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RESEARCH ARTICLE

THE EFFECTS OF EXHAUST GAS RECIRCULATION ON EMISSIONS AND PERFORMANCE OF A SPARK IGNITION ENGINE

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ABSTRACT

The development and production of modern spark-ignition engines are very important to market and regulations requirements which demand low cost, high-performance engines with low fuel consumption and reduced emissions of pollutant. Because these parameters are directly related to the combustion process in an engine cylinder, many kinds of research have been achieved to identify these parameters which affect combustion efficiency and pollutant formation in this engine cylinder. In this study, a thermodynamic cycle model has been developed and used to predict the effects of Exhaust Gas Recirculation (EGR), which is used to reduce the Nitrogen Oxide (NO) in exhaust gas, on emission levels and performance of a spark-ignition engine. The model simulates full thermodynamic cycle of a spark-ignition engine and includes heat transfer, combustion, gas exchange process, thermal dissociation of water and carbon dioxide, and chemical equilibrium in engine cylinder.

Keywords: *Cycle Model, Spark-Ignition Engine, Exhaust Gas Recirculation, Nitrogen Oxide, Emission.*

EGZOZ GAZI GERİ VERİLMESİ YÖNTEMİNİN BİR BUJİ İLE ATEŞLEMELİ MOTORUN EMİSYON DEĞERLERİ VE PERFORMANSI ÜZERİNE ETKİLERİ

ÖZ

Çağdaş buji ile ateşlemeli motorların geliştirilmesi ve üretimi, düşük maliyet, düşük yakıt tüketimi ile yüksek performanslı motorlar ve azaltılmış kirletici emisyonları talep eden pazar ve mevzuat gereksinimleri için çok önemlidir. Bu parametreler buji ile ateşlemeli bir motor silindiri içindeki yanma işlemi ile doğrudan ilişkili olduğu için, buji ile ateşlemeli bir motor silindiri içerisindeki yanma verimini ve kirletici emisyonlarını etkileyen bu parametrelerin tanımlamasını yapan birçok araştırma başarıyla yapılmıştır. Yapılan bu çalışmada, bir termodinamik çevrim modeli geliştirilerek, egzoz gazındaki azot oksit (NO) yüzdesini azaltmak amacı ile kullanılan Egzoz Gazı Geri Verilmesi Yönteminin buji ile ateşlemeli bir motorun egzoz emisyon değerleri ve performansı üzerine etkilerini tahmin etmek için kullanılmıştır. Kurulan model, buji ile ateşlemeli bir motorun tüm termodinamik çevrimini yansıtmakta ve motor silindiri içindeki yanma olayını, ısı transferini, gaz değişimini, yanma ürünlerinin ısıl ayrışmasını ve kimyasal dengeyi içermektedir.

Anahtar Kelimeler: *Çevrim Modeli, Buji ile Ateşlemeli Motor, Egzoz Gazı Geri Verilmesi, Azot Oksit, Emisyon.*

1. INTRODUCTION

The reciprocating internal combustion engine has found its widest use in the automotive industry, although this type of engine has been utilized in numerous other applications as well. The higher power to weight or volume ratio, relatively lower cost and easy maintenance of the engine have made it popular for land transport. The development and production of the modern spark-ignition engines is very important to market and legislation requirements which demand low cost, high-performance engines with low fuel consumption and reduced emissions of pollutant [1]. These factors are directly related to the combustion process in the cylinder of engine, many kinds of research have been achieved to identify the parameters which affect the combustion efficiency and pollutant formation [2, 3, 4, 5, 6].

Motor vehicles are responsible for a significant amount of environmental pollution, especially in urban areas. Road-traffic emissions come from a number of sources. They include exhaust pipe emissions and contributions from friction processes and resuspended road dust. This results in a complex mixture that includes particulate matter and gaseous pollutants, such as nitrogen oxides (nitric oxide and nitrogen dioxide), carbon monoxide and volatile organic compounds, all of which pose risks to health [7]. The relative amounts depend on engine design and operating conditions but are of order: NOx, 500 to 1000 ppm or 20 g/kg fuel; CO, 1 to 2 percent or 200 g/kg fuel; and HC, 3000 ppm or 25 g/kg fuel [8].

Figure 1 shows emissions of nitrogen oxides, which increased steadily during the 1980s, by about 25%, owing to increasing road traffic. They fell by 20% from 1991 to 1998, mainly owing to the introduction of three-way catalysts in new passenger cars. The gradual increase in sales of diesel-powered passenger cars in some countries may result in higher nitrogen oxide emissions [7].

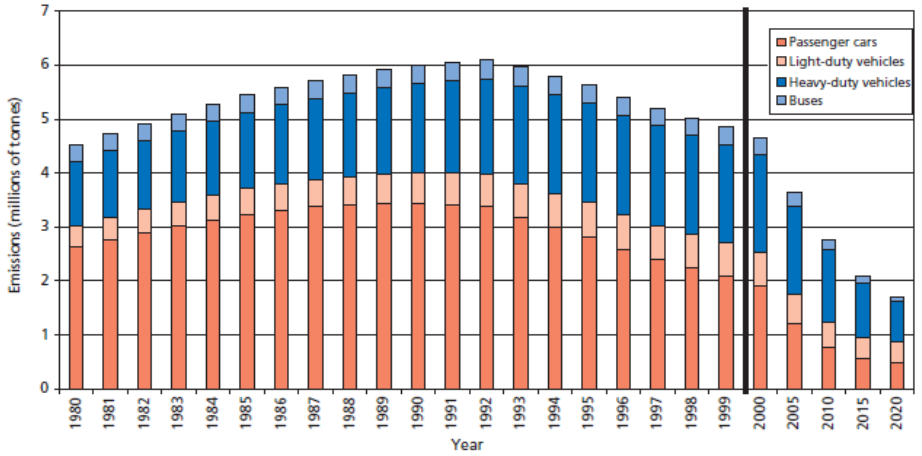

Figure 1. Total traffic emissions of nitrogen oxides in the EU countries [7].

Figure 2. shows emissions of carbon monoxide in general decreased from 1981 to 1998, mainly owing to the introduction of three-way catalysts. This trend is expected to continue [7].

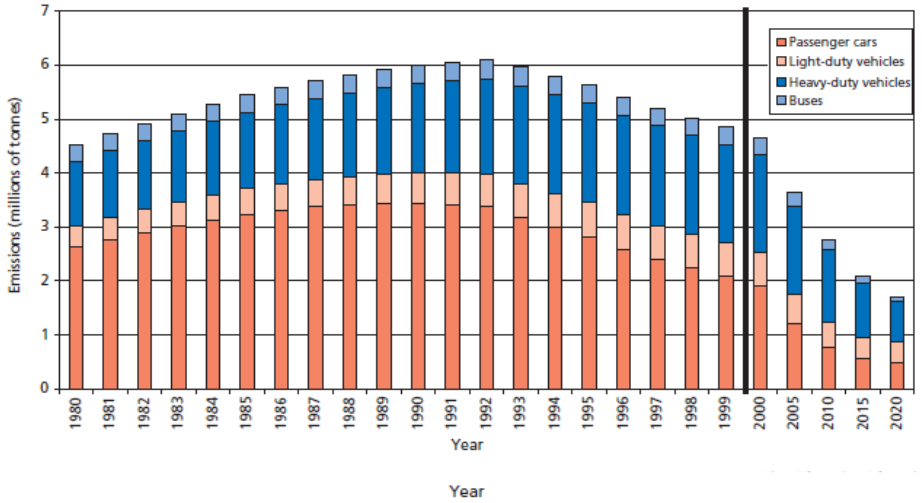

Figure 2. Total traffic emissions of carbon monoxide in the EU countries [7].

Non-stoichiometric combustion is the consequence of the mode of operation and design constraints on the reciprocating engines, which releases high toxic CO, NO and HC emissions to the atmosphere. All people are at risk for CO poisoning. Unborn babies, infants, the elderly, and people with chronic heart disease, anemia, or respiratory problems are generally more at risk than others. Breathing CO can cause headache, dizziness, vomiting, and nausea. If CO levels are high enough, you may become unconscious or die. Exposure to moderate and high levels of CO over long periods of time has also been linked with increased risk of heart disease. People who survive severe CO poisoning may suffer long-term health problems.

NO mainly impacts on respiratory conditions causing inflammation of the airways at high levels. Long term exposure can decrease lung function, increase the risk of respiratory conditions and increases the response to allergens. NO_x also contributes to the formation of fine particles (PM) and ground level ozone, both of which are associated with adverse health effects.

The design of automobile engines is very important to reduce these emissions. On the other hand, design and operating parameters affect levels of emissions, and these parameters affect engine performance and efficiency. The equivalence ratio has a strong influence on the formation of NO_x and on the oxidation of CO and unburned HCs, but the extent to which these emissions can be controlled through fuel-air ratio adjustment alone is limited. Other combustion parameters that can influence emissions include the ignition timing and design parameters. The compression ratio determines the peak pressure and hence peak temperature in the cycle. The piston and cylinder head shapes and the valve geometry influence the turbulence level in the engine and therefore the rate of heat release during combustion [17].

The processes by which pollutants form within the cylinder of a spark-ignition engine are compression, combustion, expansion, and exhaust which form four different phases of the engine operating cycle. NO forms throughout the high-temperature burned gases behind the flame through chemical reactions involving nitrogen and oxygen atoms and molecules,

which do not attain chemical equilibrium. The higher the burned gas temperature, the higher the rate of formation NO. As the burned gases cool during the expansion stroke the reactions involving NO freeze, and leave NO concentrations far in excess of levels corresponding to equilibrium at exhaust conditions. CO also forms during the combustion process. With rich fuel-air mixtures, there is insufficient oxygen to burn fully all the carbon in the fuel to CO2; also, in the high-temperature products, even with lean mixtures, dissociation ensures there are significant CO levels. Later, in the expansion stroke, the CO oxidation process also freezes as the burned gas temperature falls [8].

The unburned HC emissions have several different sources. During compression and combustion, the increasing cylinder pressure forces some of the gas in the cylinder into crevices, or narrow volumes, connected to the combustion chamber; the volumes between the piston, rings, and cylinder wall are the largest of these. Most of this gas is unburned fuel-air mixture; much of it escapes the primary combustion process because the entrance to these crevices is to narrow for the flame to enter. This gas, which leaves these crevices later in the expansion and exhaust processes, is one of unburned HC emissions. Another possible source is the combustion chamber walls. A quench layer containing unburned and partially burned fuel-air mixture is left at the wall when the flame is extinguished as it approaches the wall [8].

Mathematical modeling has been one of the tools in meeting the challenge of reduced exhaust emissions and achieving good fuel economy. Since, mathematical modeling of the engines has been a subject of research helping to define key controlling variables, giving clearer insight to the physical processes and its ability to predict behavior under different operating conditions and in general powerful tool in engine design [8].

The main purpose of this study is to develop a computer program to calculate the cylinder pressure, burnt and unburnt gas temperatures, and NO concentration rate in burnt gas of a spark-ignition engine. A thermodynamic model is developed for a SI engine cycle, which is often called Otto cycle, to obtain the engine characteristics of emissions and performance. By using this model, cylinder pressure and gas temperatures are calculated as a function of crank angle and NO formation rate and performance of engine

are investigated for the various stoichiometric ratio, λ, values. The details of the model and computer program can be found in Öğüçlü [6].

2. THERMODYNAMIC MODEL OF ENGINE CYCLE

The combustion process mathematical model is based on a homogeneous fuel-air combustible mixture, in which flame spreads from the spark plug. Engine cylinder is assumed to consist of two different regions which are separated by thin flame front. These are unburnt and burnt gas regions. The pressure in these regions is same, but all other gas mixture properties (such as temperature, specific heat values, ratio of specific heats) are different. Then, compression, combustion, and expansion processes in engine cycle are calculated using basic thermodynamic relations.

For compression process, with assumption of adiabatic compression, cylinder pressure and unburnt gas temperature are determined from relations for adiabatic compression. Thermodynamic coefficients and empirical functions for calculation of specific heat values of mixture of reactants and products are taken from Turns [9] and from Heywood [8].

For combustion and expansion processes, a relation between cylinder pressure, P, and crank angle, θ, has been obtained by applying the first law of thermodynamics to engine cylinder [10]. This equation includes volume change, combustion and heat transfer relations.

In this study, combustion rate is calculated from burnt gas mass fraction equation, $X(\theta)$ given by Vibe [11], and heat transfer rate is determined by using Annand heat transfer relationship [12]. The rate of volume change is also calculated from engine geometry. Then, to solve the cylinder pressure equation step by step for the crank angle, θ, the Euler's Method is used.

The products of combustion of fuel-air mixture are calculated by using dissociation of water and carbon dioxide, and preparing a chemical mass balance for Carbon, Hydrogen, and Oxygen. Then, with these calculated values, burnt and unburnt gas properties are determined from empirical relations.

After calculation of cylinder pressure P, unburnt and burnt gas temperatures, T_u and T_b, respectively, are determined by using basic thermodynamic relations. The heat transfer either to or from cylinder wall and burnt gas decompositions are considered. The properties of unburnt and burnt gases are calculated by using the first law of thermodynamics for engine cylinder. Then, by using these pressure and temperature values, engine performance parameters and fuel consumption are calculated.

To calculate NO formation relation, Zeldovich mechanism equations given by Hanson & Salimian [13] have been used. The assumption, that N_2, O_2, O, and OH concentrations equal equilibrium amounts and N atoms are in steady state condition, has been used. Also, to solve this equation, the Euler's Method is used.

The fuel – air mixture, which is inducted into engine cylinder at atmospheric conditions, mixes with the residual gas from the previous cycle and with the EGR gas. In this study, the EGR gas is expressed as a volume percentage of air and fuel mixture. This mixing process changes the fresh fuel–air mixture pressure and temperature. At the first stage of this study, the final mixture properties are obtained by using basic thermodynamic relations.

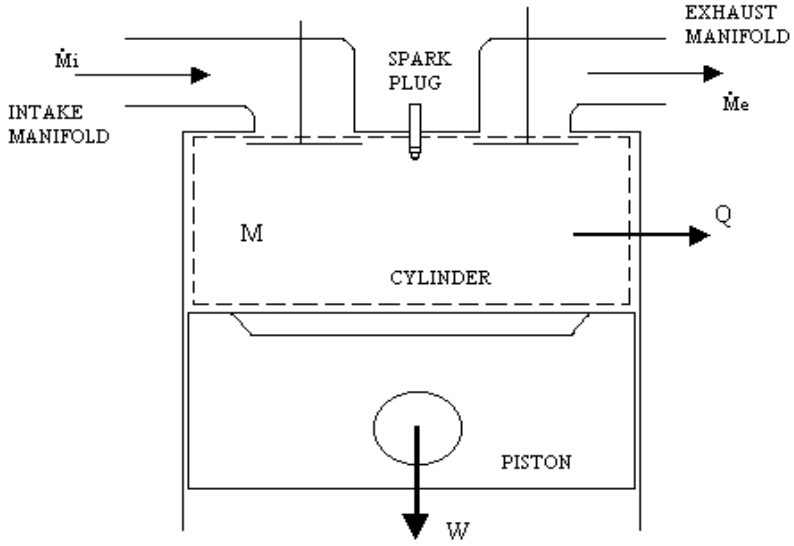

Figure 3. Engine Cylinder Thermodynamic System.

2. 1. Cycle Analysis

In this study, engine cylinder is considered as a control volume which includes all burnt and unburnt gases. Unburnt gas enters cylinder from the intake valve at flow rate, m_i and burnt gas exits cylinder from exhaust valve at flow rate, m_e , as shown in Figure 3.

There is a uniform fuel and air mixture in cylinder at end of intake time. Cylinder volume, gas pressure and gas temperature at end of intake time are P_1, V_1, and T_1. Since temperature difference between unburnt gas and cylinder wall is small, we can assume that compression of this gas is approximately adiabatic. Then cylinder pressure can be calculated from adiabatic compression equation, from crank angle at which intake valve closes to angle at which spark plug ignites fuel and air mixture.

After performing of the first law of thermodynamic for engine cylinder, we have an equation of cylinder pressure change with crank angle ($dP/d\theta$), in terms of cylinder volume (V), gas pressure and gas temperature at end of intake time (P_1 and V_1), and volume change ($dV/d\theta$), combustion rate change ($dX/d\theta$) and heat transfer change ($dQ/d\theta$) with crank angle [17],

$$\frac{\mathrm{dP}}{d\theta} = \frac{\frac{\mathrm{dQ}}{d\theta} - \frac{k_b}{k_b - 1} P \frac{\mathrm{dV}}{d\theta} - m\left[a_b - a_u - \left[\frac{k_b - k_u}{k_b - 1}\right].c_{V_u} T_1 \left(\frac{P}{P_1}\right)^{\frac{k_u - 1}{k_u}}\right]\frac{\mathrm{dX}}{d\theta}}{m.(1 - X).c_{V_u}.\left[\frac{k_b - k_u}{k_b - 1}\right].\left[\frac{k_u - 1}{k_u}\right].\frac{T_1}{P}.\left[\frac{P}{P_1}\right]^{\frac{k_u - 1}{k_u}} + \frac{V}{k_b - 1}} \quad (1)$$

where k_b and k_u are the ratio of specific heats of burnt and unburnt gases respectively, and c_{Vu} is the specific heat of unburnt gas. Parameters a_b and a_u include the reference temperature terms and the energies of formation of burnt and unburnt gases respectively and m denotes the total mass of the burnt and unburnt gases in the cylinder [17].

2. 2. Combustion Rate

The combustion rate has been calculated from burnt gas mass fraction

(m_b/m) equation, *X(θ)* given by Vibe [11]. It is a simple function and it forms of three different parts which are (i) a delay from time spark is fired until cylinder pressure increases, which is the result of combustion, (ii) an accelerating combustion rate in which a large part of air-fuel mixture is burned, (iii) and slowing combustion rate until the end of combustion duration. Vibe equation is given as below,

$$X(\theta) = 1 - \mathrm{Exp}\left[-6.908\left(\frac{\theta - \theta_0}{\Delta\theta_c}\right)^4\right] \tag{2}$$

where θ_0 is the crank angle at which the spark is fired and $\Delta\theta_c$ is the combustion duration as crank angle degrees.

2. 3. Heat Transfer Calculation

In the first law (see Equation (1)), Q is net heat transfer either to or from engine cylinder liner wall. In this cycle modeling, heat transfer is calculated by using Annand heat transfer relationship [12]. This heat transfer relation consists of convection and radiation heat transfer terms and is given as below,

$$\frac{\mathrm{dQ}}{\mathrm{dt}} = \mathrm{hA}_t\left(T_g - T_w\right) + \mathrm{CA}_t\left(T_g^4 - T_w^4\right) \tag{3}$$

where h is the convective heat transfer coefficient (W/m^{2}K), A_t is the total heat transfer area (m^2), T_g and T_w represent the mean gas temperature (K) and the mean wall temperature (K) respectively. The radiation coefficient C is given as 4.5x10^{-9} W/m^{2}K^4 by Annand [12].

2. 4. Rate of Volume Change

The compression ratio is given by

$$\varepsilon = \frac{V_c + V_d}{V_c} \tag{4}$$

where V_c is clearance volume (m^3) in which cylinder piston is at Top Dead Center (TDC) and V_d is displacement volume (m^3) between TDC and Bottom Dead Center (BDC).

Engine cylinder volume can be calculated from Equation (5) and stroke length deviation for crank angle can be calculated by Equation (6);

$$V(\theta) = V_c + \frac{\pi D^2}{4} S(\theta) \tag{5}$$

where,

$$S(\theta) = r\left[1 - \mathrm{Cos}\theta + \frac{1}{\lambda}\left(1 - \sqrt{1 - \lambda^2 \mathrm{Sin}^2\theta}\right)\right] \tag{6}$$

where λ = r / L, and L is piston connecting rod length (m) and r is crank shaft length (m).

Then, displacement volume change for the crank angle can be calculated by Equation (7);

$$\frac{\mathrm{dV}}{d\theta} = \frac{\pi D^2}{4} \mathrm{rSin}\theta \left[1 + \frac{\lambda \mathrm{Cos}\theta}{\sqrt{1 - \lambda^2 \mathrm{Sin}^2\theta}}\right] \tag{7}$$

and total wall area can be calculated by Equation (8);

$$A_t = \frac{4V_c}{D} + \pi D\left[r(1 - \mathrm{Cos}\theta) + L\left(1 - \sqrt{1 - \lambda^2 \mathrm{Sin}^2\theta}\right)\right] \tag{8}$$

2. 5. Combustion Stoichiometry

The burnt gas properties are calculated by assuming chemical equilibrium among six combustion products. The products of the reaction are numerous. Major products of lean combustion are H_2O, CO_2, O_2, and N_2; while for rich combustion, they are H_2O, CO_2, CO, H_2, and N_2. On the other hand, there are the minor species of equilibrium combustion of hydrocarbons in air. These are the atoms O and H, and the diatomic species OH and NO. But in this study, only the stoichiometric equation (see Equation (9)) is considered,

$$C_mH_n + a(O + 3.762N_2 + 7.656\mathrm{w}H_2O) \rightarrow \mathrm{b}CO_2 + \mathrm{c}CO + \mathrm{d}H_2O + \mathrm{e}H_2 + \mathrm{f}O_2 + 3.762\mathrm{a}N_2 \quad (9)$$

Equation (9) includes dissociations of water and carbon dioxide. In this equation, a is the ratio of moles number of O_2 in air-fuel mixture to moles number of fuel. a can be associated with the stoichiometric ratio, λ ; as $a=\lambda(m+n/4)$. When fuel type and λ are given, a is calculated.

The numbers of moles; b, c, d, e and f are dependent on the degree of dissociation of the reacting substances. To solve for the five unknowns, five simultaneous equations are required. The way to obtain these equations is preparing a chemical mass balance by considering the basic equilibrium reactions.

With these known values, the gas mixture properties can be calculated and the first law of thermodynamics for the modeling can be solved. The fuel, which is indicated by the formula "C_mH_n", is assumed to be iso-octane; where m = 8 and n = 18.

2. 6. Gas Exchange Processes

The fuel-air mixture, which is introduced into the engine cylinder at atmospheric pressure, P_a, and temperature, T_a, conditions, mixes with residual gas from previous cycle and with recycled gases from EGR. Therefore, this process changes pressure and temperature of final mixture, before compression stroke. At the first stage of this study, thermodynamic properties of the final mixture are calculated from basic thermodynamic relations. To calculate the final mixture properties, parameters such as induction air pressure, P_i and exhaust discharge pressure, P_e are kept constant. Figure 4 shows Gas Exchange Processes in the Engine Cylinder.

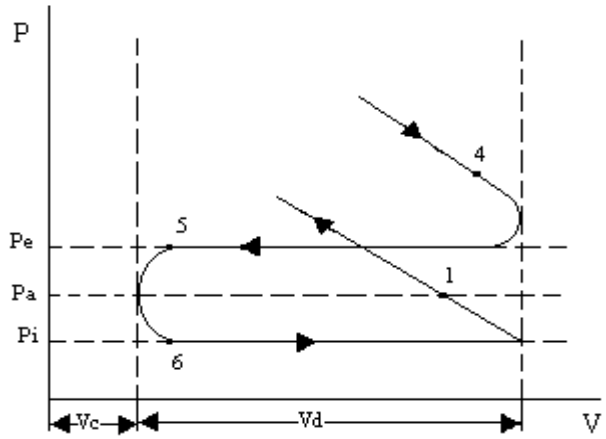

Figure 4. Gas Exchange Processes in the Engine Cylinder.

In the Figure 4, point 1 represents the crank angle where the intake valve closes (IVC), point 4 represents the crank angle where the exhaust valve opens (EVO), point 5 represents the crank angle where the inlet valve opens (IVO) and point 6 represents the crank angle where the exhaust valve closes (EVC).

2. 7. Solution Procedure

The cylinder pressure, P can be calculated by using Equation (1) with the combustion rate, $X(\theta)$, given by Vibe, and with the expression for heat transfer given by Annand. After cylinder pressure, P is calculated, unburnt and burnt gas temperatures, T_u and T_b, are determined respectively. In this study, to calculate cylinder pressure from the Equation (1), the Euler's Method is used. The unburnt gas temperature, T_u, is calculated from adiabatic compression equation and then the burnt gas temperature, T_b, is calculated. Further details of the cycle model can be found in Öğüçlü [6]. Euler method consists of the following formulas;

$$\frac{\mathrm{dP}}{d\theta} = \frac{P_{i+1} - P_i}{\Delta\theta} = f(\theta_i, P_i)$$
$$P_{i+1} = f(\theta_i, P_i)\Delta\theta + P_i \quad (10)$$

where P_i denotes Pressure value at the current step (kPa), P_{i+1} is Pressure value at next step (kPa) and $\Delta\theta$ denotes step size in crank angle degrees. For θ_1 = Spark Timing, θ_0 ; first Pressure value, P_1 is calculated from relation between pressure and volume in adiabatic compression.

3. POLLUTANT EMISSION FORMATION AND CONTROL IN COMBUSTION

The combustion products are known as a source of environmental damage, with the continuous increase in the combustion of hydrocarbon fuels. The most important combustion products are carbon dioxide and water. Now the carbon dioxide is just being a significant source in atmosphere for the greenhouse effects. On the other hand, Nitrogen Oxides (NO_x) are less known products of combustion. In the last half of the 20th century, it has become apparent that NO and NO_2, collectively called NO_x, is a major contributor of photochemical smog and ozone in the urban air, more general, the troposphere. Furthermore, NO_x participates in a chain reaction that removes ozone from strarosphere with the consequence of increased ultraviolet radiation reaching the earth's surface. Consequently, minimization of NO_x production has become a most important topic in combustion [15].

3. 1. Nitrogen Oxides

Most important air pollutants are nitrogen oxides, and their most important source is combustion. Motor vehicles are responsible from a large partition of nitrogen oxides emissions, but electric power plants also release nitrogen oxides. Nitric oxide, NO, and nitrogen dioxide, NO_2 are called as NO_x. Combustion generates both nitric oxide, NO, and nitrogen dioxide, NO_2, but large partition of nitrogen oxides are spreaded as NO. Because NO is turned into NO_2 in atmosphere. NO is formed through several mechanisms. These mechanisms are classified into the following three categories [16]:

1. The extended Zeldovich (or thermal) mechanism in which O, OH, and N_2 species have their equilibrium values and N is in steady state condition

2. Mechanisms whereby NO is formed more rapidly than predicted by the thermal mechanism above, either by (i) the Fenimore CN and HCN pathways, (ii) the N_2O-intermediate route, or (iii) as a result of superequilibrium concentrations of O, and OH radicals in conjunction with extended Zeldovich scheme.

3. Fuel nitrogen mechanism, in which fuel-bound nitrogen is converted to NO.

3. 2. Thermal NO_x Formation

The thermal or Zeldovich mechanism has two chain reactions as shown in Equations (11) and (12).

$$N_2 + O \leftrightarrow NO + N \tag{11}$$

$$N + O_2 \leftrightarrow NO + O \tag{12}$$

which can be extended by adding the reaction (see Equations (13)).

$$NO + H \leftrightarrow N + OH \tag{13}$$

The constants for these reactions mentioned in Equations (11), (12) and (13) are given in the following equations [13].

$$k_{1f} = 1.8 \times 10^{11} \exp[-38{,}370 / T(K)] \ (m^3 / kmol\text{-}s) \tag{14}$$

$$k_{1r} = 3.8 \times 10^{10} \exp[-425 / T(K)] \ (m^3 / kmol\text{-}s) \tag{15}$$

$$k_{2f} = 1.8 \times 10^{7} \ T(K) \exp[-4{,}680 / T(K)] \ (m^3 / kmol\text{-}s) \tag{16}$$

$$k_{2r} = 3.8 \times 10^{6} \ T(K) \exp[-20{,}820 / T(K)] \ (m^3 / kmol\text{-}s) \tag{17}$$

$$k_{3f} = 7.1 \times 10^{10} \exp[-450 / T(K)] \ (m^3 / kmol\text{-}s) \tag{18}$$

$$k_{3r} = 1.7 \times 10^{11} \exp[-24{,}560 / T(K)] \ (m^3 / kmol\text{-}s) \tag{19}$$

The reaction constants R_{NO} and R_N can be calculated by Equations (20) and (21);

$$R_{NO} = k_{1f}[N_2][O] - k_{1r}[NO][N] + k_{2f}[N][O_2] - k_{2r}[O][NO] + k_{3f}[N][OH] - k_{3r}[NO][H] \quad (20)$$

$$R_N = k_{1f}[N_2][O] - k_{1r}[N][NO] - k_{2f}[N][O_2] + k_{2r}[O][NO] - k_{3f}[OH][N] + k_{3r}[H][NO] \quad (21)$$

To calculate R_{NO} and R_N, we need concentrations of O, H, and OH. Most of the reaction occurs after the combustion reactions completed and before important heat is released with the flame due to the reaction rate, which is rapid simply at the highest temperatures. Therefore, we can assume that N_2, O_2, O, H, and OH concentrations have their equilibrium amounts and N atoms are in steady state condition.

Now, the reaction constants can be written as Equation (22),

$$k_{1f}[O]_e[N_2]_e = k_{1r}[NO]_e[N]_e \quad (22)$$

Then, reaction constants become,

$$R_1 = k_{1f}[O]_e[N_2]_e = k_{1r}[NO]_e[N]_e \quad (23)$$

similarly, at equilibrium,

$$R_2 = k_{2f}[O_2]_e[N]_e = k_{2r}[O]_e[NO]_e \quad (24)$$

$$R_3 = k_{3f}[OH]_e[N]_e = k_{3r}[H]_e[NO]_e \quad (25)$$

and the quantities α and β are defined as Equation (26),

$$\alpha = \frac{[\mathrm{NO}]}{[\mathrm{NO}]_e}$$
$$\beta = \frac{[N]}{[N]_e} \tag{26}$$

therefore, reaction constants Equations (20) and (21) are expressed as,

$$R_{\mathrm{NO}} = R_1 - R_1\alpha\beta + R_2\beta - R_2\alpha + R_3\beta - R_3\alpha$$
$$R_N = R_1 - R_1\alpha\beta - R_2\beta + R_2\alpha - R_3\beta + R_3\alpha \tag{27}$$

Then, by using the assumption that N atoms are in steady-state condition, $R_N = 0$, β_{SS} becomes as Equation (28)

$$\beta_{\mathrm{SS}} = \frac{R_1 + R_2\alpha + R_3\alpha}{R_1\alpha + R_2 + R_3} = \frac{\kappa + \alpha}{\kappa\alpha + 1} \tag{28}$$

where

$$\kappa = \frac{R_1}{R_2 + R_3} \tag{29}$$

Then using β_{SS} into R_{NO} equation,

$$R_{\mathrm{NO}} = \frac{d([\mathrm{NO}])}{\mathrm{dt}} = \frac{2R_1(1-\alpha^2)}{1+\kappa\alpha} \tag{30}$$

For constant temperature and pressure, Equation (30) is written as a differential equation for α ;

$$\frac{d\alpha}{\mathrm{dt}} = \frac{1}{[\mathrm{NO}]_e}\frac{2R_1(1-\alpha^2)}{1+\kappa\alpha} \tag{31}$$

and,

$$[\mathrm{NO}] = c.y_{\mathrm{NO}}$$
$$[\mathrm{NO}]_e = c.y_{\mathrm{NOe}} \quad (32)$$
$$c = \frac{P}{\mathrm{RT}}$$

Equation (32) can be written into Equation (26),

$$\alpha = \frac{[\mathrm{NO}]}{[\mathrm{NO}]_e} = \frac{y_{\mathrm{NO}}}{y_{\mathrm{NOe}}} \quad (33)$$

and into Equation (31).

$$\frac{d\alpha}{\mathrm{dt}} = \frac{1}{y_{\mathrm{NOe}}} \frac{\mathrm{dy_{NO}}}{\mathrm{dt}} \quad (34)$$

Therefore, the rate equation for NO formation and decomposition is obtained as Equation (35).

$$\frac{\mathrm{dy_{NO}}}{\mathrm{dt}} = \frac{1}{c}\left[\frac{2R_1(1-\alpha)}{1+\kappa\alpha}\right] \quad (35)$$

and Equation (35) is arranged for crank angle,

$$\frac{\mathrm{dy_{NO}}}{d\theta} = \frac{\mathrm{RT}}{P\omega}\left[\frac{2R_1(1-\alpha^2)}{1+\kappa\alpha}\right] \quad (36)$$

where, y_{NO} is NO mole fraction (kmol / kmol), y_{NOe} denotes NO equilibrium mole fraction (kmol / kmol) and c ; concentration in moles (kmol / m^3).

When $\alpha < 1$ and $dy_{NO}/d\theta > 0$, NO tends to compose; when $\alpha > 1$ and $dy_{NO}/d\theta < 0$, NO tends to dissociate [17].

3. 3. Calculation of Nitrogen Oxide Formation

In this study, to calculate Nitrogen Oxide mole fraction, y_{NO} from Equation (36), the Euler's Method is used. This method consists of the following formulas;

$$\frac{dy_{NO}}{d\theta} = f(\theta, y_{NO}) \tag{37}$$

$$\frac{dy_{NO}}{d\theta} = \frac{(y_{NO})_{i+1} - (y_{NO})_i}{\Delta\theta} = f[\theta_i, (y_{NO})_i] \tag{38}$$

$$(y_{NO})_{i+1} = f[\theta_i, (y_{NO})_i].\Delta\theta + (y_{NO})_i \tag{39}$$

where, for θ_1 = Spark Timing, θ_0 ; $(y_{NO})_1 = 0$.

3. 4. NOx Control Strategies

For processes in which thermal NO formation is important; time, temperature, and oxygen availability are main factors which influence NO_x yields. NO_x emissions are maximum at $\Phi = 1$ and decrease fast with increasing or decreasing equivalence ratio. On the other hand, maximum efficiency also is achieved near this equivalence ratio for many practical devices.

The NO_x control strategies in the internal combustion engines can be classified into four stages:

1. Reducing peak temperatures can significantly reduce NO_x emissions. In spark ignition engines, this can be achieved by mixing exhaust gases with the fresh air or fuel.

2. Another way to lower combustion temperature in spark ignition engines is to retard the spark timing.

3. The amount of thermal NO_x produced in a device is strongly linked to time that combustion products spend at high temperatures. Therefore, in the design of a combustion system, temperature – versus – time relationship is key to the control of NO emissions.

4. Staged combustion, in which a rich – lean or lean – rich combustion sequence takes place, is also a NO_x control strategy.

If maximum temperature in the cylinder can be decreased, NO_x emissions decrease. One of the ways to decrease maximum temperature is to mix fuel-air mixture with combustion products. This is known as Exhaust Gas Recirculation (EGR) in spark ignition engines [12]. The using of combustion products instead of excess air has two benefits [9]:

1. the addition of excess O_2 increases NO_x formation,

2. because of the presence of H_2O and CO_2, the specific heat of the gas increase. This reduces the combustion temperature.

3.5. Validation of Model

To show the validity of presented model, the predictions of cycle pressure values are compared with experimental data reported in the literature [10] for the conditions and the engine specifications given in Table 1. Figure 5 shows a comparison of cylinder pressure values as a function of crank angle, which are taken from presented model and experimental data reported in Taylor [10], for the stoichiometric ratio, $\lambda = 0.84$.

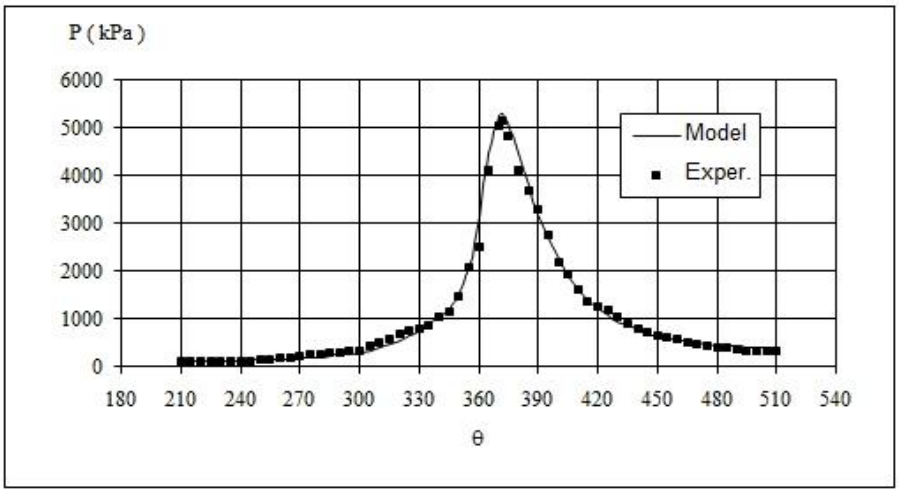

Figure 5. Comparison of Cylinder Pressure Predictions of Presented Model and Experimental Results from Taylor [10].

Table 1. Cooperative Fuel Research (CFR) Engine specifications [10].

Bore	D = 0.08255 m
Stroke	S = 0.1143 m
Rod Length	L = 0.2 m
Displacement Volume	$V_d = 0.000612\ m^3$
Compression Ratio	$\varepsilon = 8.35$
Engine Speed	n = 1200 rpm
Fuel	iso-octane
Stoichiometric Ratio	$\lambda = 0.84$
Spark Timing	$\theta_0 = 20^o$ Before Top Dead Center
Combustion Duration	$\Delta\theta_c = 40^o$
Inlet Temperature	$T_i = 353$ K
Inlet Pressure	$P_i = 99.3$ kPa
Exhaust Pressure	$P_e = 104.11$ kPa
Inlet Valve Opens	IVO= 15^o Before Top Dead Center
Inlet Valve Closes	IVC= 30^o After Bottom Dead Center
Exhaust Valve Opens	EVO= 30^o Before Bottom Dead Center
Exhaust Valve Closes	EVC= 15^o After Top Dead Center

From the Figure 5, we can see that the presented model predicts higher pressure values than the experimental results. The peak pressure calculated in the model is significantly higher than the measured peak pressure in the experiment. This result may be partly due to the assumptions used in the combustion model. The model assumes complete combustion of all the fuel. However, in the actual engine cycle, partial combustion and sometimes no combustion can occur particularly under marginal conditions. The higher pressure predicted by the model may be resulted from the higher energy release from the complete combustion of all the fuel. Consequently, the comparison between the presented model and experimental results reported in the literature, appears satisfactory. The presented model's calculations are in a good deal with experimental data, as seen in the Figure 5, so it can be said that the presented cycle model allows the conduct of this parametric study with acceptable accuracy.

4. PERFORMING CYCLE MODEL AND RESULTS

The computer program, which is used to calculate the values of the cylinder pressure, unburnt and burnt gas temperature, and NO formation rate in this study, consists of three stages. In the first stage, the values of Engine Geometry and Operating Conditions, and Fuel and Air Properties are put into program. Then, the unknown values of pressure and temperature are calculated in the second stage of program, according to values given in the first stage. After the calculating of pressure and temperature values with the given tolerance, the NO formation rate and Engine Performance values are obtained. In the last stage of the program, these calculated values are shown in the various graphics and tables. The details of computer program can be found in Öğüçlü [6]. The efficiency of an internal combustion engine is usually reported in terms of the Specific Fuel Consumption (SFC) which is the mass of fuel consumed per unit of work output (g/kWh or kg/MJ). It is inversely proportional to the thermal efficiency of the engine [19]. The work output per engine cycle is presented in terms of the Mean Effective Pressure (MEP) which is the work done on the piston divided by the displacement volume. It increases as manifold pressure increases [19].

4. 1. Engine Geometry and Operating Conditions

The parameters of Engine Geometry and Operating Conditions, Fuel and Air Properties are chosen as follows,

Stoichiometric Ratio	; $\lambda = 1.05$
Engine Speed	; n = 3000 rpm
Spark Timing	; $\theta_0 = 27^o$ Before Top Dead Center (BTDC)
Combustion Duration	; $\Delta\theta_c = 51$ Crank Angle Degrees
Compression Ratio	; $\varepsilon = 8$
Bore	; D = 73 mm
Stroke	; S = 72 mm
Rod Length	; L = 120 mm
Crank Arm Length	; r = 36 mm
Number of Cylinders	; z = 4
Fuel	; Iso-octane (C_8H_{18})
Intake valve opening time	; 20^o Before Top Dead Center (BTDC)
Intake valve closing time	; 30^o After Bottom Dead Center (ABDC)
Exhaust valve opening time	; 30^o Before Bottom Dead Center (BBDC)
Exhaust valve closing time	; 20^o After Top Dead Center (ATDC)
Inlet Temperature	; $T_i = 330$ K
Inlet Pressure	; $P_i = 95$ kPa
Exhaust Pressure	; $P_e = 105$ kPa
Atmosphere Temperature	; $T_a = 300$ K
Atmosphere Pressure	; $P_a = 101.325$ kPa
Saturation Pressure of Water	; $P_g = 3.169$ kPa (at 300 K)
Relative Humidity	; ϕ = % 40

4. 2. Results

With given parameters in Section 4.1., the computer program calculates the cylinder pressure, gas temperatures, and NO concentration rate in burnt gas. Figure 6 and Figure 7 show the Cylinder Pressure and NO Concentrations in the Burnt Gas for a various percentage of EGR, respectively.

From these results, we can see that the Exhaust Gas Recirculation can reduce NO formation in spark ignition engines. The effect of the recirculated gases is to decrease the maximum temperatures in the flame zone [20]. The effect of EGR is to increase the heat capacity of the burned gases for a given quantity of heat release, thus lowering the combustion temperature [9]. Due to the use of EGR, NO concentration reduces significantly. This can be seen clearly from Figure 7. Recirculation of exhaust gases is a common technique which is used to control oxides of nitrogen in internal combustion engines. And, the exhaust gas recirculation is effective measure for NO emission control. But, the degree of control of NO by this method is limited. Because, the use of the EGR in spark ignition engines causes the fuel consumption and the power output penalties. The EGR reduces the cylinder pressure, hence, it reduces engine power output. This reduction can be seen from clearly Figure 6. We can see that the loss of power (or pressure) is important, while the EGR percentage increases the loss of pressure increases. If the EGR is employed to control NO emissions, the engine size must be increased to meet a particular power requirement.

For 10% EGR, the computer program gives Engine Performance Results as;

Mean Effective Pressure	; MEP = 938.6 kPa
Specific Fuel Consumption	; SFC = 224.344 g / kW-h
Efficiency	; $\eta = 0.3656$
Power	; P = 32.34 kW
Peak Cylinder Pressure	; $P_{max} = 5070.68$ kPa
Peak Burned Gas Temperature	; $T_{bmax} = 2698$ K
Peak Unburned Gas Temperature	; $T_{umax} = 927$ K
Exhaust NO Concentration	; $y_{NO} = 6989$ ppm

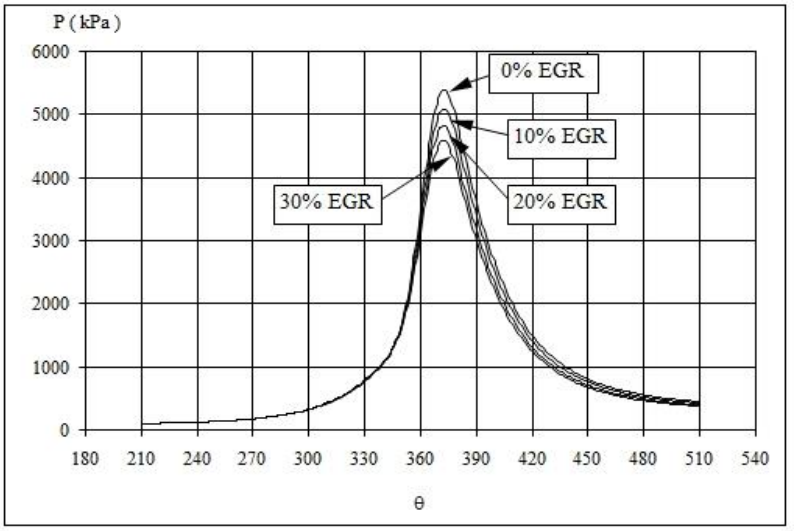

Figure 6. Cylinder Pressure for various percentage of EGR.

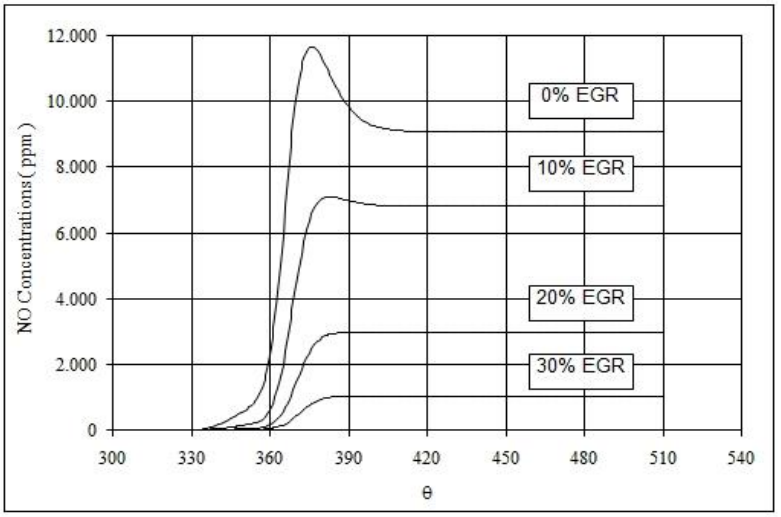

Figure 7. NO Concentrations for various percentage of EGR.

5. CONCLUSION AND FURTHER WORKS

A computer program for the simulation of thermodynamic processes, which take place in a spark ignition engine cylinder, is developed. This computer program can calculate the cylinder pressure, burnt and unburnt gas temperatures, and NO concentration rate in burnt gas of a spark ignition engine. And the Exhaust Gas Recirculation in the spark ignition engine is also employed. The hypotheses developed in the literature for the formation mechanism of NO_x emissions were reviewed and used to calculate the NO formation rate in the burnt gas. The graphical representation of the cylinder pressure, burnt and unburnt gas temperatures, and NO concentration in burnt gas as a function of crank angle is achieved.

The comparison between model and experimental results shows that model satisfactorily simulates the cycle of a spark ignition engine. However, several areas in the model need further development. Therefore, the inclusion of detailed calculations of the gas exchange processes, the blow-by gas model, and the heat transfer coefficient into the cycle simulation model can provide more detailed results. With the extensions mentioned, the computer program can be used as a useful design tool.

Consequently, this thermodynamic model and the computer program can be used by automotive engineers for predicting engine performance, Nitric Oxide emission level, and effects of Exhaust Gas Recirculation in spark ignition engines. Hence, by using these results, they can select the optimum spark timing and fueling schedules or improve combustion chamber design.

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