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THERMODYNAMIC MODEL OF THE CYCLE OF SPARK IGNITION ENGINE WITH EXHAUST GAS RECIRCULATION

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Abstract

A thermodynamic model has been developed and applied to predict the emission levels and performance of a spark ignition engine with using Exhaust Gas Recirculation (EGR) gas. The model simulates the full thermodynamic cycle of the engine and includes heat transfer, combustion, gas exchange process, thermal dissociation of water and carbon dioxide, and chemical equilibrium.

EGZOZ GAZI GERİ VERİLMESİ UYGULANAN BUJİ İLE ATEŞLEMELİ MOTOR ÇEVRİMİNİN TERMODİNAMİK MODELİ

Özetçe

Yapılan çalışmada, bir termodinamik model geliştirilerek, buji ile ateşlemeli bir motorun egzoz emisyon değerlerini ve performansını tahmin etmek için kullanılmıştır. Ayrıca bu modelde, egzoz gazındaki NO yüzdesini azaltmak amacı ile kullanılan Egzoz Gazı Geri Verilmesi Yöntemi de uygulanmıştır. Kurulan model, motorun tüm termodinamik çevrimini yansıtmakta ve motordaki yanma olayını, ısı transferini, dolgu değişimini, yanma ürünlerinin ısıl ayrışmasını ve kimyasal denge şartlarını içermektedir.

Key Words: *Cycle model, spark ignition engine, exhaust gas recirculation*
Anahtar Kelimeler: *Buji ile ateşlemeli motor, egzoz gazı geri verilmesi*

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 reciprocating 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. Because these factors are directly related to the combustion process in the cylinder of engine, many researches have been achieved to identify the parameters which affect the combustion efficiency and pollutant formation.

Motor vehicles are responsible for a significant amount of environmental pollution, especially in urban areas. Non-stoichiometric combustion is the consequence of the mode of operation and design constraints on the reciprocating engines, producing high toxic CO, NO_x and HC emissions to the atmosphere. After the realization of the fact that the motor vehicles are one of the major contributors to high toxic emissions in the atmosphere in urban areas, tough measures have been introduced to control and reduce such emissions from vehicles. Thus, the design of automobile engines is very important to reduce emissions of these pollutants. On the other hand, design and operating variables not only influence the levels of pollutant emissions, but also these parameters affect the engine power output and efficiency. Thus, while we investigate various emission control strategies, we must also consider their effects on engine performance.

A number of sources for NO_x emissions from spark ignition engines has been identified through experimental and theoretical work and some useful information obtained and adopted in engine design. The research works still continue on this subject.

Mathematical modelling has been one of the tools in meeting the challenge of reduced exhaust emissions and achieving good fuel economy.

Since, mathematical modelling 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 behaviour under different operating conditions and in general powerful tool in engine design [1] .On the other hand, succesful mathematical modelling offers some advantages over traditional experimental procedures. It has proved to be cost effective and requiring shorter analysis times in design over experimental methods. In addition, increasing computer power has given rise to improvement in the numerical methods applied to the simulation of the relevant thermodynamic and gas dynamic phenomena.

In this study, a thermodynamic model has been developed for the spark ignition engine cycle, to obtain the engine characteristics of emissions and performance. Then, by using this model, the pressure and temperature values have been computed as a function of crank angle and, thus, NO formation rate and performance of engine have been invastigated for the various stoichiometric ratio, λ, values.

For the thermodynamic model, the engine cylinder is assumed to consist of two very distinct zones separated by the infinitely thin flame front. These are the unburned gas zone and burned gas zone. The pressure in these zones is assumed the same, but all other properties are different. Then, compression, combustion, and expansion processes are calculated using basic thermodynamic relation.

For the compression process, with the assumption of adiabatic compression, the pressure in the cylinder and the temperature of the unburned gas are determined from the relations for the adiabatic compression. Thermodynamic coefficients and empirical functions for the calculation of specific heat values of the mixture of reactants and products are taken from Turns [2] and from Heywood [1] .

For the combustion and expansion processes, a relation between the cylinder pressure, P, and the crank angle, θ, has been obtained by applying the first law of thermodynamic to the engine cylinder. This relation includes the rate of volume change, and the combustion and heat transfer rates, and is in the form of the following equation,

$$\frac{dP}{d\theta} = f(\theta, P) \tag{1}$$

In this study, the combustion rate has been calculated from the burned gas mass fraction equation, X(θ) given by Vibe [3], and the heat transfer rate has been determined by using Annand heat transfer relationship [4]. Also, the rate of volume change is calculated from the engine geometry. Then, to solve the above equation step by step for the crank angle, θ, the Euler’s Method has been used.

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

After the calculation of the cylinder pressure P, the unburned and burned gas temperatures, T_u and T_b, respectively, have been determined by using the basic thermodynamic relations. Then, by using these pressure and temperature values, the engine power output (or mean effective pressure) and specific fuel consumption are calculated.

To calculate the rate of NO formation, the rate constants for the Zeldovich mechanism given by Hanson & Salimian [5] have been used. Also, the assumption, that the N_2, O_2, O, and OH concentrations are at their equilibrium values and N atoms are in steady state, has been used. Thus, the NO formation rate has been calculated from the following equation,

$$\frac{dy_{NO}}{d\theta} = g(\theta, y_{NO}) \tag{2}$$

Also, to solve this equation, the Euler’s Method has been used.

The fuel-air mixture, which is inducted into the 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 has been expressed as a volume percentage of the air and fuel. Thus, this mixing process changes the fresh fuel-air mixture pressure and temperature. At the first stage of this study, the final mixture properties have been obtained by using basic thermodynamic relations.

2. THERMODYNAMIC MODEL OF THE ENGINE CYCLE

The mathematical modelling of the combustion process is based upon a homogeneous gas-air combustible mixture, through which the flame propagates from the spark. This introduces the concept of two very distinct zones separated by the infinitely thin flame front. The pressure in the reactant and product zones is same, but all other properties are different. However, the properties are assumed homogeneous within the zones. The heat transfer to the cylinder wall and product dissociations are considered. The properties of the reactants and products are determined by balancing the first law of thermodynamic for the engine cylinder.

2. 1. Cycle Analysis

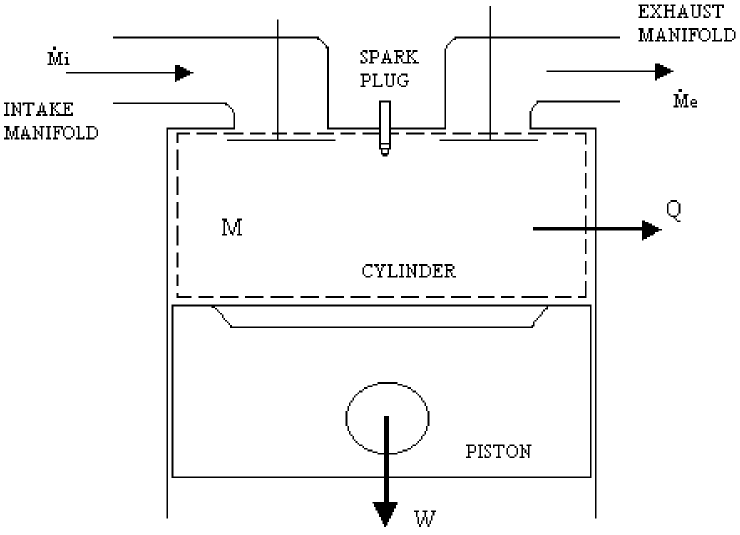

Figure 1. Engine Thermodynamic System

We consider a control volume that encloses all the gases in the cylinder. Mass enters the control volume through the intake valve at flow rate, m_i . And mass leaves through the exhaust valve at flow rate, m_e , as shown in Figure 1. The first law of thermodynamics for this control volume is,

$$\frac{dU}{dt} = \dot{m}_i h_i - \dot{m}_e h_e + \frac{dQ}{dt} - \frac{dW}{dt} \qquad (3)$$

where

U ; the total internal energy of the gases contained in the cylinder (kJ)

h_i, h_e; the mass specific enthalpies of the incoming and exiting flows (kJ / kg)

Q ; the heat that is transferred to the surroundings from the gases (kJ)

W ; the work which is done by the gases (kJ).

If we consider the time between closing the intake valve and opening the exhaust valve, and assume that there are no leaks from the cylinder, no mass enters or leaves the cylinder. And, the engine frequency is

$$\omega = \frac{d\theta}{dt} \qquad (4)$$

then, the energy equation is

$$\frac{dU}{d\theta} = \frac{dQ}{d\theta} - \frac{dW}{d\theta} \qquad (5)$$

where θ is the crank angle.

The work done by the gases is computed assuming the pressure in the cylinder is uniform,

$$\frac{dW}{d\theta} = P\frac{dV}{d\theta} \qquad (6)$$

where P ; pressure and V ; volume.

Consequently, the energy equation for the cylinder is

$$\frac{dU}{d\theta} = \frac{dQ}{d\theta} - P\frac{dV}{d\theta} \qquad (7)$$

The total internal energy of the gas can be written, by characterizing both the burned and unburned gases by mass average properties, with a mass fraction of burned gas, X;

$$U = mX\langle u_b \rangle + m(1 - X)\langle u_u \rangle \qquad (8)$$

where < > denotes an average over the entire mass of burned or unburned gas in the cylinder, and

m; the total mass of the charge (kg)

X; the mass fraction of burned gas, $X = m_b / m$, (kg / kg)

$<u_b>$, $<u_u>$; the average specific internal energy of the burned and unburned gas, respectively (kJ / kg) .

The unburned gas is quite uniform in temperature, the burned gas is not. Because, there are temperature gradients in the burned gas caused by the progressive burning and by the boundary layer heat loss. Thus, we can write,

$$\langle u_u \rangle = u_u \qquad (9)$$

While the specific heats vary with temperature, that variation is small over a limited temperature range. If we assume constant specific heats, this assumption will simplify our analysis of the engine cycle. To minimize the errors introduced by this simplification, the specific heats will be evaluated for the actual composition of the gases in the cylinder as an average over the temperature range encountered by those gases.

At the end of the intake stroke, the cylinder is filled with a uniform mixture of fuel and air. The pressure, cylinder volume, and gas temperature at the time the intake valve closes are P_1, V_1, and T_1, respectively. Because temperature difference between the unburned gas and the cylinder wall is small, we can assume that the compression of this gas is approximately adiabatic. Then the pressure in the cylinder can be determined from the formula for the relation between pressure and volume in adiabatic compression, from the crank angle at which intake valve closes to the angle at which the spark plug ignites the mixture.

Thus, we have the rate of change of the cylinder pressure in terms of the conditions at the end of the intake stroke, the rate of volume change, and the combustion and heat transfer rates,

$$\frac{dP}{d\theta}=\frac{\frac{dQ}{d\theta}-\frac{k_b}{k_b-1}P\frac{dV}{d\theta}-m\left[a_b-a_u-\left[\frac{k_b-k_u}{k_b-1}\right].c_{V_u}T_1\left(\frac{P}{P_1}\right)^{\frac{k_u-1}{k_u}}\right]\frac{dX}{d\theta}}{m.(1-X).c_{V_u}.\left[\frac{k_b-k_u}{k_b-1}\right].\left[\frac{k_u-1}{k_u}\right].\frac{T_1}{P}.\left[\frac{P}{P_1}\right]^{\frac{k_u-1}{k_u}}+\frac{V}{k_b-1}} \tag{10}$$

2. 2. Combustion Rate

Instead of developing detailed fluid mechanical of combustion process, we can specify a simple functional form for the mass fraction of burned gas, $X(\theta)$ that shows the essential features of actual combustion profiles. This profile is a delay from the time the spark is fired until the pressure rise, which is associated with combustion, becomes appreciable, an accelerating combustion rate until a large fraction of the charge is burned, followed by a decreasing burn rate. In this study, the following empirical relation, which is given by Vibe [3] , has been used ,

$$X(\theta)=1-Exp\left[-6.908\left(\frac{\theta-\theta_0}{\Delta\theta_c}\right)^4\right] \tag{11}$$

then, the combustion rate is

$$\frac{dX}{d\theta}=27.632\frac{(\theta-\theta_0)^3}{(\Delta\theta_c)^4}Exp\left[-6.908\left(\frac{\theta-\theta_0}{\Delta\theta_c}\right)^4\right] \tag{12}$$

where

θ_0 ; the crank angle at which the spark is fired (degrees)

$\Delta\theta_c$; the combustion duration (crank angle degrees)

2. 3. Heat Transfer Calculation

In the first law equation, Q is the net heat transfer to the cylinder that is the heat transfer either to or from the cylinder. In this cycle modelling, heat transfer is calculated using Annand heat transfer relationship [4] . This heat transfer relation consists of convection and radiation heat transfer terms,

$$\frac{dQ}{dt} = hA_t\left(T_g - T_w\right) + CA_t\left(T_g^4 - T_w^4\right) \tag{13}$$

where

h ; the convective heat transfer coefficient (W / m^2K)
C ; the radiation coefficient
A_t ; the total heat transfer area (m^2)
T_g ; the mean gas temperature (K)
T_w ; the mean wall temperature (K)

Then, the combustion rate is

$$\frac{dQ}{d\theta} = \frac{1}{\omega}\left(\frac{dQ_b}{dt} + \frac{dQ_u}{dt}\right) \tag{14}$$

and with the assumption of dQ_u / dt = 0 ,

$$\frac{dQ}{d\theta} = \frac{{dQ_b}/{dt}}{\omega} \tag{15}$$

where,

$$\frac{dQ_b}{dt} = h_b A_b\left(\langle T_b\rangle - T_w\right) + CA_b\left(\langle T_b\rangle^4 - T_w^4\right) \tag{16}$$

and $A_b = A_t.X^{1/2}$ suggested by Ferguson et. al. [6] , also because of dQ_u / dt = 0, $T_w = T_u$. The radiation coefficient C is given as 4.5x10^{-9} W/m^2K^4 by Annand [4].

At early times, when very little of the charge has burned, the burned gas temperature is particularly sensitive to small errors and modelling inadequacies. Because, it is difficult to say what the heat losses are during the early part of the burn. Hence, for the very first crank angles, from the time at which the spark is fired until the time when approximately 5 or 7 percent of the charge is burned, the adiabatic flame temperature is used for the burned gas temperature.

On the other hand, for the expansion stroke, the time-dependent wall temperature is modelled by assuming a conductive resistance, R_w, for the walls with a coolant temperature T_c . Then,

$$T_w = T_c + R_w \frac{dQ_b}{dt} \tag{17}$$

where

R_w ; the conductive resistance (= 0.005 K / W)

T_c ; the effective coolant temperature (= 350 K)

2. 4. Rate of Volume Change

The compression ratio is

$$\varepsilon = \frac{V_c + V_d}{V_c} \tag{18}$$

where

V_c ; the clearance volume (m^3)

V_d ; the displacement volume (m^3)

The volume in the cylinder can be expressed as a simple function of the crank angle θ;

$$V(\theta) = V_c + \frac{\pi D^2}{4} S(\theta) \tag{19}$$

where,

$$S(\theta) = r\left[1 - Cos\theta + \frac{1}{\lambda}\left(1 - \sqrt{1 - \lambda^2 Sin^2\theta}\right)\right] \tag{20}$$

where

$\lambda = r / L$

L ; the piston rod length (m)

r ; the length of the crank arm (m)

Then, the rate of change of volume is

$$\frac{dV}{d\theta} = \frac{\pi D^2}{4} r Sin\theta \left[1 + \frac{\lambda Cos\theta}{\sqrt{1-\lambda^2 Sin^2\theta}} \right] \qquad (21)$$

and the total wall area is

$$A_t = \frac{4V_c}{D} + \pi D \left[r(1 - Cos\theta) + L\left(1 - \sqrt{1-\lambda^2 Sin^2\theta}\right) \right] \qquad (22)$$

2. 5. Combustion Stoichiometry

The burned gas properties are computed assuming chemical equilibrium amongst six products of combustion. 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 research, only the following stoichiometric equation is considered,

$$C_m H_n + a(O_2 + 3.762 N_2 + 7.656 w H_2O) \rightarrow bCO_2 + cCO + dH_2O + eH_2 + fO_2 + 3.762 aN_2 \qquad (23)$$

in which the dissociations of water and carbon dioxide are considered. In this equation, the coefficient *a* represent the ratio of the number of moles of O_2 in the reactants to the number of moles of fuel. We can relate *a* to the equivalence ratio, Φ ;

$$a = \frac{m + n/4}{\Phi} = \lambda . \left[m + \frac{n}{4} \right] \qquad (24)$$

thus, given the fuel type and Φ (or λ) , *a* is a known quantity.

In addition, in the above equation, w is the specific humidity,

$$w = 0.622 \frac{\phi P_g}{P_a - \phi P_g} \tag{25}$$

where,

ϕ ; the relative humidity
P_a ; the air pressure at the temperature T_a (kPa)
P_g ; the saturation pressure of water at the temperature T_a (K)

and,

$$M_{ha} = M_a \frac{(1+w)}{(1+1.608.w)} \tag{26}$$

where, M_{ha} ; the molecular weight of the humid air (kg / kmol).

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 and by considering the following basic equilibrium reactions;

$$\begin{aligned} &CO + H_2O \Leftrightarrow H_2 + CO_2 \\ &CO + \frac{1}{2}O_2 \Leftrightarrow CO_2 \end{aligned} \tag{27}$$

The first equation, which is water-gas shift reaction, states that in equilibrium the rate of formation of H_2 and CO_2 is equal to the rate of formation of CO and H_2O. Their proportions in the mixture can be determined from the equilibrium equation of the form;

$$K_{P1} = \frac{P_{CO_2} P_{H_2}}{P_{H_2O} P_{CO}} \tag{28}$$

where P_{CO2}, P_{H2}, P_{H2O}, P_{CO} are the partial pressure of CO_2, H_2, H_2O, and CO, respectively.

Similarly for the second dissociation equation, which is the carbon monoxide reaction, the equilibrium equation is of the form;

$$K_{P2} = \frac{P_{CO_2}}{P_{CO} P_{O_2}^{1/2}} \tag{29}$$

where P_{O2} is the partial pressure of O_2.

Because of $y_i = N_i / N_t = P_i / P$, we can write;

$$K_{P1} = \frac{y_{CO_2} y_{H_2}}{y_{H_2O} y_{CO}} = \frac{b.e}{d.c} \tag{30}$$

and,

$$K_{P2} = \frac{y_{CO_2}}{y_{CO} y_{O_2}^{1/2} . P^{1/2}} = \frac{b}{c.f^{1/2}} \frac{N_t^{1/2}}{P^{1/2}} \tag{31}$$

where, $N_t = b + c + d + e + f + 3.762a$.

K_{P1} and K_{P2} are equilibrium constants and are function of temperature only. And, their values are calculated from the Gibbs function or given in tables. Similar tabulations are found in the JANAF tables [7] . In this research, they are given as a function of temperature in a polynomial of 5th degree;

$$\log_{10} K_{P1} = -4.275 - 7.776591x10^{-3} T + 5.18659x10^{-6} T^2 - 1.83203x10^{-9} T^3$$
$$+ 3.31748x10^{-13} T^4 - 2.42387x10^{-17} T^5$$
$$\log_{10} K_{P2} = 41.75367 - 5.78096x10^{-2} T + 3.69976x10^{-5} T^2 - 1.28456x10^{-8} T^3$$
$$+ 2.30571x10^{-12} T^4 - 1.67704x10^{-16} T^5$$

Other relations involving *b*, *c*, *d*, *e*, and *f* are obtained by using a chemical mass balance for carbon, hydrogen, and oxygen;

$$\begin{aligned}
&\text{Carbon;} && m = b + c \\
&\text{Hydrogen;} && n/2 + 7{,}656w.a = d + e \qquad (33)\\
&\text{Oxygen;} && 2a + 7{,}656w.a = 2b + c + d + 2f
\end{aligned}$$

and, with,

$$K_{P1} = \frac{b.e}{d.c}$$
$$K_{P2} = \frac{b}{c.f^{1/2}}\frac{N_t^{1/2}}{P^{1/2}} \qquad (34)$$

Combining these five equations above gives,

$$N_t = m + \frac{n}{2} + 7.656wa + f + 3.762a$$

$$c = \frac{m}{\left(1 + K_{P2}\left(\frac{P.f}{N_t}\right)^{1/2}\right)}$$

$$e = \frac{K_{P1}c\left(\frac{n}{2} + 7.656wa\right)}{(m-c)\left(1 + \frac{K_{P1}c}{m-c}\right)} \qquad (35)$$

$$f = a - m + \frac{c+e}{2} - \frac{n}{4}$$

Firstly, we can obtain *f, c, e*, and N_t by solving these equations iteratively by using first value of $f = a - m - n / 4$ from the stoichiometric combustion. Then, *b* and *d* can be calculated from the equations;

$$\begin{aligned} b &= m - c \\ d &= \frac{n}{2} + 7.656wa - e \end{aligned} \qquad (36)$$

Thus, with these known values, we can calculate the mixture properties and solve the first law of thermodynamics for the modelling. The fuel, which is indicated by the formula "C_mH_n", is assumed to be iso-octane; thus, m = 8 and n = 18 .

2. 6. Gas Exchange Processes

The fuel-air mixture, which is introduced into the cylinder of the engine at atmospheric pressure, P_a, and temperature, T_a, conditions, mixes with the residual gas from the previous cycle and with the recycled gases from the EGR. Thus, this process changes the pressure and temperature of the final mixture, before the 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.

2. 7. Solution Procedure

The pressure in the cylinder, P can be calculated by using equation (10) with the combustion rate given by equation (12), and with expression for heat transfer given by equation (15) . After the pressure in the cylinder, P is calculated, the mean unburned and burned gas temperatures can be determined respectively.

In this research, to calculate the pressure in the cylinder from the equation (10), the Euler’s Method is used. This method consists of the following formulas;

$$
\begin{aligned}
&\frac{dP}{d\theta} = f(\theta, P) \\
&\frac{dP}{d\theta} = \frac{P_{i+1} - P_i}{\Delta\theta} = f(\theta_i, P_i) \qquad (37) \\
&P_{i+1} = f(\theta_i, P_i)\Delta\theta + P_i
\end{aligned}
$$

where,

P_i ; the value at the current step (kPa)
P_{i+1} ; the value at the next step (kPa)
$\Delta\theta$; the step size (crank angle degrees)

The temperature of the unburned gas throughout the cycle is computed by adiabatic compression,

$$T_u(\theta) = T_1\left[\frac{P(\theta)}{P_1}\right]^{\frac{k-1}{k}} \qquad (38)$$

and the temperature of the burned gas throughout the cycle is computed by

$$\langle T_b \rangle = \frac{PV - m(1-X)R_u T_u}{mXR_b} \qquad (39)$$

where < > denotes an average over the entire mass of burned gas in the cylinder, and

$$
\begin{aligned}
R_b &= (k_b - 1)c_{vb} \\
R_u &= (k_u - 1)c_{vu}
\end{aligned}
\qquad (40)
$$

where k is the ratio of specific heats.

3. POLLUTANT EMISSION FORMATION AND CONTROL IN COMBUSTION

The products of combustion are identified as a source of environmental damage, with the steady increase in combustion of hydrocarbon fuels. The major combustion products are carbon dioxide and water. Although, these products were considered harmless, now, the carbon dioxide is becoming a significant source in atmosphere for the greenhouse effects. On the other hand, Nitric Oxides (NO_x) are less obvious products of combustion [8].

Control of pollutant emissions is a major factor in the design of modern combustion systems. Pollutants of concern include particulate matter, such as soot, fly ash, metal fumes, and various aerosols; the sulfur oxides, SO_2 and SO_3 ; unburned or partially burned hydrocarbons; oxides of nitrogen, NO_x which consist of NO and NO_2; carbon monoxide; and greenhouse gases such as N_2O, but particularly CO_2 [2].

3. 1. Nitrogen Oxides

Nitrogen oxides are important air pollutants, the most important source of which is combustion. Motor vehicles account for a large fraction of the nitrogen oxide emissions, but stationary gas sources ranging from electric power generating stations to gas-fired cooking stoves also release nitrogen oxides. Both nitric oxide, NO, and nitrogen dioxide, NO_2, are produced in combustion, but the majority of nitrogen oxides are emitted as NO. Because NO is converted to NO_2 in the atmosphere, emissions of both species frequently are called NO_x.

NO is formed through several mechanisms and variations. These mechanisms are classified into the following three categories [9] :

1. The extended Zeldovich (or thermal) mechanism in which O, OH, and N_2 species are at their equilibrium values and N atoms in steady-state
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 the extended Zeldovich scheme.

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

The thermal mechanism dominates in high-temperature combustion over a fairly wide range of equivalence ratios, while the Fenimore mechanism is particularly important in rich combustion. On the other hand, the N_2O-intermediate mechanism plays an important role in the production of in very lean, low temperature combustion processes. The third NO-formation mechanism is not generally important in premixed combustion applications, because most fuels used in premixed combustion contain little or no bound nitrogen.

3. 2. Thermal NO_x Formation

The thermal or Zeldovich mechanism consists of the two chain reaction:

$$N_2 + O \Leftrightarrow NO + N \qquad (41)$$
$$N + O_2 \Leftrightarrow NO + O \qquad (42)$$

which can be extended by adding the reaction:

$$N + OH \Leftrightarrow NO + H \qquad (43)$$

the rate constants for the extended Zeldovich mechanism are [5];

$$k_{1f} = 1.8 \times 10^{11} \exp [-38{,}370 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (44)$$
$$k_{1r} = 3.8 \times 10^{10} \exp [-425 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (45)$$
$$k_{2f} = 1.8 \times 10^{7}\ T (K) \exp [-4{,}680 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (46)$$
$$k_{2r} = 3.8 \times 10^{6}\ T (K) \exp [-20{,}820 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (47)$$
$$k_{3f} = 7.1 \times 10^{10} \exp [-450 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (48)$$
$$k_{3r} = 1.7 \times 10^{11} \exp [-24{,}560 / T (K)] \ (m^3 / kmol\text{-}s) \qquad (49)$$

then, the net rates of formation of NO and N are;

$$R_{NO} = k_{1f}[N_2][O] - k_{1r}[N][NO] + k_{2f}[N][O_2] - k_{2r}[NO][O] + k_{3f}[N][OH] - k_{3r}[NO][H] \qquad (50)$$

$$R_N = k_{1f}[N_2][O] - k_{1r}[N][NO] - k_{2f}[N][O_2] + k_{2r}[NO][O] - k_{3f}[N][OH] + k_{3r}[NO][H] \qquad (51)$$

The concentrations of O, H, and OH are required for calculation of the N and NO formation rates. Because the reaction rate is fast only at the highest temperatures, most of the reaction takes place after the combustion reactions are complete and before significant heat is transferred from the flame. This allows us to make an important simplification. Therefore, the reasonable acceptance is to assume that the N_2, O_2, O, H, and OH concentrations are at their equilibrium values and N atoms are in steady-state.

At thermodynamic equilibrium, we can write

$$k_{1f}[N_2]_e[O]_e = k_{1r}[N]_e[NO]_e \qquad (52)$$

Thus, we may define the equilibrium, one-way rate of reaction as,

$$R_1 = k_{1f}[N_2]_e[O]_e = k_{1r}[N]_e[NO]_e \qquad (53)$$

similarly, at equilibrium,

$$R_2 = k_{2f}[N]_e[O_2]_e = k_{2r}[NO]_e[O]_e \qquad (54)$$

$$R_3 = k_{3f}[N]_e[OH]_e = k_{3r}[NO]_e[H]_e \qquad (55)$$

and, we define the quantities,

$$\alpha = \frac{[NO]}{[NO]_e} \qquad \beta = \frac{[N]}{[N]_e} \qquad (56)$$

thus, the rate equations may now be expressed as,

Then, by using the assumption that N atoms are in steady sta (57) $= 0$, we find

$$\beta_{SS} = \frac{R_1 + R_2\alpha + R_3\alpha}{R_1\alpha + R_2 + R_3} = \frac{\kappa + \alpha}{\kappa\alpha + 1} \qquad (58)$$

$$R_{NO} = R_1 - R_1\alpha\beta + R_2\beta - R_2\alpha + R_3\beta - R_3\alpha$$

$$R_N = R_1 - R_1\alpha\beta - R_2\beta + R_2\alpha - R_3\beta + R_3\alpha$$

$$\kappa = \frac{R_1}{R_2 + R_3} \qquad (59)$$

where

Thus, by using β_{SS} into R_{NO} equation, we find

$$R_{NO} = \frac{d([NO])}{dt} = \frac{2R_1(1-\alpha^2)}{1+\kappa\alpha} \qquad (60)$$

For constant temperature and pressure, equation (60) may be written as a differential equation for α ;

$$\frac{d\alpha}{dt} = \frac{1}{[NO]_e}\frac{2R_1(1-\alpha^2)}{1+\kappa\alpha} \qquad (61)$$

and,

$$[NO] = c.y_{NO}$$

$$[NO]_e = c.y_{NOe} \qquad (62)$$

$$c = \frac{P}{RT}$$

then,

$$\alpha = \frac{[NO]}{[NO]_e} = \frac{y_{NO}}{y_{NOe}} \qquad (63)$$

and,

$$\frac{d\alpha}{dt} = \frac{1}{y_{NOe}} \frac{dy_{NO}}{dt} \tag{64}$$

$$\frac{dy_{NO}}{dt} = \frac{1}{c}\left[\frac{2R_1(1-\alpha)}{1+\kappa\alpha}\right] \tag{65}$$

Therefore, we can obtain the following rate equation for NO formation and decomposition;

and,

$$\frac{dy_{NO}}{d\theta} = \frac{RT}{P\omega}\left[\frac{2R_1\left(1-\alpha^2\right)}{1+\kappa\alpha}\right] \tag{66}$$

where,

y_{NO} ; the mole fraction of NO (kmol / kmol)
y_{NOe} ; the equilibrium mole fraction of NO (kmol / kmol)
c ; the concentration in moles (kmol / m^3)

When $\alpha < 1$ and $dy_{NO} / d\theta > 0$, NO tends to form; when $\alpha > 1$ and $dy_{NO} / d\theta < 0$, NO tends to decompose [10] .

3. 3. Calculation of the Formation of NO

In this study, to calculate the y_{NO} from equation (66), the Euler's Method is used. This method consists of the following formulas;

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

$$\frac{dy_{NO}}{d\theta} = \frac{(y_{NO})_{i+1} - (y_{NO})_i}{\Delta\theta} = f\left[\theta_i, (y_{NO})_i\right] \tag{67}$$

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

where,

$(y_{NO})_i$; the value at the current step (kmol / kmol)

$(y_{NO})_{i+1}$; the value at the next step (kmol / kmol)

$\Delta\theta$; the step size (crank angle degrees)

and, for $\theta_1 = \theta_0$, $(y_{NO})_1 = 0$.

3. 4. NO_x Control Strategies

For processes dominated by thermal NO formation, time, temperature, and oxygen availability are the primary variables affecting NO_x yields. NO_x emissions are maximums at $\Phi = 1$ and decrease rapidly as the equivalence ratio is increased or decreased. On the other hand, maximum efficiency also is achieved near this equivalence ratio for many practical devices. Thus, design and operating variables not only influence the levels of pollutant emissions, but also directly affect the engine power output and efficiency.

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, the 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.

To reduce NO_x emissions significantly, it is necessary to reduce the peak temperature significantly. One of the ways to reduce the peak temperatures is by mixing the charge with combustion products. In spark ignition engines, this process is called Exhaust Gas Recirculation (EGR) . Figure 2 shows the EGR system for the spark ignition engines[2].

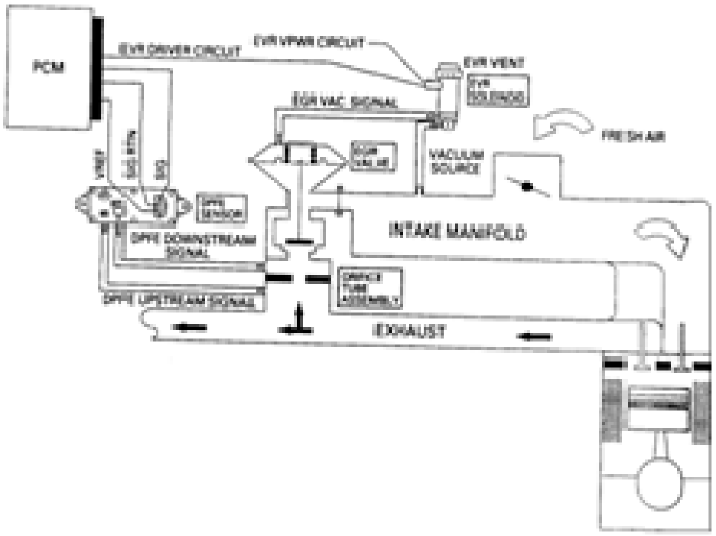

Figure 2. Exhaust Gas Recirculation System for the Spark Ignition Engines

4. PERFORMING OF THE CYCLE MODELLING AND RESULTS

4. 1. Engine Geometry and Operating Conditions

Stoichiometric Ratio ; $\lambda = 1.05$
Percentage of EGR ; EGR = % 10
Engine Speed ; n = 3000 rpm
Spark Timing ; $\theta_0 = 27$ Deg. Before Top Dead Center
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 opens ; 20 Deg. Before Top Dead Center
Intake valve closes ; 30 Deg. After Bottom Dead Center
Exhaust valve opens ; 30 Deg. Before Bottom Dead Center
Exhaust valve closes ; 20 Deg. After Top Dead Center
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 Humudity ; ϕ = % 40

4. 2. Results

Figure 3 , 4 , and 5 show the cylinder pressure, unburned and burned gas temperatures, and NO concentration in the burned gas as a function of crank angle, respectively.

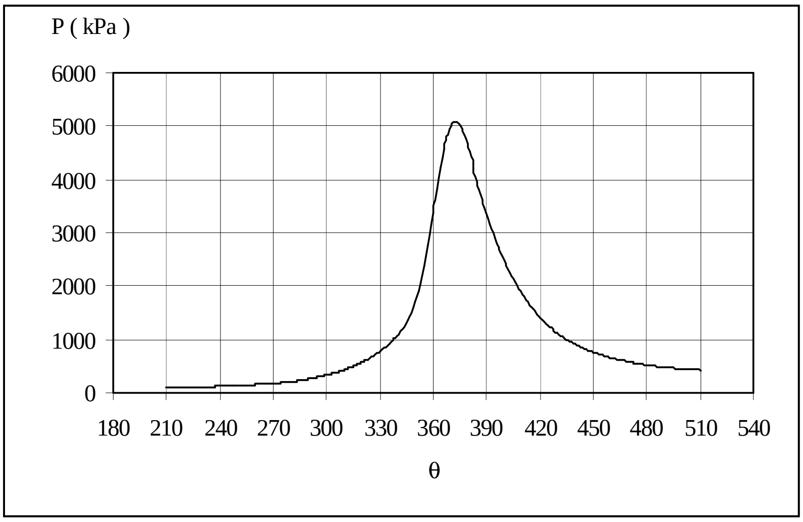

Figure 3. Cylinder Pressure

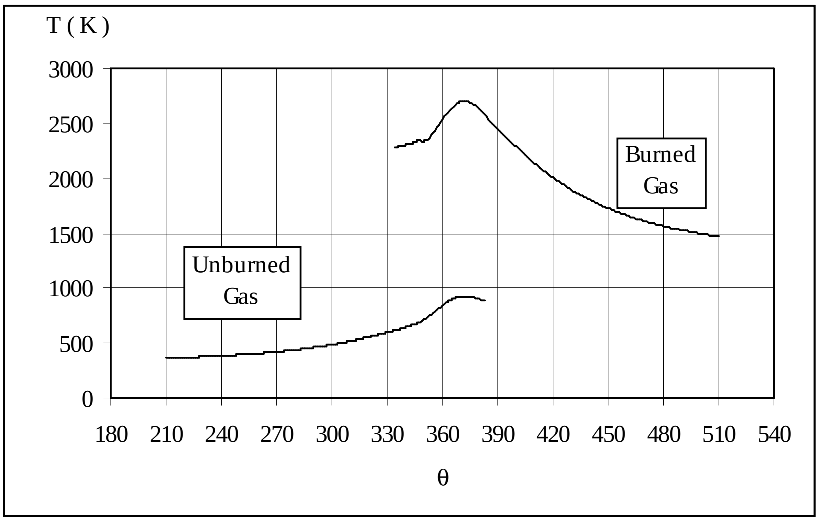

Figure 4. Unburned and Burned Gas Temperatures

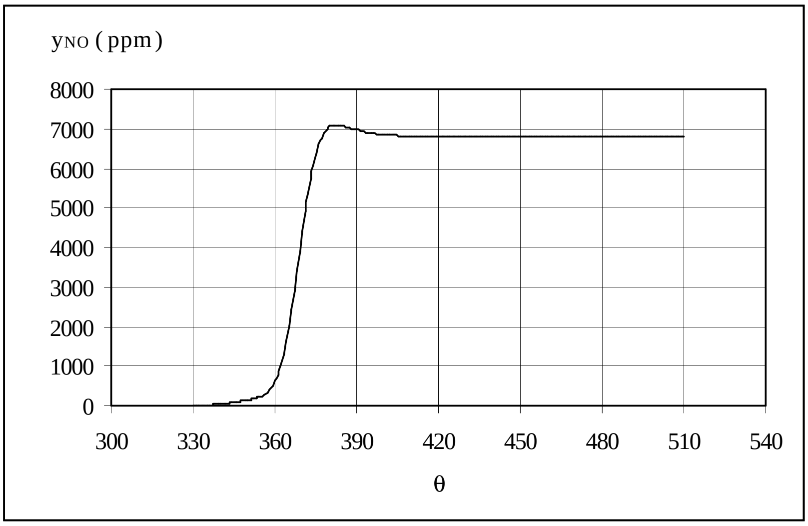

Figure 5. NO Concentration in the Burned Gas

Engine Performance Results ;

Indicated Mean Effective Pressure	; IMEP = 938.6 kPa
Indicated Specific Fuel Consumption	; ISFC = 224.344 g / kW-h
Indicated Efficiency	; $\eta_i = 0.3656$
Indicated Power	; $P_i = 32.34$ 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

4. 3. Conclusion

A computer code for the simulation of thermodynamic processes, which take place in the cylinder of a spark ignition engine, was developed. The main objective of the present work was to develop a computer code to calculate the cylinder pressure, burned and unburned gas temperatures, and NO concentration rate in the burned gas of a spark ignition engine. And, the Exhaust Gas Recirculation in the spark ignition engines was 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 burned gas. A good agreement was obtained in the comparison of calculated and measured cylinder pressure. The graphical representation of the cylinder pressure, burned and unburned gas temperatures, and NO concentration in the burned gas as a function of crank angle was achieved [11].

The comparison between the analytical and experimental results shows that the model satisfactorily simulates the cycle of spark ignition engine. Thus, the methodology, which is used to develop the model, can be applied to the actual spark ignition engines with minimum difficulty. However, several areas in the model need further development. Therefore, the inclusion of detailed calculations of the gas exchange processes, the blowby gas model, and the heat transfer coefficient into the cycle simulation model can provide more detailed results. With the extensions mentioned, the computer code could be used as a useful design tool.

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

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