SEPARATE DIRECT INJECTION OF DIESEL AND ETHANOL A Numerical Analysis

by

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The purpose of this study is to investigate the theoretical possibility of using a pilot diesel injection for the auto-ignition of a main ethanol injection in a compression ignition engine. To this effect a predictive simulation model has been built based on experimental results for a diesel cycle (pilot and main injection) at 1500 and 2500 min⁻¹, respectively. For every engine speed, in addition to the diesel reference cycle, two more simulations were done: one with the same amount of fuel injected into the cylinder and one with the same amount of energy, which required an increase in the quantity of ethanol proportional to the ratio of its lower heating value and that of diesel. The simulations showed that in all cases the pilot diesel led to the auto-ignition of ethanol. The analysis of the in-cylinder traces at 1500 min⁻¹ showed that combustion efficiency is improved, the peak temperature value decrease with approximately 240 K and, as a result, the NO emissions are 3.5-4 times lower. The CO and CO₂ values depend on the amount of fuel injected into the cylinder. At 2500 min⁻¹ there are similar trends but with the following observations: the ignition delay increases, while the pressure and temperature are lower.

Key words: diesel, ethanol, simulation, combustion, direct injection, dual-fuel

Introduction

For year 2020 the European Directive 2009/28/EC stipulates a minimum share of 20% bioenergy for every country of the European Union [1], while for transportation it sets a target of minimum 10% biofuel. This requires that vehicle manufacturers adapt their engines to the new regulations with respect to the most commonly used biofuels (currently): biodiesel and bioethanol [2, 3]. The main objective of the current study is to investigate the possibility of increasing the biofuel percentage inside a compression ignition engine by employing a separate direct injection of diesel and ethanol. For this engine cycle, the diesel fuel would be used as a pilot injection that can create favorable auto-ignition conditions for a main injection of ethanol. When it comes to the use of ethanol in compression ignition engines there are numerous studies that investigate several possibilities:

ethanol fumigation [4-9], ethanol is added to the intake air as a low reactivity fuel, while a pilot diesel injection is used to initiate combustion. The disadvantages of this method are the limited compression ratio (in order to prevent knock) and the ethanol quantity that can be added (determined by the amount of ethanol that can evaporate into the intake air),

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mixing of ethanol and diesel fuel [10-18], ethanol is injected into the cylinder with the diesel fuel as blend. The main disadvantage of this method is the occurrence of phase separation (determined by temperature, water content, and the presence of an additive – biodiesel can be used).

However, there are very few studies regarding the separate direct injection of ethanol in the compression ignition engine. A Diesel engine running on only ethanol is presented in [19] but, in order to achieve reasonable ignition delays, it was required that the compression ratio of the engine be increased as well as an ignition additive be added to ethanol (the fuel used was designated ED95, which contains 5% ignition improver). In contrast, this theoretical study aims to use a pilot diesel injection and no alterations of the compression ratio to achieve ethanol auto-ignition. However, this technology is not available at the moment and therefore, the simulations can not be supported by experimental results. In addition to a brief description of the current methods of adding ethanol in Diesel engines, the possibility of employing a separate direct injection of diesel and ethanol is presented in [20] but, this is done by analogy with a dual-fuel engine running on diesel and natural gas (only one injector, capable of injecting both fuels is used). Even so it highlights the possible advantages of using a separate direct injection of diesel and ethanol: increased efficiency (dependent on engine speed and load), very low CO₂ emissions (considering the fuel life cycle analysis), lower smoke and particulate emissions, and in the end, a better energy security. By employing a separate direct injection of diesel and ethanol, the disadvantages of the other methods (fumigation blends) are avoided. Also due to the fact that ethanol injection continues even after auto-ignition, this leads to a diffusive combustion of the fuel. As a result, the pressure gradients are much lower than in the case of premixed combustion of ethanol. The main drawbacks of this method are the more complicated engine management and the necessity of using to fuel tanks and injection systems, the latter can be solved by employing a dual-fuel injector [20].

Methodology

This theoretical study is based on experimental research performed in the Laboratory for testing of internal combustion engines that run on biofuels (TESTECOCEL) managed by the Department of Automotive Engineering and Transportation of the Faculty of Mechanics, Technical University of Cluj-Napoca, Romania. The tests were done on a single cylinder compression ignition engine built for research purposes, namely the AVL 5402 [4]. The relevant test parameters set in the engine control software, tab. 1, were chosen from the engine operation map provided by the manufacturer.

Engine speed [min ⁻¹]	Load [–]	Rail pressure [MPa]	Pilot quantity [mg]	Pilot timing [°CA]	Main quantity [mg]	Main timing [°CA]
1500	High	80	0.5	25.125	15.2	4.875
2500				28.125	11.8	12.000

Table 1	l. Test	parameters
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After obtaining the necessary experimental data, the simulation models were built using the AVL Fire [21] software. As a first step, simulations were performed on a model with complete intake and combustion chamber geometry, fig. 1, described in [22]. Due to the high computational costs (approx. 72 hours per run), the purpose of these simulation was only to determine the temperature and charge motion inside the cylinder after intake valve closing.

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These values would then be used as input data for the cycle simulation in a secondary, more simplified model. To this end, because of a symmetrical combustion chamber with respect to the cylinder axis, it was possible to run an engine sector simulation, fig. 2, corresponding to one injector hole which, in this case means 1/8 of the whole cylinder. However, elements like the valve cuts in the piston can not be represented and therefore, in order to match the engine compression ratio, a compensation volume has to be used. The models used to predict the physical phenomenon in these simulations are:

- combustion model: ECFM-3Z,
- spray calculations: WAVE breakup and multi-component evaporation,
- NO formation: extended Zeldovich model, and
- soot formation: kinetic model.





Figure 1. Complete intake and cylinder geometry model

Figure 2. Engine sector mesh (75 800 cells)

To be able to use the simulation model as a predictive model it was validated with the experimental results for the following parameters: in-cylinder pressure and temperature, rate of heat release, and NO_x emissions. It must be noted that the simulation model is not capable of predicting all the components that form nitric oxides, only the NO values but, because NO_x consists of 90-98% NO [23] it can be considered to be representative.

For the comparison with the simulation, the experimental values were analyzed using thermodynamic relations available in the literature [12, 24]. The experiment-simulation comparison for 1500 min⁻¹ (M1500) is presented in figs. 3-6. It can be seen that there is a good agreement between the traces (there is a difference of less than 3% between the mean values). For the phase without combustion there is an almost complete overlap of the curves, while for combustion phase some differences arise which can be argued by:



Figure 3. The M1500 validation vs. cylinder pressure



Figure 4. The M1500 validation vs. cylinder temperature



Figure 5. The M1500 validation vs. rate of heat release

Figure 6. The M1500 validation vs. NO emissions

- uncertainties concerning the actual amount of fuel injected into the cylinder compared to the values chosen by the user in the engine control software,
- differences between the actual injection rate and the one used in simulations, which was
 estimated using the AMESim software,
- the actual in-cylinder conditions after intake valve closing and the values obtained through simulation might differ, and
- simplified hypothesis used by the employed simulation models and for thermodynamic analysis of the experimental values.

For the 2500 min⁻¹ case (M2500) presented in figs. 7-10 there is a similar experiment-simulation trend but with somewhat higher differences due to bigger uncertainties regarding fuel injection. However, the error remains under 3%.



Figure 7. The M2500 validation vs. cylinder pressure



Figure 9. The M2500 validation vs. rate of heat release



Figure 8. The M2500 validation vs. cylinder temperature



Figure 10. The M2500 validation vs. NO emissions

As a result of the good agreement between experiment and simulation it was considered that the models can be used as predictive models. As a first step the pilot injection quantity was changed to 1 mg and the simulations were ran again for both engine speeds. The results were considered as the diesel reference cycles and were assigned the following notations: D100_D100_1mg_15mg (for the 1500 min⁻¹ case) and D100_D100_1mg_12mg (for the 2500 min⁻¹ case) where 15 mg and 12 mg depict the main injection quantities presented in tab. 1. The next step involved the simulation of the pilot diesel, main ethanol injection cycles. For each engine speed, two different cases were considered:

- (a) the ethanol quantity injected in the cylinder is the same as for the diesel reference cycle, which led to the following notations: D100_E100_1mg_15mg (for the 1500 min⁻¹ case) and D100_E100_1mg_12mg (for the 2500 min⁻¹ case), and
- (b) the energy quantity introduced in the cylinder is equal to that of the reference cycle, which requires increasing the ethanol quantity with the ratio of its lower heating value and that of diesel fuel. This led to the following notations: D100_E100_1mg_24mg (for the 1500 min⁻¹ case) and D100_E100_1mg_19mg (for the 2500 min⁻¹ case).

If detailed chemistry is not used, the classic combustion simulation models can not predict a correct combustion for two different fuels injected separately into the cylinder at different times of the engine cycle. Although the spray models can consider the different parameters of the fuels and their influence on the jet, the combustion models are unable to calculate a correct heat release. This is due to the fact that only one fuel can be selected for species transport (be it a blend or a pure fuel). In order to simulate the cycle with pilot diesel and main ethanol injection, a different simulation strategy was employed. As a first step, for each engine speed, the simulation parameters were saved after the pilot injection and its combustion, just before the main injection with 0.5 and 0.25 °CA, respectively. This way, the simulation can be restarted from the saved point without any loss of information inside the cylinder. As a second step, the transported fuel was changed to ethanol and the main injection quantity was corrected – see point (b). The last step was to restart the simulation from the saved point with the new parameters. The simulation/injection strategy is presented in fig. 11. It must be noted that this strategy introduces an error in the total amount of energy, which depends on the quantity of pilot fuel that did not burn before the point of restart and for a large enough interval between the injections, this can significantly decrease. By relating the pilot energy loss



Figure 11. Simulation strategy for the pilot diesel and main ethanol injection cycle

to the theoretical amount of energy that was supplied to the cylinder, this leads to an error of 1.16% for 1500 min⁻¹ and 3.1% for 2500 min⁻¹.

Results and discussions

In order to assess the differences between the reference diesel cycle and the pilot diesel, main ethanol injection cycle the following parameters have been compared: cylinder pressure and temperature, heat release, and pollutant emissions (CO, CO₂, NO, and soot). Several combustion chamber cuts are studied for a more clear understanding of the phenomenon (equivalence ratio, NO mass fraction, and temperature).

The 1500 min⁻¹ case (C1500)

In the D100_E100_1mg_24mg case the same amount of energy as in the reference diesel cycle (D100_D100_1mg_15mg) is supplied to the cylinder. However, due to an improved combustion efficiency of ethanol as well as a prolonged heat release, the peak cylinder pressure increases, fig. 12. As a result of the lower heating value of ethanol, if the same amount of fuel is injected into the cylinder (D100_E100_1mg_15mg), the pressure drops below that of the reference cycle. The temperature traces, fig. 13, for the studied cases are similar to that of pressure, considering that the two thermodynamic values are proportional. As for pressure, the highest mean in-cylinder temperature was obtained in the D100_E100_1mg_24mg case. The heat release rates, fig. 14, do not differ considerably. However, that is not the case with the accumulated heat released. While for the D100_E100_1mg_15mg case the end value increases, fig. 15, which is a result of the higher burning efficiency of ethanol. Compared to a maximum theoretical value of 694 J, the pilot diesel, main ethanol cycle produced 690.5 J, a value significantly higher than that of the diesel cycle which produced only 648.6 J. The advantage of using ethanol was reported by many authors [25-29].

Although the use of ethanol has its advantages when it comes to efficiency, there are some drawbacks in terms of pollution. On the one hand, in the D100_E100_1mg_15mg the in-



Figure 12. The C1500 vs. cylinder pressure

cylinder temperature is significantly lower than in the reference case and as a result, the CO oxidation is stopped, fig. 16, leading to higher end values. On the other hand, by injecting the same fuel quantity inside the cylinder - point (a) the CO₂ emissions drop significantly, fig. 17, because of an incomplete oxidation of CO and a much lower carbon (C) content of ethanol (C_2H_5OH) . In the D100 E100 1mg 24mg case the mean temperature is above that of diesel, thus favoring CO oxidation. Combined with the lower C content this leads to lower CO and CO_2 values. As can be seen in fig. 18, soot production is well under the value for diesel in both pilot diesel and main ethanol cases. This can be argued, as in the case of CO₂, by the lower C content of ethanol, which sustains the idea of a more clean combustion. Consequently, the end values for D100 E100 1mg 15mg and D100 E100 1mg 24mg are approx. 2 times smaller.





Figure 13. The C1500 vs. cylinder temperature

800

700

600

500

400

300

200

100

0

released [J]

Accumulated heat

Figure 14. The C1500 vs. rate of heat release



Figure 15. The C1500 vs. accumulated heat release

Crank angle [°CA]

Figure 16. The C1500 vs. CO emissions

In addition to the fact that ethanol can be produced from renewable sources, the main advantage of the D100 E100 cycles are much lower NO values. In fig. 19 it can be seen that, compared to the diesel reference cycle, the NO values are about 3.5-4 times smaller. Considering that the parameters important for NO formation are temperature, the dissociation of O_2 and N_2 molecules into atomic oxygen (O) and atomic nitrogen (N) as well as the production of OH radicals, in the D100 E100 1mg 15mg case, lower NO values are to be expected. For the



D100_E100_1mg_24mg this requires a more detailed analysis, because the mean temperature curve is in a 20 °CA interval (from 728 °CA to 748 °CA) above that of diesel.

1600

Figure 17. The C1500 vs. CO₂ emissions



Figure 19. The C1500 vs. NO emissions



Figure 18. The C1500 vs. soot emissions

To explain these trends, several cuts in the combustion chamber for the diesel reference case, as well as for the pilot diesel, main ethanol cases are presented in figs. 20-25. This is considered to be a more facile way to highlight the differences between the cycles. The parameters for comparison are: the equivalence ratio (for fuel distribution and mixture formation), NO mass fractions (provide information regarding the locations where nitric oxides are formed), and in-cylinder temperature (the temperature fields highlight not only the fuel combustion evolution but also the favorable locations for NO formation). The image

analysis led to the following conclusion concerning the two cycles with pilot diesel and main ethanol injection:

- ethanol is better distributed inside the combustion chamber due to its lower density and due the motion of the charge; this favors a stoichiometric combustion (figs. 20 and 23),
- as a result of its inferior lower heating value ethanol produces through combustion a smaller quantity of heat; combined with its higher enthalpy of vaporization this leads to lower temperatures inside the combustion chamber,
- lower temperatures positively affect NO emissions because the conditions required for the dissociation of O₂ and N₂ are not achieved;
- NO emissions start to form where the equivalence ratio is close to 0.9 and the temperatures are higher than 1800 K, and
- ethanol combustion starts in a location close to where the pilot diesel burned.

There are, however, some differences between the two ethanol cycles described at points (a) and (b) in the section Methodology. On the one hand, in the D100 E100 1mg

_15mg case the CO emissions increase as a result of the lower temperature. On the other hand, in the D100_E100_1mg_24mg case the following can be highlighted:





- a detailed analysis of fig. 25 revealed lower peak temperatures compared to the diesel reference cycle values (with approx. 240 K, which leads to NO formation rates that are 3.5 times smaller); also, the temperature is more evenly distributed (fig. 25 at 740 °CA) in the combustion chamber it justifies the increase of the mean value,
- higher temperatures favor CO oxidation, which leads to lower end values,
- the NO emissions increase compared to the D100_E100_1mg_15mg case but they remain well under those of D100_D100_1mg_15mg, and
- injection duration is increased due to the higher ethanol quantity required to match the energy values of diesel; as the cycle proceeds the heat released through combustion is used for ethanol evaporation and this way a lower temperature is maintained.

It has to be noted that in both cases, the use of a pilot diesel injection favored the auto-ignition of the main ethanol injection. Because only a small part of ethanol and air are mixed before the start of combustion and the injection continues during the process, ethanol burns diffusively.

The 2500 min⁻¹ case (C2500)

For the 2500 \min^{-1} case there are similar trends to those of the 1500 \min^{-1} case, but there are also some observations:

- the higher engine speed leads to a reduced time for the combustion of the pilot injection and also to a higher ignition delay; in both pilot diesel, main ethanol injection cases the pressure traces are slightly retarded due to the higher auto-ignition delay; as a result, the peak pressure values are below those of D100 D100 1mg 12mg,

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- the temperature curve is in both situations under that of the diesel reference case; this is due to the higher ignition delay combined with the combustion in the expansion stroke (the cylinder volume increases and consequently the temperature drops),
- the analysis of the accumulated heat release compared to the theoretical value (547 J) revealed that the advantage of the pilot diesel, main ethanol case decreased (528 J for D100_E100_1mg_19mg compared to 521 J for D100_D100_1mg_12mg),
- the lower temperature values led to a poorer conversion of CO to CO₂ in both cases, and
- as in the 1500 min⁻¹ case, the use of ethanol for the main injection led to lower NO values.
 For this case, only the parameters for which there is a noticeable difference between

the reference diesel cycle and the pilot diesel main ethanol cycle are presented (figs. 26-29).

350

300

250

200

150

100

50

0

NO [ppmv





Figure 26. The C2500 vs. cylinder pressure

Figure 27. The C2500 vs. cylinder temperature



Figure 28. The C2500 vs. rate of heat release



640 660 680 700 720 740 760 780 800 820

Crank angle [°CA]

Conclusions

The objective of this study was to investigate the characteristics of an engine cycle with a pilot diesel that can create the necessary auto-ignition conditions for a main ethanol injection, with both fuels injected directly into the cylinder. By employing a specific simulation strategy it was possible to simulate such a cycle without the use of detailed chemistry models. The analysis of the obtained results led to the following conclusions:

- In all cases the pilot diesel injection favored the auto-ignition of ethanol.
- If the same quantity of fuel is injected into the cylinder, point (1) in the section Methodology, the following conclusions can be drawn:
- the peak in-cylinder pressure decreases,
- the temperature curve is below that of the reference diesel case,
- CO emissions increase, and
- CO₂ and NO emissions decrease;
- If the same quantity of energy is supplied to the cylinder, point (2) in previous section, the conclusions that can be drawn are:
- the peak in-cylinder pressure increases,
- the mean temperature curve is above that of diesel in small interval, but the peak values are with approx. 240 K lower,
- the total amount of heat released is higher due to an improved combustion of ethanol, and
- CO, CO₂, and NO emissions decrease;
- Raising the engine speed from 1500 to 2500 min^{-1} led to:
- higher CO and CO₂ emissions in both pilot diesel, main ethanol injection cases, and
- an increased ignition delay.

Based on the results of this study, future experimental research can be developed to validate the concept.

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