Simulation of a Diesel Engine Operating with Ethanol to Reduce Pollutant Emissions

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In this study a computational model to simulate the operation of a diesel engine fuelled by blends of 95% diesel oil + 5 % biodiesel (B5) and anhydrous ethanol was developed. The model was developed using the Engineering Equation Solver (EES) software and calculates fuel and air properties and the thermodynamic processes of the engine cycle. Ethanol injection was investigated by two different techniques: direct injection in the combustion chamber, together with B5, and indirect injection in the intake air system, with B5 being directly injected in the combustion chamber. Fuel/air mixture equivalence ratio, compression ratio, and the injected amount of ethanol were varied to obtain the cycle temperature and pressure diagrams, fuel consumption, indicated power, and exhaust gas composition. Fuel/air mixture equivalence ratio was varied from 0.7 to 0.9, compression ratio was varied from 15:1 to 19:1, directly injected ethanol concentration was varied up to 20 % of the total fuel amount injected, and intake system injected ethanol concentration was varied up to 50 % of the total fuel amount injected. The results demonstrate that the use of ethanol can reduce carbon monoxide (CO) and oxides of nitrogen (NO_X) emissions, slightly penalizing the net cycle work and increasing fuel consumption. Direct ethanol injection in the combustion chamber was shown to be more advantageous technique than indirect ethanol injection in the intake system.

1. Introduction

There is a growing fuel demand to meet the increasing number of vehicles and, as a consequence, there is a need to minimize the environmental impacts generated by fuel burning. The two main challenges faced in relation to internal combustion engines are reducing emissions and fuel consumption (Payri et al., 2011). In the case of diesel engines, new technologies such as those presented by Di Natale et al. (2013) can help to solve the emissions issue. There are two strategies that together are capable of reaching satisfactory results: the addition of biofuels to diesel oil and engine optimization. One of the most promising fuels to replace petroleum fuels are alcohols, mainly ethanol and methanol. Ethanol is an attractive alternative fuel because it is renewable, has a high latent heat of vaporization, is an oxygenated fuel, sulfur-free and has high burning rate, with high potential to reduce oxides of nitrogen (NO_X) and particulate matter (PM) emissions from compression ignition engines (Hansen et al., 2005).

Ajav et al. (1999) presented an experimental study of some performance parameters of a constant speed stationary diesel engine using ethanol-diesel oil blends as fuel. Tests with 5 %, 10 %, 15 % and 20 % of ethanol were carried out. The lesser amount of carbon and the presence of oxygen in ethanol composition contributed to the reduction of carbon monoxide (CO) emission. The lower fuel/air ratio and the higher latent heat of vaporization of ethanol compared to diesel oil lead to lower flame temperature and reduced NO_X emissions. The authors concluded that the diesel engine at constant speed can operate satisfactorily with the addition of up to 20 % ethanol without modifications.

Zhang et al. (2013) investigated the influence of methanol fumigation on combustion and PM emissions from a diesel engine. The authors concluded that the use of methanol increased the total fuel consumed and decreased the in-cylinder pressure at low to medium engine load. Yilmaz et al. (2014) investigated the diesel engine emissions in biodiesel-ethanol-diesel oil blends using ethanol concentrations of 3 %, 5 %,

15 % and 25 %. The results showed that nitric oxide (NO) emissions and exhaust gas temperature decreased with the increase of ethanol concentration.

Besides experimental studies, computer simulation has widely been used in the study of internal combustion engines. Numerical simulation is an important tool for new engine technology development, assisting in improving performance and enabling more efficient control systems to reduce emissions. The predictive capability of current models is sufficient to eliminate inefficient settings and reduce the time and costs of the prototype development phase (Mittal et al., 2012).

D'errico et al. (2000) developed a one-dimensional model to simulate a cylinder of a spark-ignition engine using hydrogen. The comparison between the model results and the experimental results showed that the model was satisfactory. Payri et al. (2011) developed a zero-dimensional thermodynamic model for a diesel engine in which the conservation equations of mass and energy were solved to obtain the instantaneous state of the gas in the combustion chamber. The adjusted model was able to satisfactorily provide the evolution of cylinder pressure, and the use of sub-models to consider other phenomena (blow-by, chamber deformation and heat transfer) improved the accuracy of the model.

This study presents a computational model developed to simulate the operation of a diesel engine fuelled by blends of diesel oil containing 5 % biodiesel (B5) and anhydrous ethanol. The model was developed using the Engineering Equation Solver (EES) software and calculates fuel and air properties and the thermodynamic processes of the engine cycle. Ethanol injection was investigated by two different techniques: direct injection in the combustion chamber, together with B5, and indirect injection in the intake air system, with B5 being directly injected in the combustion chamber.

2. Mathematical model

The mathematical model was developed to simulate the operation of a diesel engine considering two different methods of ethanol injection:
  a. Directly injection of anhydrous ethanol diesel oil containing 5 % biodiesel (B5) in the combustion chamber;
  b. Anhydrous ethanol fumigation in the intake air charge.

The following considerations were made:
  − the engine is a closed system and isentropic (adiabatic and reversible), comprising the steps of compression, incremental combustion at constant pressure and expansion;
  − the mixture inside the engine is always uniform (air, ethanol, biodiesel, diesel oill and burned gas);
  − the intake air consists of 21 % oxygen and 79 % nitrogen;
  − the reactants (air, ethanol and diesel oil) and the combustion products are ideal gases;
  − the effects of kinetic and potential energy are negligible;
  − ambient pressure (P_0) and ambient temperature (T_0) are equal to 101.325 kPa and 25 °C, respectively;
  − Anhydrous ethanol is represented by C_2H_5OH, diesel oil is represented by $C_{10,8}H_{18,7}$, and biodiesel is represented by $C_{19}H_{36}O_2$.

The reactants chemical equation is showed by Eq(1). The air/fuel equivalence ratio is represented as $\emptyset$.

$$n_F \left(\alpha_{diesel} C_{n_1} H_{m_1} + \alpha_{biodiesel} C_{n_2} H_{m_2} O_{r_2} + \beta C_{n_3} H_{m_3} O_{r_3} + \gamma \frac{1}{\emptyset} O_2 + \gamma \frac{3,76}{\emptyset} N_2 \right) \tag{1}$$

Where:

$$\gamma = \alpha_{diesel} n_1 + \alpha_{biodiesel} n_2 + \beta n_3 + \frac{\alpha_{diesel} m_1 + \alpha_{biodiesel} m_2 + \beta m_3}{4} - \frac{\alpha_{biodiesel} r_2 + \beta r_3}{2} \tag{2}$$

$n_1 = 10,8 \, ; m_1 = 18,7 \, ; n_2 = 19 \, ; m_2 = 36 \, ; r_2 = 2 \, ; n_3 = 2 \, ; m_3 = 6 \, ; r_3 = 1$
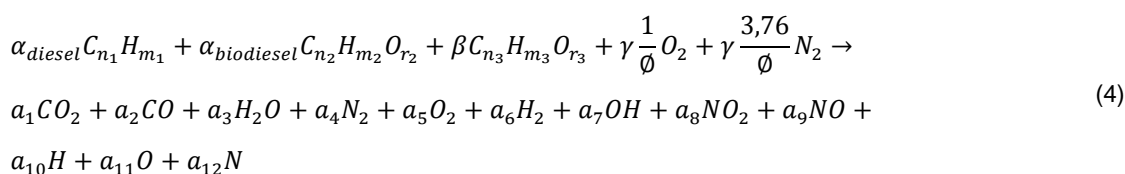
The parameters α_{diesel}, $\alpha_{biodiesel}$ and β represent, respectively, diesel oil, biodiesel and ethanol ratio in the fuel blend. The calculation starts by the mixture initial state, at the start of the compression stroke, where pressure, temperature and volume are related by the Ideal Gas Law.

To model the following state, obtained at the end of the isentropic compression, the gas composition is considered constant, small volumetric variations during the compression stroke are considered and the internal energy (U_R) is only a function of temperature (T). Applying the First Law of Thermodynamics the internal energy is obtained. The internal energy of the next state is obtained by adding the previous total internal energy to the work performed, as shown by Eq(3):

$$U_{n+1} = U_n +_n W_{n+1}$$

(3)

At the end of the compression stroke, instantaneous fuel injection occurs and fuel burning begins throughout the expansion process. It is considered that fuel injection and combustion occur at constant pressure. For modeling of the next state, obtained at the end of the fuel burning process small volumetric variations are considered, with combustion occurring with gas expansion at constant pressure.

When considering instantaneous fuel injection, the fuel at ambient temperature is injected directly into the combustion chamber at constant pressure. After injection of the total fuel amount, a uniform gas temperature is achieved and fuel burning immediately starts and continues throughout gas expansion at constant pressure. The amount of burned fuel corresponds to the energy required to increase the gas temperature and maintain constant pressure during gas expansion. The combustion process is taken as between instantaneous and adiabatic for small volume increments, and it is modeled by the chemical reaction shown by Eq(4):

$$\alpha_{diesel} C_{n_1} H_{m_1} + \alpha_{biodiesel} C_{n_2} H_{m_2} O_{r_2} + \beta C_{n_3} H_{m_3} O_{r_3} + \gamma \frac{1}{\emptyset} O_2 + \gamma \frac{3{,}76}{\emptyset} N_2 \rightarrow$$

$$a_1 CO_2 + a_2 CO + a_3 H_2 O + a_4 N_2 + a_5 O_2 + a_6 H_2 + a_7 OH + a_8 NO_2 + a_9 NO +$$

$$a_{10} H + a_{11} O + a_{12} N$$

(4)

The combustion product coefficients for the above chemical reaction are achieved by mass balance for carbon, hydrogen, oxygen and nitrogen and additional instantaneous reactions involving the combustion product components.

From the energy conservation equation, where the total internal energy of the combustion products (u_p) is considered to be equal to the total internal energy of the reactants, the burned gas temperature is found. The modeling of the remainder of the expansion process was done in a similar manner to the compression stroke, with the same considerations, but with the presence of burned gas.

The computational model developed consists of a zero-dimensional model of an engine cylinder operating on the diesel cycle. The model was developed in the Engineering Equation Solver (EES) program using 12 combustion products. All simulations consist of a cycle of one cylinder of a naturally aspirated diesel engine with the following dimensions: 102 mm bore, 60 mm crankshaft radius, 207 mm connecting rod length, and 17:1 compression ratio. In the baseline condition the engine operates with B5 and fuel/air mixture equivalence ratio of 0.8. Fuel/air mixture equivalence ratio, compression ratio, and the injected amount of ethanol were varied to obtain the cycle temperature and pressure diagrams, fuel consumption, indicated power, and the exhaust gas composition. The Table 1 shows the simulations parameters.

Table 1: Varied parameters during simulation.

Mode	Ethanol [%]	Compression ratio (r)	Fuel/air equivalence ratio (∅)
Simulation 1	0	17	0.7, 0.8, 0.9
Simulation 2	0	15,17, 19	0.8
Simulation 3 (direct injection)	0, 10, 20	17	0.8
Simulation 4 (indirect injection)	0, 10, 50	17	0.8

3. Results

Figure 1 shows cylinder pressure and temperature variation as function of crankshaft position for equivalence ratios of 0.7, 0.8 and 0.9. When ∅ was increased, an increase of cylinder gas temperature at the end of combustion and expansion process is observed. This is explained by the higher fuel amount injected in the cylinder, making longer the heat release process during combustion and, consequently, increasing the temperature along the expansion process.

Figure 2 shows the behavior of cylinder pressure and temperature as function of crankshaft position for compression ratios of 15:1, 17:1 and 19:1. As the compression ratio (CR) is increased cylinder pressure is

substantially increased, while the duration of peak pressure is reduced. Higher compression ratios cause increased temperature after fuel injection and shift the peak temperature closer to the top dead center (TDC) position.

Figure 3 shows the cylinder gas pressure and temperature variation as function of crankshaft position and the amount of anhydrous ethanol directly injected in the combustion chamber. The variation of the ethanol amount in the mixture caused no significant change on cylinder pressure and temperature. Furthermore, the duration of the combustion process does not changed significantly with increasing concentration of ethanol in the fuel. It is important to note that this model does not predict the likely increase in the ignition delay caused by the use of ethanol, which affect the combustion duration, due to the lower ethanol cetane number in comparison with diesel oil. The experiments carried out by Fang et al. (2013) also showed that the in-cylinder pressure has similar shape with the use of different diesel oil and ethanol blend concentrations.

Figure 4 shows the variation of cylinder gas pressure and temperature as function of crankshaft position and the amount of anhydrous ethanol fumigated in the intake air. Increasing the amount of fumigated ethanol resulted in reduced cylinder peak pressure and reduced cylinder temperature. The high ethanol latent heat of vaporization causes the reduction of the cylinder temperature and, consequently, the cylinder pressure. Similar results were found by Zhang et al. (2013) in experiments with a diesel engine.

Figure 5 shows that with increasing the ethanol concentration in the direct injection mode leads to a reduction of oxygen (O_2), nitrogen (N_2), NO and nitrogen dioxide (NO2) formation, while atomic nitrogen (N) concentration is increased. The reduction of the concentrations of O_2 and N_2 occurs due to the reduction of air in the cylinder. The reduction of molecular nitrogen (N_2) contributes to the reduction of NO_X (NO and NO2). The presence of oxygen in the ethanol molecule contributes to increase the oxidation rate
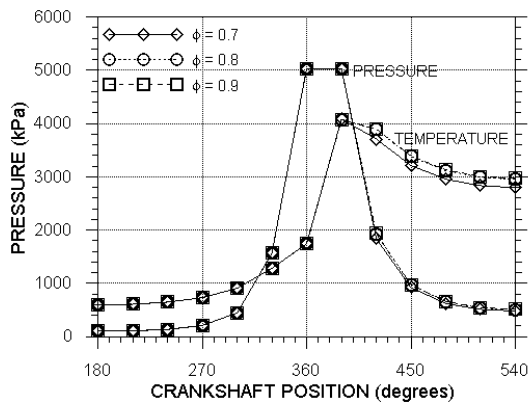

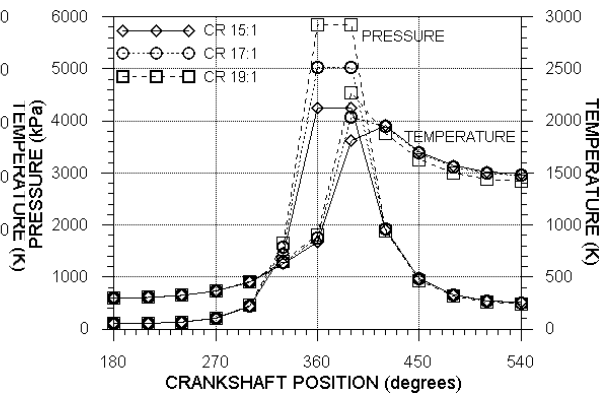*Figure 1: Variation of cylinder gas pressure and temperature with fuel/air mixture equivalence ratio*

Figure 2: Variation of cylinder gas pressure and temperature with compression ratio (CR)
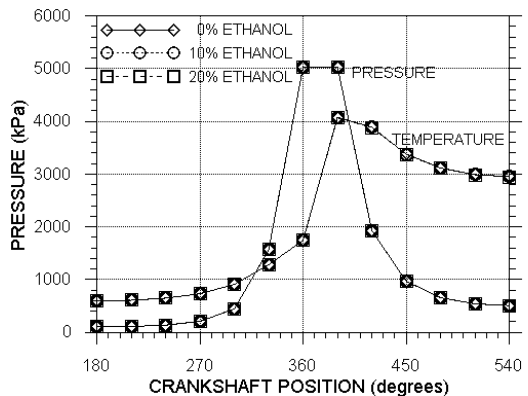

Figure 3: Variation of cylinder gas pressure and temperature with directly injected ethanol concentration
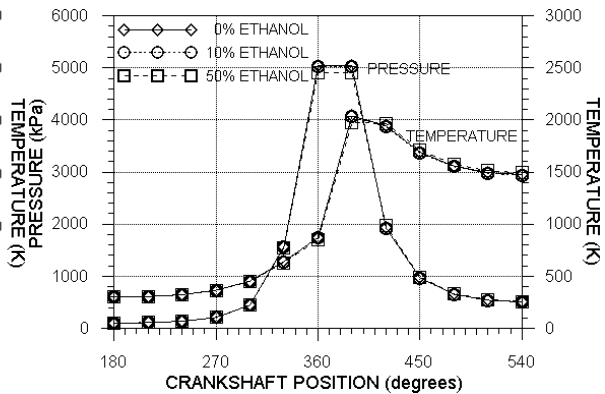

Figure 4: Variation of cylinder gas pressure and temperature with indirectly injected ethanol concentration

of CO in carbon dioxide (CO_2). Increasing the concentration of ethanol in the fuel also leads to a decrease of hydroxyl (OH), water (H_2O), atomic hydrogen (H) and atomic oxygen (O) concentrations, while hydrogen (H_2) concentration remains constant. Yilmaz et al. (2014), Zhu et al. (2010) and Park et al. (2011) also showed reduction of NO_X emissions with the use of ethanol blended to diesel oil and in diesel engines. Increased CO_2 and decreased CO emissions were also shown in the experiments by Park et al. (2011) and Hulwan and Joshi (2011) with the use of ethanol in diesel engines.

Figure 6 showed that increasing the amount of ethanol vaporized in the intake manifold causes a reduction in the concentration of CO and NO_X and increases the concentration of CO_2. The presence of oxygen in the ethanol molecule increases the oxidation rate of CO in CO_2. It was also noticed a decrease in the concentration of OH and an increase in the concentrations of H_2O and H, while H_2 concentration remained constant. The reduction in NO and NO_X emissions were also noticed by Yao et al. (2010) and Surawski et al. (2010) in experiments with ethanol fumigation in diesel engines and can be justified by the reduced in-cylinder temperatures, once NO formation is strongly dependent on high temperatures.
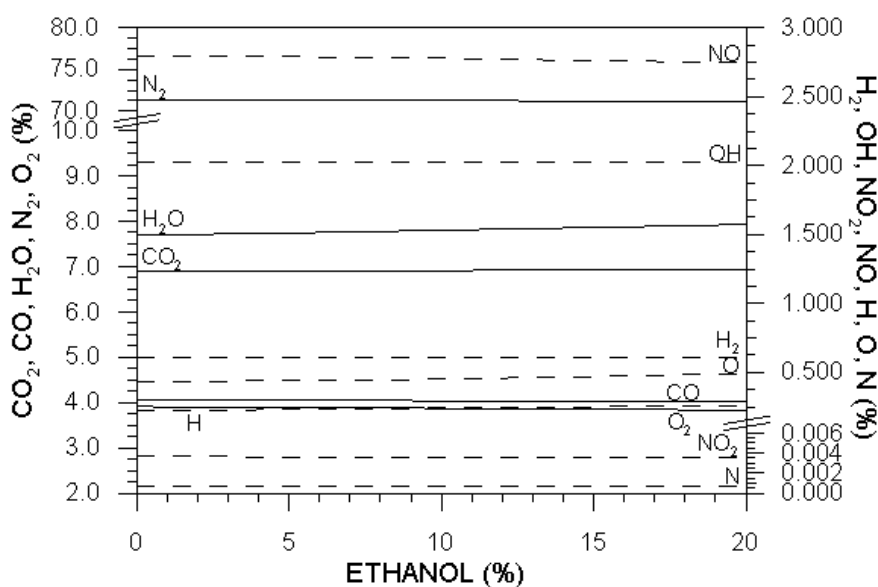

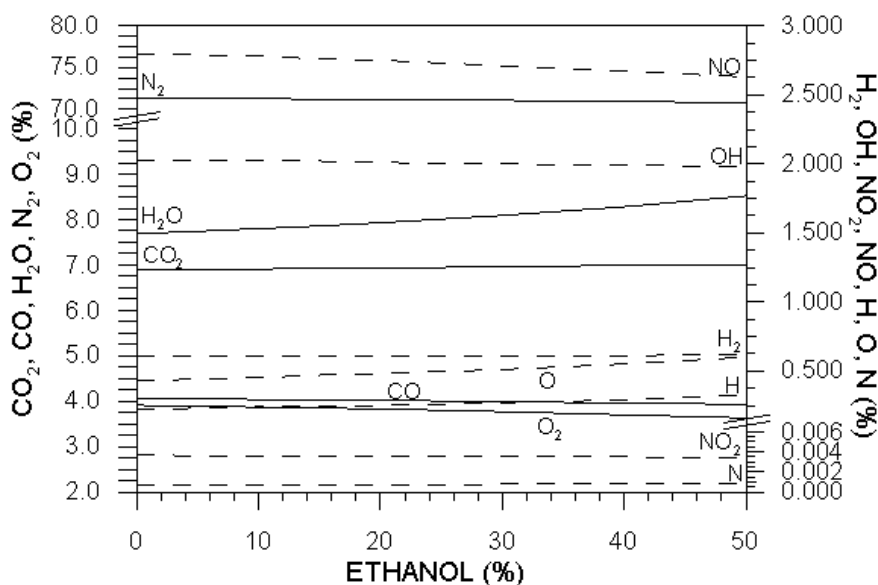*Figure 5: Variation of combustion products with directly injected ethanol concentration*

Figure 6: Variation of combustion products with indirectly injected ethanol concentration

4. Conclusions

The computational model developed was shown to be adequate to partially reproduce the behavior of the diesel engine operating with diesel oil and ethanol varying different parameters. The results indicated that the engine operates in best combination of results when configured with equivalence ratio of 0.7 and compression ratio of 19:1, in the range investigated. The direct injection of ethanol in the cylinder showed better results regarding pollutant emissions, in comparison with indirect injection of ethanol in the intake manifold, slightly penalizing the net cycle work and increasing fuel consumption. Ethanol injection in the intake manifold allows for the use of higher concentrations of this fuel; however, it decreases the amount of air charge into the engine and, consecutively, reduces engine power output. If ethanol is injected separately from the pilot fuel (B5 in this case) it will require a second fuel tank and fuel injection system. Several experimental works by other authors reported similar results to the ones obtained by simulation, presented in this work.

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