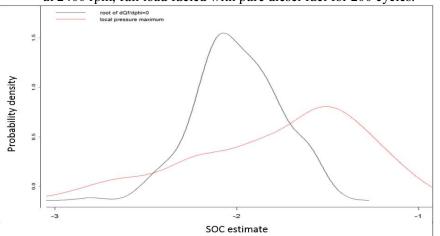


Figure 12. SOC distribution estimated from the rate of heat release (zero root) and from second order derivative of cylinder pressure at 2400 rpm under full load fueled with pure diesel fuel for 200 cycles.

5.3. Ignition delay period

Ignition delay period (ID) as mention before, is the duration between the start of fuel injection SOI and the start of combustion SOC [11]. In this study, the start of injection was taken as the time when the injector needle lifts off (threshold value was equal to 0.002 mm) while the start of combustion corresponds to the zero root of the heat release rate. The variations of needle lift versus the crankshaft position for diesel fuel at the engine speed of 2400 rpm and full load operating conditions for 200 cycles are presented in figure 13. The experimental tests were repeated three times in different days trying to keep the same ambient initial conditions (temperature 35°C and barometric pressure 1bar in the test cell) to verify the consistency of experimental data. At engine speed of 2400 rpm the start of injection for the average of cycles was 5 degrees before top dead center (BTDC).

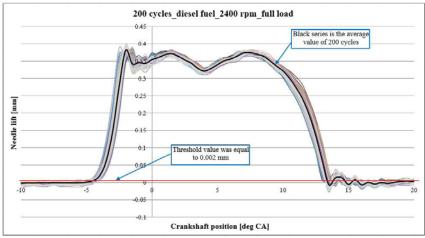


Figure 13. Needle lift vs. crankshaft position at full load conditions and 2400 rpm engine speed, the black series is the average value comprised in the envelope of 200 cycles, the SOI was considered at the threshold value equals to 0.002 mm.

The start of combustion (SOC) was placed at the zero root for the rate of heat release characteristic profile for tested regime, as presented in figure 14. Thus, the start of combustion point (average of cycles) was identified at 0.375 degree after top dead center (ATDC) at 2400 rpm speed. These values (SOI and SOC) for both engine operating conditions were taken into consideration to calculate the ignition delay period.

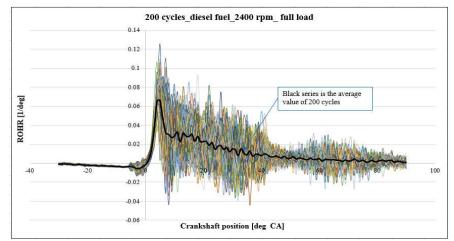


Figure 14. Rates of relative heat release vs. crank angle at full load and 2400 rpm engine speed, the black series is the average value comprised in the envelope of 200 cycles.

The mean cylinder pressure and temperature during the ignition delay period were used to estimate the ignition delay from different correlations. The results obtained from these correlations were compared to the experimental data. The ignition delay period for pure diesel and biodiesel B20 fuels, calculated from different correlations, are listed in table 3. Regarding diesel fuel, there are some deviations between the results that were obtained from these correlations with the experimental data. However, the correlation proposed by Assanis [14] is the closest to the experimental results, with relative deviations of 13% and 14.5% at engine speeds 1400 rpm and 2400 rpm, respectively. Concerning biodiesel B20, there is a significant difference between the experimental results and the results that were obtained from the correlation previously proposed by Al-Kasaby [21], with relative deviations of up to 75% and 80.54% at engine speeds 1400 rpm and 2400 rpm, respectively. The ignition delay period for biodiesel B20 was shorter than that of pure diesel fuel at the same operating conditions. This behavior may be due to the fact that the biodiesel has higher cetane number compared to pure diesel fuel.

Table 3. Ignition delay estim	nated from different correlations
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For pure diesel fuel											
Engine speed	SOI	SOC	Duration	ID EXP	Р	Т	Phi	Assanis [14]	Watson [20]	Rodriguez [13]	EL-Kasaby [21]
[rpm]	[deg CA]	[deg CA]	[deg CA]	[ms]	[bar]	[K]	[-]	[ms]	[ms]	[ms]	[ms]
1400	-6	-0.33	5.67	0.394	44.39	994.5	0.64	0.453	0.595	1.065	1.38
2400	-5	0.375	5.37	0.37	46.93	1008.4	0.52	0.433	0.546	1.046	1.69
For biodiesel B20 fuel											
	SOI	SOC	Duration	ID EXP	Р	Т	Phi				EL-Kasaby [21]
1400	-6	-0.25	5.75	0.39	41.61	957.15	0.64	-	-	-	1.56
2400	-5	0.125	5.125	0.356	44.7	990.38	0.52	-	-	-	1.83

6. Conclusions

The ignition delay period for a compression ignition engine fueled with pure diesel fuel and biodiesel B20 at engine speeds 1400 rpm and 2400 rpm under full load operating conditions were experimentally determined. The experimental results were compared to that obtained from different correlations proposed in several studies by different authors. The main conclusions of this study are the following:

- The root of the rate heat release is a sensitive and proper method to identify the start of combustion compared to other methods that were considered.
- The correlation proposed by Assanis [14] seems to the closest to the experimental results for pure diesel fuel at tested operating conditions with relative deviations lower than 15%.
- The ignition delay period for B20 was shorter than that of pure diesel at same operating conditions.
- The correlation proposed by El- Kasaby [21] to predict the ignition delay period for biodiesel B20 is far than experimental results.
- This work marks a starting point which has to be followed by the efforts to investigate the combustion process of the diesel engine fueled with pure diesel fuel and biodiesel B20 at other engine speeds and full load condition.

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