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RESEARCH ARTICLE OPEN

A computational study on nonlinear curve-fitted equation for estimating gasoline –engine exhausts emissions

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I. INTRODUCTION

The control and reduction of emissions in automobile sources of pollution have been carried out for vehicles by several researchers. taking advantage of control devices, the levels of emissions of automobiles have been reduced substantially in the last twenty years. those indexes reached a reduction of 87% for new cars and 78% for used cars [2]. for example, in the united states, cars, trucks and off road vehicles are responsible for about 40—50% of HC or VOC emissions, 50 % of NOX emissions and 80—90% of the co emissions [3]. the largest contribution (90%) to HC emission from spark-ignition (SI) engines during a standard test was found to occur during the first minute of operation [4].

Traffic-related pollution emission is of great concern because of the hazards to health and the environment. Consecutive series of more stringent regulations have oriented technology projects devoted to the understanding of species and radicals formation in engine combustion in order to reduce these emissions. Poor air quality leads to health problems such as respiratory and cardiovascular disease. The pollutant emissions of SI engines, mainly hydrocarbon (HC), carbon monoxide (CO), and nitrogen oxide (NOX), greatly exceed the limits imposed by most regulatory boards, and future emission legislation will require substantial additional reductions and control of pollutant emission levels. There is a general agreement to world scientists and engineers that upstream emissions of electric drive vehicles that are of interest.

To maintain air quality, vehicle emissions must meet certain standards for exhaust emissions before they can be approved for use. Up to the author knowledge, successive "Kuwaiti" emission standards for passenger cars and light vehicles have not been initiated yet in the country. These standards will definitely help achieving considerable reduction in air pollution from cars. Reducing vehicle emissions should be part of a larger strategy to tackle the negative health and environmental effects of air pollution created by all sectors.

The relative amounts of various emission pollutants depend on fuel composition (especially fuel —air equivalence ratio), engine design and operating conditions. Many authors [1, 5, 6] found that the leaner mixtures give lower quantities of CO and NO. However, if the mixture is made too lean the engine may misfire, giving rise to higher HC emissions. They also suggested that for obtaining maximum power the engine needs to operate near stoichiometric (slightly rich), while the best economy is obtained with a mixture somewhat leaner than stoichiometric.

In engine emission species, specially NO formation, there are many reaction mechanisms proposed by different authors namely Heywood [1], Horlock-Benson [5], Millar et al. [7] Zeldovich (2 reactions), Extended Zeldovich (3 reactions), super extended Zeldovich (67 reactions) and Lavoie (7 reactions). These equations depend upon the engine operating conditions and accuracy of predictions. Similarly, CO concentrations in exhaust gases are recognized to be kinetically controlled, because CO concentrations are lower than the maximum value measured within the combustion chamber but higher than the corresponding equilibrium value. For this, Benson2, Sher et al. [8] introduced COFAC factor, used to predict CO concentrations, which lies between the peak and exhaust equilibrium values. The more detailed information concerning pollution formation mechanism and their chemical kinetic rate of carbon monoxides, organic compounds, and particulates are adequately discussed in the book of: Horlock-Benson [5], Heywood [1], Turns [9]. Along with reduction of engine emission, the efficiency and power of the engine are also equally important.

The difference between rich, lean, and stoichiometric engine operation lies in the air to fuel ratio. Stoichiometric engine operation is defined as having the chemically correct amount of air in the combustion chamber during combustion. Hence, perfect combustion would result in the production of carbon dioxide (C02) and water. However, perfect combustion not being possible results in the production of HC, CO, NOX, PM, and water as well. A rich-burn engine is characterized by excess fuel in the combustion chamber during combustion. A lean-burn engine, on the other hand, is characterized by excess air in the combustion chamber during combustion which results in an oxygen rich exhaust. Gasoline engines can be operated in all three modes of operation.

As can be seen in the relevant literature, providing a simple equation of the effect of equivalence ratio on performance of Otto cycle does not appear to have been published. Therefore, the objective of this present work involves a theoretical approach to develop a computational model of combustion in SI engine in order to generate curve-fitted equations for estimating emission and performance of gasoline operated internal combustion engines. The validation of model is being compared by Ferguson et al. [6].

II. ANALYSIS

Understanding the performance and emission of internal combustion engines require a satisfactory thermodynamic model. Simulations software is a powerful tool for studying and optimizing internal combustion engines systems. In this section the thermodynamics of combustion and suitable models for application to internal combustion engines is presented. The multicomponent ideal gas property and computational of equilibrium combustion component and properties is given.

3.1 General Chemical Equilibrium

In general, a combustion problem that has many product species is often considered. The fuel is initially mixed with air with an equivalence ratio (D and then the products of reaction are assumed to be in equilibrium at temperature T and pressure P after the combustion process. The composition and thermodynamic properties of the products are to be determined. The overall combustion reaction per mole of fuel is:

$$\begin{aligned}&CC_{\alpha}H_{\beta}O_{\gamma}N_{\delta}+\frac{as}{\phi}(O2+3.76\,N_2)\rightarrow\\&n_1CO_2+n_2H_2O+n_3N_2+n_4O_2+n_5CO+n_6H_2\\&+n_7H+n_8O+n_9OH+n_{10}NO+n_{11}N+n_{12}C(S)\\&+n_{13}NO_2+n_{14}CH_4+\dots\end{aligned}\qquad(1)$$

The condition for equilibrium is usually stated in terms of thermodynamic functions such as the minimization of the Gibbs or Helmholtz free energy or the Maximization of entropy. If temperature and pressure are used to specify a thermodynamic state, the Gibbs free energy is most easily minimized since temperature and pressure are its fundamental variables. For a product mixture of n species, the Gibbs free energy is:

$$g=\sum_{j}^{n}=1\ \mu_j n_j\quad(kJ)\qquad(2)$$

where the chemical potential, gj, of species j is defined by

$$\mu j=\left(\frac{\delta g}{\delta n_j}\right)T_1P_1n_i\neq j\ (KJ/Kmol)\qquad(3)$$

The equilibrium state is determined by minimizing the Gibbs free energy subject to the constraints imposed by atom conservation, that is,

$$B^{'}_{i}=\sum_{j=1}^{n}a_{ij}n_j\qquad i=1,\dots,l\qquad(4)$$

Or

$$b_i-b^{'}_i=0\qquad i=1,\dots,l\qquad(5)$$

where I is the number of atom types, aij is the number of atoms of element i in species j, bi is the number of atoms of element i in the reactants, and

$$b_i=\sum_{j=1}^{n}a_{ij}n_j\qquad(6)$$

is the number of atoms of element i in the products.

Defining a term G to be

$$G=g+\sum_{i=1}^{l}\lambda_i\left(bi-b'_i\right)\qquad(7)$$

Where n are Lagrangian multipliers, the condition for equilibrium become

$$\delta G=\sum_{j=1}^{n}\left(\mu_j+\sum_{i=1}^{l}\lambda_i a_{ij}\right)\delta n_j+\sum_{i=1}^{l}(b_i-b_i)\,\delta\lambda_i=0$$

Treating the variations ónj and ô1i as independent

$$\mu_j+\sum_{i=1}^{l}\lambda_i a_{ij}=0\qquad j=1\dots n$$

For ideal gases

$$\mu_j=\mu_j^{0}+R_uT\ln\left(\frac{n_j}{N}\right)+R_uT\ln\left(\frac{P}{P_0}\right)\qquad(8)$$

(9)

(10)

So that

$$\frac{\mu_j^{\circ}}{R_uT}+\ln\left(\frac{n_j}{N}\right)+\ln\left(\frac{P}{P_0}\right)+\sum_{i=1}^{l}\pi_i a_{ij}=0\qquad j=1,\dots,n\qquad(11)$$

where

$$\pi=\lambda_i/R_uT\qquad(12)$$

To determine the equilibrium composition using the Lagrange multiplier approach, we have to solve a set of (n + I + 1) equations. For a given temperature and pressure (T, P) Equation 11 is a set of n equations for the n unknown n_j, I unknown πi , and N

Equation 5 provides an additional I equation and we close the set with

N

$$\sum_{j=1}^{n} \cdot\cdot_{ij} n_j$$

Once the composition of the products has been determined, we can now compute the thermodynamic properties of the equilibrium mixture. Recall that any two of the independent properties T, P, H, S, U, and V specify the thermodynamic state. For example, for constant pressure combustion, the enthalpy is known instead of the temperature. For this case we include an equation for known enthalpy to our set of equations,

$$H=\sum_{j=1}^{n} n_j \bar{h}_j \tag{14}$$

For an isentropic compression or expansion, or expansion to a specified pressure, the entropy is given instead of enthalpy or temperature. In this case we have

$$S=\sum_{j=1}^{n} n_j\left[s_j^{\circ}-R_u\ln\left(\frac{n_j}{N}\right)-R_u\ln\left(\frac{P}{P_0}\right)\right] \tag{15}$$

Finally, if in any case specific volume rather than pressure is known, then we have to minimize the Helmholtz free energy. In this case a similar analysis (Gordon and McBride, 1971) shows that Equation 11 is replaced by

$$\frac{\mu_j^{*}}{R_u T}+\ln\left(\frac{n_j}{N}\right)+\ln\left(\frac{RT}{P_0 v}\right)+\sum_{i=1}^{\ell}\pi_i a_{ij}=0 \qquad j=1,\ldots,n \tag{16}$$

For constant volume combustion, the internal energy is known, so we include

$$U=\sum_{j=1}^{n} n_j\left(\bar{h}_j-R_u T\right) \tag{17}$$

For an isentropic expansion or compression to a specified volume v we include

$$S=\sum_{j=1}^{n} n_j\left[s_j^{\circ}-R_u\ln\left(\frac{n_j}{N}\right)-R_u\ln\left(\frac{RT}{P_0 v}\right)\right] \tag{18}$$

Solution of these problems for practical application requires numerical iteration on a computer, i.e., TRANS72 for hydrocarbon-air mixtures [10].

3.2 Four-stroke Otto Cycle

In this work, it is instructive to consider the Otto fuel-air cycle with the ideal inlet and exhaust processes. Hence, the intake pressure Pi, the exhaust pressure P_e, and the intake temperature T_i are the independent variables. Hence the cycle is consisted of the following processes:

1 to 2 Isentropic compression
2 to 3 Constant pressure heat addition
3 to 4 Isentropic expansion
4 to 5 Constant cylinder volume blowdown
5 to 6 Constant pressure exhaustion
6 to 7 Constant cylinder volume reversion
7 to 1 Constant pressure induction

Define the residual fraction as follows

$$f=\frac{1}{r}\frac{V_4}{V_6} \tag{19}$$

The energy equation applied to the cylinder control volume during intake is given by

$$h_1=f\left[h_5+\left(P_i-P_e\right)v_6\right]+\left(1-f\right)h_i \tag{20}$$

and, of course, it is still true that if the pressure drop across the intake valves is neglected

$$P_1=P_i \tag{21}$$

The volumetric efficiency and pumping work are

$$\eta_{vol}=\frac{m_i}{\rho_i V_d}=\frac{r\left(1-f\right)}{\left(r-1\right)v_1} \tag{22}$$

$$Pmep = p_e - p_i$$

Finally, the net imep and thermal efficiency are

$$(imep)_{net} = imep - pmep \tag{24}$$

$$\eta_{net}=\eta\left(1-\frac{pmep}{imep}\right) \tag{25}$$

The inputs to a four-stroke Otto fuel-air cycle are the compression ratio r, the fuel-air equivalence ratio 4, the intake pressure Pi, the exhaust pressure Pe, the intake temperature Ti, and the fuel type. This analysis of the four-stroke fuel-air requires iteration.

j=1,…,n

Nitrogen oxidizes are generally formed at high temperatures when N2 is oxidized in air. This reaction is governed by the Zeldovich Mechanism as shown by the following equations:

Typically, if combustion temperature and residence time are minimized and the appropriate amount of air is used, NO emissions will be small [11].

$$O_2 \Longleftrightarrow O + O \tag{26a}$$

$$O + N_2 \Longleftrightarrow NO + N \tag{26b}$$

$$N + O_2 \Longleftrightarrow NO + 0 \tag{26c}$$

III. RESULTS AND DISCUSSIONS

Figure 4 shows the effect of equivalence ratio on the maximum temperature of an SI engine. The maximum temperature increased as the equivalence ratio increased until it reached maximum value slightly above stoichiometric condition and then decreased. The maximum temperature is at slightly rich equivalence ratio mixture which is a consequence of both the heat of combustion and the heat capacity of the generated products compositions $(N^{*}Cp)_P$ reducing beyond the stoichiometric condition. The decrease in heat capacity of the mixture is dominated by the decrease in number of product moles formed per mole of fuel burned. It should be noted that the maximum temperature occurs at stoichiometric @ = 1) in the absence of dissociation. With dissociation effects, the maximum temperature occurs when the mixture is slightly rich. In addition, the dissociation decreases the maximum temperature.

The computed peak pressure in a spark ignition engine dependence on equivalence ratio is shown in Figure 5. The maximum pressure increases monotonically with the equivalence ratio. The peak pressure inside an engine depends on several factors. This includes inlet charge conditions, compression ratio, and amount of heat supplied by fuel and others. In this work, the engine speed, compression ratio, and inlet conditions are kept constant. Hence the main reason for the increase of peak pressure with equivalence ratio is the high heat generated inside the engine at higher values of equivalence ratios. The advantage of increasing the peak pressure is the increase of specific power which improves the acceleration of the vehicle.

Figure 6 shows the main calculated emission species from an SI engine and its variation with fuel-air equivalence ratio. The spark-ignition engines are normally operated close to stoichiometric or slightly fuel-rich mixture in order to ensure smooth operation. CO_2 is one of the major components of the exhaust in the hydrocarbon fuel combustion. It is considered a major greenhouse gas. As the equivalence ratio increases, CO_2 levels increases until it reaches its maximum value close to stoichiometric and then decreases. The reason of the increase level is that more fuel is oxidized and converted to CO_2 with the increase in equivalence ratio level. However, increasing more fuel (beyond stoichiometric) will result in insufficient oxygen to burn all the carbon in fuel to CO_2 and starts to generate CO and unburned hydrocarbon.

The carbon monoxide (CO) is generated when the engine is operated with a fuelrich equivalence ratio significantly, as shown in Figure 6. The main reason for this generation is that there is no enough oxygen to convert all carbon in the fuel to CO_2; some fuel does not get burned and some carbon ends up as CO. In addition, the presence of CO in the exhaust indicates lost chemical energy that was not fully utilized in the engine.

The oxygen level also varies with equivalence ratio. At low equivalence ratio levels more oxygen presents in the engines while this levels start to decrease at higher levels of equivalence ratio because more oxygen is consumed to convert the carbon in the fuel into CO_2 and CO. The presence of CO_2 and CO in the gas mixture tends to prevent the dissociation of CO_2 at high temperatures, which is noticeable in the fuel-rich mixture. However, dissociation of burnt gases does not occur in the lean-fuel mixture due to the relatively low temperature produced by the combustion process which is too low for dissociation.

Figure 7 presents the minor species distributions for gasoline-air combustion at the maximum temperature and pressure. It can be seen that the level of the hydroxyl radical OH is more than an order of magnitude greater than the O atom and that both peak slightly lean of stoichiometric condition ($0.9 < \Phi < 1$). The high levels of O and OH radicals in the lean region result in enhancing the kinetics of NO formation. Equilibrium NO concentration is decreased with the increase in equivalence ratio. However, in realistic internal combustion engines, NO levels are well below the equilibrium concentration because of the relatively slow formation reaction. When the engine runs under lean conditions, the reduction of nitrogen oxide stops almost completely, because the now abundant free oxygen in the exhaust gas is used to oxidize the unburned hydrocarbon and the carbon monoxide.

Figure 8 shows the effect of equivalence ratio on the indicated mean effective pressure of an SI engine. As is evident in Figure 8, the indicated mean effective pressure increases with increasing the equivalence ratio, peaks at slightly rich mixture and then decreases. At very low equivalence ratios the combustion process is limited by the available fuel. At equivalence ratios that are too high the combustion process is limited by the availability of oxygen in the gas mixture to complete the combustion. At intermediate equivalence ratios, the combustion process is limited, to a degree, by the ease of forming free radicals. Running slightly rich means that there is more fuel available to accomplish this. These factors combine to cause the observed maximum in the IMEP as a function of equivalence ratio. The decrease afterwards in the IMEP may have to do with the poor turbulence and mixing characteristics of the combustion chamber as well as mixture preparation and charge cooling.

Figure 9 presents the specific net work output in a spark ignition engine as a function of equivalence ratio. It is shown from the Figure 9 that the specific net work output increases with the equivalence ratio over the studied range [0.8 (Þ ≤1.21. For the value of equivalence ratio below stoichiometric ($0 < 1$), the specific net work output increases more rapidly than values the rich mixture values of equivalence ratio. This is due to the higher pressure and temperature values generated inside the engine cylinder operating at higher equivalence ratio.

Figure 10 shows that thermal efficiency (77th) and the volumetric efficiency (qvol) as a function of equivalence ratio. As it shown, the thermal efficiency tends to decrease with equivalence ratio over the range studied. Thermal efficiency is work-out divided by energy-input. In this case the input energy is the product of the mass of fuel and the lower heating value. As the mixture is made richer a greater amount of the fuel does not burn. The energy contained in the bonds of this fuel is counted in the energy-input term but does not contribute to the workout since it does not burn, and hence the thermal efficiency decreases. At equivalence ratios that are too lean, the power output drops significantly causing the thermal efficiency to decrease. These two factors cause a maximum value of thermal efficiency at an intermediate equivalence ratio. This maximum is achieved Slightly rich of stoichiometric.

The correlation between volumetric efficiency (TIVOI) and equivalence ratio is shown to be very weak. There is a weak trend that the volumetric efficiency tends to increase slightly as you move to values of the equivalence ratio that are either very rich or very lean. At very lean conditions there is very little fuel in the mixture. This means that the cylinder takes in a greater amount of air for a given amount of mixture. At very high equivalence ratios the effects of charge cooling may be significant. This decrease in temperature increases the density of the mixture, thus increasing volumetric efficiency. These trends are not strong and more tests would be warranted as confirmation.

Finally, all the above emissions values have been plotted against the equivalence ratio and then curve fitted assuming 2nd and 3 rd degree quadratic functions with (t) as follows:

$$\Lambda = a_0 + a_1\Phi + a_2\Phi^2 + a_3\Phi^3 \tag{27}$$

where A = {CO_2, H_2O, N_2, O_2, CO, H_2, H, O, OH, NO). The curve fitting coefficients, i.e. m, al, etc..., for the several functions are given in Table 1 and found by EES program.

IV. CONCLUSIONS

A general gasoline engine simulation technique has been used to model power cycle and emission, The equivalence ratio has been changed from lean mixture conditions to rich mixture condition. Linear regression technique has been used to derive simple equations that can estimate pollution emissions. Thermal efficiency, volumetric efficiency and specific work have also been derived. The following conclusions are drawn from the present work:

a) The peak temperature and the indicated mean effective pressure increases with equivalence ratio up to a slightly rich mixture and then decreases.

b) The maximum pressure and the specific net work increase monotonically with equivalence ratio.

c) The CO and 1-12 emissions increase towards rich mixture.

d) NO concentration varies with equivalence ratio and it increases at slightly lean stoichiometric mixture and reduces toward richer mixture.

e) Both the volumetric efficiency and the net thermal efficiency decreases with equivalence ratio.

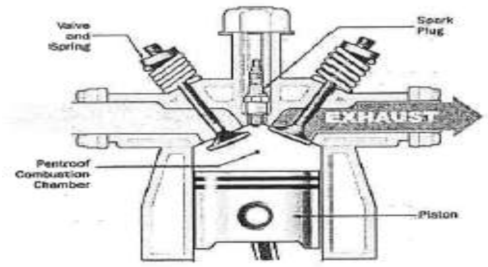

Figure 1: Schematic diagram of an internal combustion engine (From HowStuffWorks 2003)

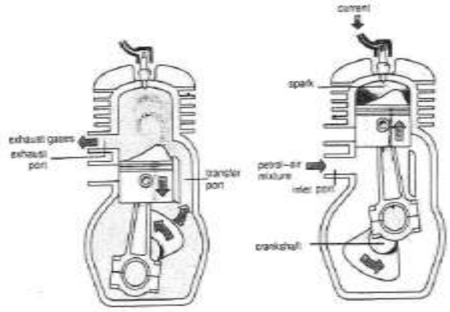

Figure 2: Two-stroke internal combustion engine (From schoolworkhelper.net)

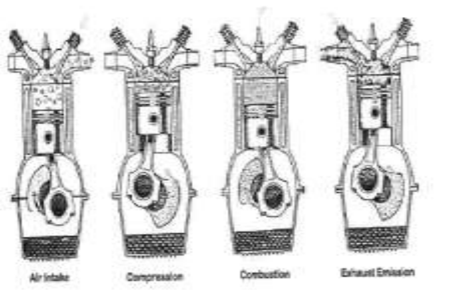

Figure 3: Four-stroke internal combustion engine (Fromschoolworkhelper.net)

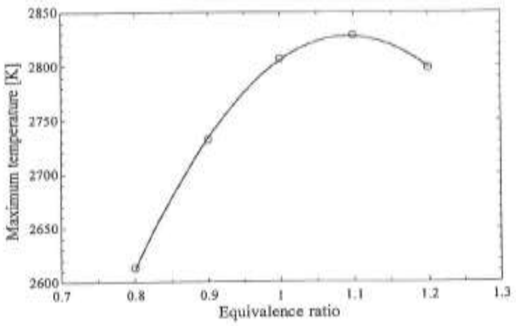

Figure 4: The maximum temperature in a spark ignition Engine as a function of equivalence ratio

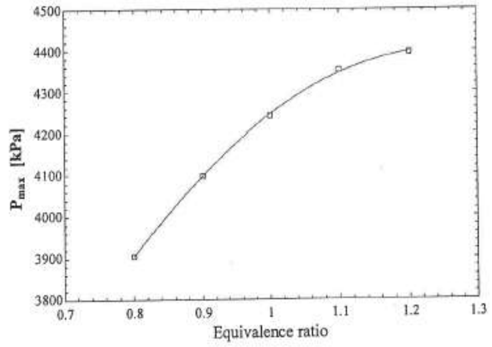

Figure 5: The maximum pressure in a spark ignition Engine as a function of equivalence ratio

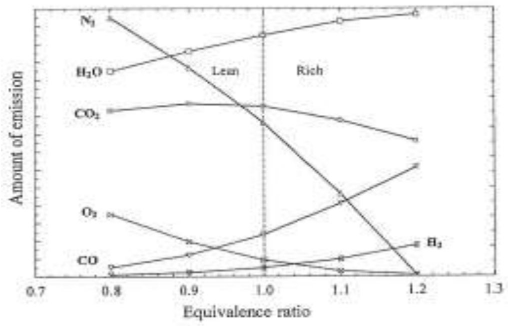

Figure 6: Calculated emmision species from SI Engine as a function of equivalence ratio

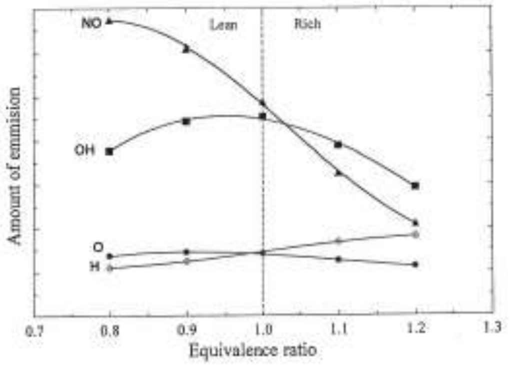

Figure 7: Minor species distribution of gasoline-air combustion as a function of equivalence ratio

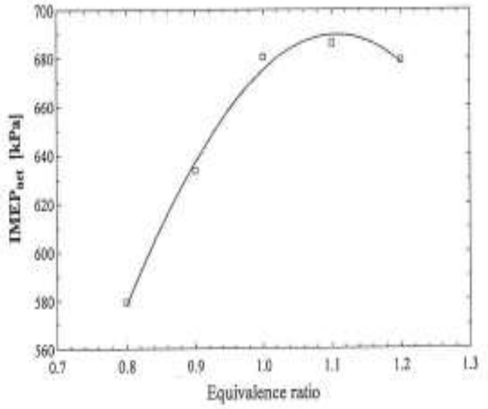

Figure 8: The indicated mean effective pressure in a spark ignition Engine as a function of equivalence ratio

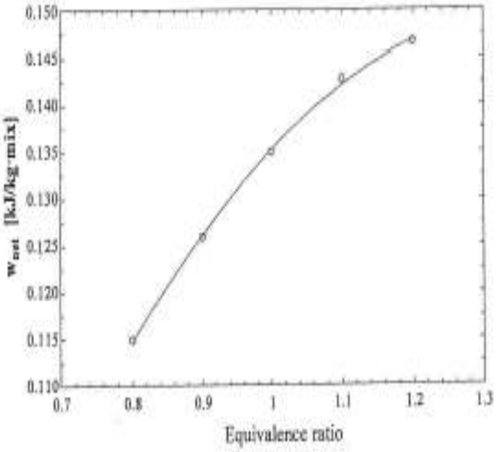

Figure 9: The specific net work output in a spark ignition Engine as a function of equivalence ratio

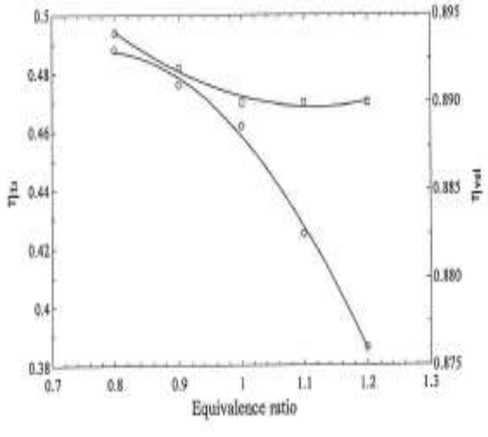

Figure 10: The thermal efficiency and the volumetric efficiency in a spark ignition Engine as a function of equivalence ratio

Table 1: Constant coefficients for the 2nd degree polynomial fit for calculating equilibrium composition species [$A = a_o + a_1\Phi + a_2\Phi^2 + a_3\Phi^3$]

Species	a_0	a_1	a_2	a_3
CO_2	-0.12518	0.48240	-0.26244	o.oooo
H_2O	-0.05721	0.30487	-0.11241	o.oooo
N_2	0.72780	0.08310	-0.09530	o.oooo
O_2	0.40063	-0.79427	0,49581	-0.0930
CO	0.11649	-0.32621	0.23365	o.oooo
H2	-0.06062	023177	-0.30227	0.1361
H	0.02261	-0.07424	0.07879	-0.0263
O	-0.02875	0.08507	-0.07927	0.0238
OH	-0.09015	0.24637	-0.19534	0.0461
NO	-0.16013	0.54262	-0,55168	0.1768

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