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A Computer-Based Air-Fuel Model for Analysing the Performance of Spark-Ignition Internal Combustion Engines

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Abstract: This paper presents a computer-based thermodynamic model of spark-ignition (SI) internal combustion engines. The air-fuel formulation enables the model to analyse the engine's performance with conventional and alternative fuels. The paper describes the mathematical formulation of the model and outlines the main features of its computer code. The model was verified against published results of earlier fuel-inducted air-fuel models and then used to analyse the performance of a SI engine with ethanol and ethanol-gasoline mixture. The engine's efficiency and indicated mean effective pressure were evaluated at different engine speeds, compression ratios and equivalence ratios.

Keywords: *Air-fuel model; Thermodynamic models; Spark-ignition engines; Alternative fuels.*

1. INTRODUCTION

The depletion of the world oil reserves together with the environmental pollution and global warming problems caused by large-scale use of fossil-fuels are deriving interest in alternative fuels for automotive engines. Alcohols and gaseous fuels are two categories of alternative fuels that have received much consideration. Alcohols, such as ethanol and methanol, can be produced from renewable bio-resources and, giving less polluting exhausts. Gaseous fuels, such as natural gas and liquefied petroleum gas, offer cleaner combustion due to improved fuel-air mixture preparation and higher hydrogen to carbon ratios compared to conventional liquid fuels [1]. Although the suitability of these types of alternative fuels has been demonstrated by many research groups [2]-[7], the drive to convert to an alternative fuel has been stronger in some countries than others depending on the availability of the alternative fuel at a competitive cost. A successful experience in this respect is that of Brazil which used ethanol as fuel for passenger car since the 1973 oil crisis. The large-scale production of ethanol as a by-product of sugar industry has made it available at costs that can compete with gasoline.

The recent political and economical developments in Sudan urge the country to follow the Brazilian example by using ethanol as an alternative fuel for passenger cars. Producing about 700,000 tonnes per crop, Sudan is the largest producer

of sugarcane in Africa and the Arab World. The availability of water and land enables the country to join the top-five world sugar producers alongside Brazil, India and the European Union. A by-product of the sugar industry is the production of ethanol. Kenana Sugar Company, the biggest sugar producer in the country, which currently produces about 50 million litre per season, plans to increase its ethanol production to about 250 million litre per season in the near future [8]. Sudan, which produces about 115,000 barrels per day of crude oil, is expected to legalise the blending of ethanol with petrol and there are also plans to produce ethanol-fuelled vehicles by the local car assembly company GIAD.

Numerous experimental studies investigated the suitability of alcohols in general, and ethanol in particular, as fuels for internal combustion (IC) engines. Brusstar *et al* [2] reported high efficiency and low emissions from a port-injected engine with neat alcohol fuels. Al-Hasan, [3], Yanju *et al.* [4], and Abdalla and Abushousha [5] investigated the effects of ethanol or methanol-gasoline blends on the performance and exhaust emission of spark-ignition (SI) engines. Costa and Sodré [6] and Munsin *et al.* [7] conducted experimental studies on the effect of hydrous ethanol on the engines' performance and emissions. Computer-based models have also been used to analyse the performance of IC engines with conventional and alternative fuels [9]-[14]. Heywood [10] and Ferguson [11] described such models for both fuel-

inducted and fuel-injected engines. By adopting the fuel-air approximation rather the standard-air approximation, these models take into account the type of fuel used and the outputs of the combustion process such as the composition of the exhaust gas. The models also apply the principles of thermodynamics to allow for the effects of suction and discharge of the fluids involved and take account of the heat-transfer and mass transfer losses that take place.

Experimental studies require costly research engine test beds and skilful technicians to run them. Since such facilities are currently unavailable, the present paper presents an air-fuel model that can be used to analyse the performance of SI engines with fuel mixtures as well as pure fuels. The paper describes the mathematical formulation of the model and outlines the main features of its computer program. The model is verified against published results of fuel-inducted air-fuel models using gasoline [10],[11]. The paper also analyses the performance of a SI engine fuelled with ethanol and ethanol-gasoline mixture. Performance parameters of the engine are evaluated at different engine speeds, compression ratios and equivalence ratios.

2. MATHEMATICAL FORMULATION OF THE MODEL

The principal governing equations of the model are the mass and energy conservation relations, the equation of state (assuming perfect gases), and the second-law of thermodynamics. In the mathematical formulation of governing equations the crank angle is taken as the independent variable. Thus, the differential form of the energy conservation equation (the first-law of thermodynamics) applied to an open system encasing the cylinder contents is [10],[11]:

$$m \frac{du}{d\theta} + u \frac{dm}{d\theta} = \frac{dQ}{d\theta} - P \frac{dV}{d\theta} - \frac{\dot{m}_l h_l}{\omega} \quad (1)$$

where θ is crank-angle, m mass, u internal energy, Q net heat added to the system, P pressure, V volume, and ω the rotational speed. In the last term of the equation (\dot{m}_l) stands for the instantaneous leakage or blowby rate. Early in the combustion process, unburned gas leaks past the rings while late in the combustion process burnt gas leaks past the rings. The model assumes the leakage to be always out of the cylinder taking with it the gas characterised by the enthalpy (h_l) of the cylinder contents (which in turn depends on the temperature, pressure, and composition of the fluid).

A two-zone combustion model is adopted whereby the combustion chamber is divided into two zones containing unburned gases and burned gases [10]-[12]. Accordingly, the specific volume of the system (v) is expressed as:

$$v = \frac{V}{m} = xv_b + (1-x)v_u \quad (2)$$

where x is the mass fraction of the cylinder contents that has been burned, v_b is the volume of the burnt gas that is at a

temperature T_b and v_u is the volume of the un-burnt gas at a temperature T_u . The mass fraction (x) is determined by an empirical cosine burning law. While the unburned gases are a mixture of fuel, air and residual gas, the burned gases are assumed to be a mixture of 10 combustion products (O_2 , N_2 , CO_2 , H_2O , H_2 , OH , NO , CO , O , H). Furthermore, the burned gases are assumed to be in chemical equilibrium during combustion and the main part of the expansion stroke. Near the end of the expansion stroke the mixture is assumed frozen.

Unlike standard gas cycles, the model takes into consideration the relative timing of the heat addition by using an empirical relationship that expresses the fraction of the heat added at any time to the crank angle. Empirical relationships are also used to express the terms involving $\frac{dm}{d\theta}$ and $\frac{dQ}{d\theta}$ in Eq. (1). The energy equation (1) is thus seen to be a relationship among three parameters and their derivatives, i.e. the equation can be put in the form:

$$f\left(\theta, \frac{dP}{d\theta}, \frac{dT_b}{d\theta}, \frac{dT_u}{d\theta}, P, T_b, T_u\right) = 0 \quad (3)$$

Therefore, two more equations are needed to complete the mathematical formulation of the model. One of the requisite equation is derived by differentiating Eq. (2) for the specific volume of the system. The second requisite equation comes from introducing the un-burnt gas entropy into the analysis. The three equations are then rearranged in the standard form used to numerically integrate a set of ordinary differential equations:

$$\frac{d\xi_i}{d\theta} = f_i(\theta, P, T_b, T_u) \quad (4)$$

where ξ_1 , ξ_2 , ξ_3 refer to P , T_b , T_u , respectively. The three equations are supplemented by three other equations for the work done, the heat loss, and the enthalpy loss. The model then consists of a set of six ordinary differential equations (ODEs) describing the rates of change of six parameters with respect to crank angle. By simultaneously integrating these equations from the start of the compression until the end of the expansion, indicated efficiency and indicated mean effective pressure can be determined.

The model needs thermodynamic properties of the combustion reactants and products at different stages of the engine's cycle. To evaluate these properties, the following formulae are used [10]-[12]:

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (5.a)$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + a_6 \frac{1}{T} \quad (5.b)$$

$$\frac{s}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (5.c)$$

where cp is the specific heat at constant pressure, R is the gas constant, T is the temperature in Kelvin, h is the specific enthalpy and s is the specific entropy. The coefficients a_6 in the enthalpy equation and a_7 in entropy equation are constants resulting from the relevant integration of Eq. (5.a) [10]-[12]. To evaluate the thermodynamic properties of the fuels (in vapour phase) simplified versions of Eqs. (5) are used in which both a_4 and a_5 are set to zero.

3. THE COMPUTER PROGRAM

Ferguson [11] provided FORTRAN computer programs for air-fuel models of both fuel-induced and fuel-injected engines. For the solution of the system of ODEs, he adopted the subroutine DVERK from the (IMSL) package which uses

fifth and sixth order Runge-Kutta_Verner method. Buttsworth [12] developed a fuel-induced computer program based on that of Ferguson [11] but used Matlab in order to use its in-built function ODE45.m as a solver. Matlab is also more user-friendly than FORTRAN and provides its user with many powerful graphical utilities. The present model is also based on the fuel-induced engine model of Ferguson [11], but it has been developed with an in-built ODE solver that applies the classical fourth order Runge-Kutta method [15] in order to make the model self-contained. The computer code has been developed in Visual Basic in order to make the model more user-friendly by developing a suitable graphical user interface (GUI) [16]. The graphical-user interface allows the fuel to be selected from a library of fuels as shown in Fig. 1.

Fig. 1. Fuel properties GUI.

Engine Parameters	Value	Step	Max
Compression Ratio, R	10	~	~
Bore, B [cm]	10	~	~
Stroke, S [cm]	8	~	~
Half Stroke To Rod Ratio, Eps	0.25	~	~
Engine Speed, Rpm [rad/s]	2000	~	~
Heat Transfer Coefficient, H [J/s/m**2/K]	500	~	~
Blowby Coefficient, C [1/s]	0.8	~	~
Equivalence Ratio, Phi	0.8	~	~
Residual Fraction, F	0.1	~	~
Initial Pressure, P1 [bar]	1	~	~
Initial Temperature, T1 [K]	350	~	~
Wall Temperature, TW [K]	420	~	~
Burn Angle, ThetaB [deg]	60	~	~
Start Of Heat Release, ThetaS [deg atdc]	-35	~	~

Fig. 2. Engine specifications and operating conditions

A new fuel can be added to the model's library by using the "Edit Fuel" option shown in Fig. 1. The fuel properties that have to be provided for the new fuel include its content of carbon, hydrogen, oxygen and nitrogen. A general formula for fuels is $C_aH_bO_cN_d$. Fig. 1 shows the respective values of these coefficients for gasoline (C_7H_{17}) [11]. The required fuel properties also include the values of coefficients a_1 – a_7 used to determine the fuel's thermodynamic properties from Eq. (5). Fig. 1 also shows the values of these coefficients for gasoline (shown as A_0 , B_0 , etc instead of a_1 , a_2 , etc.). After the fuel is selected, the GUI allows the user to specify the engine's specifications and operation parameters. Fig. 2 shows that values of 14 parameters have to be specified.

As shown in Fig. 2, the model's GUI allows single or multi runs to be performed. If a single-cycle simulation is chosen, the model will proceed to integrate the ODEs starting from a crank angle of -180° until 180° to obtain the variation of the cycle parameters with crank-angle over the complete cycle. At the end of the cycle the simulation also gives the values of four overall parameters which are the indicated thermal efficiency (η), the indicated mean effective pressure (IMEP), the error in the conservation of mass (Error 1), and the error in the conservation of energy (Error 2). The results are stored in a normal text file. The multi-cycle option gives the variation of the four overall parameters (η , IMEP, Error 1,

and Error 2) with the variation of any of the 14 parameters shown in Fig. 2. If this simulation is selected, the model does the cycle integration for each value of the selected parameter but only stores the values of the four parameters for the cycle in a second text file.

Following the specification of the fuel and engine properties, the model may be triggered to run the required simulation mode by pressing the "next" button shown in Fig. 2. The results can then be plotted with Microsoft Excel. Fig. 3 shows the results of a single-cycle simulation by the present model for the engine with the specifications shown in Fig. 2 with gasoline as fuel. The figure shows the variation of the pressure, work, temperature, and heat leakage with crank angle. The model results, which are compared with those provided by Ferguson [11] for the same case, confirm that the two models yield almost identical results. Table 1 compares the values obtained by the present model for the four overall parameters η , IMEP, Error 1, and Error 2 to the corresponding values given by Ferguson [11] and Buttsworth [12]. The figures show that the first three of the parameters are in a strong agreement with their corresponding values given by Ferguson [11]. Although the error in energy conservation (Error2) shows a significant difference from the corresponding value given by Ferguson [11] and Buttsworth [12], its absolute value is still insignificant.

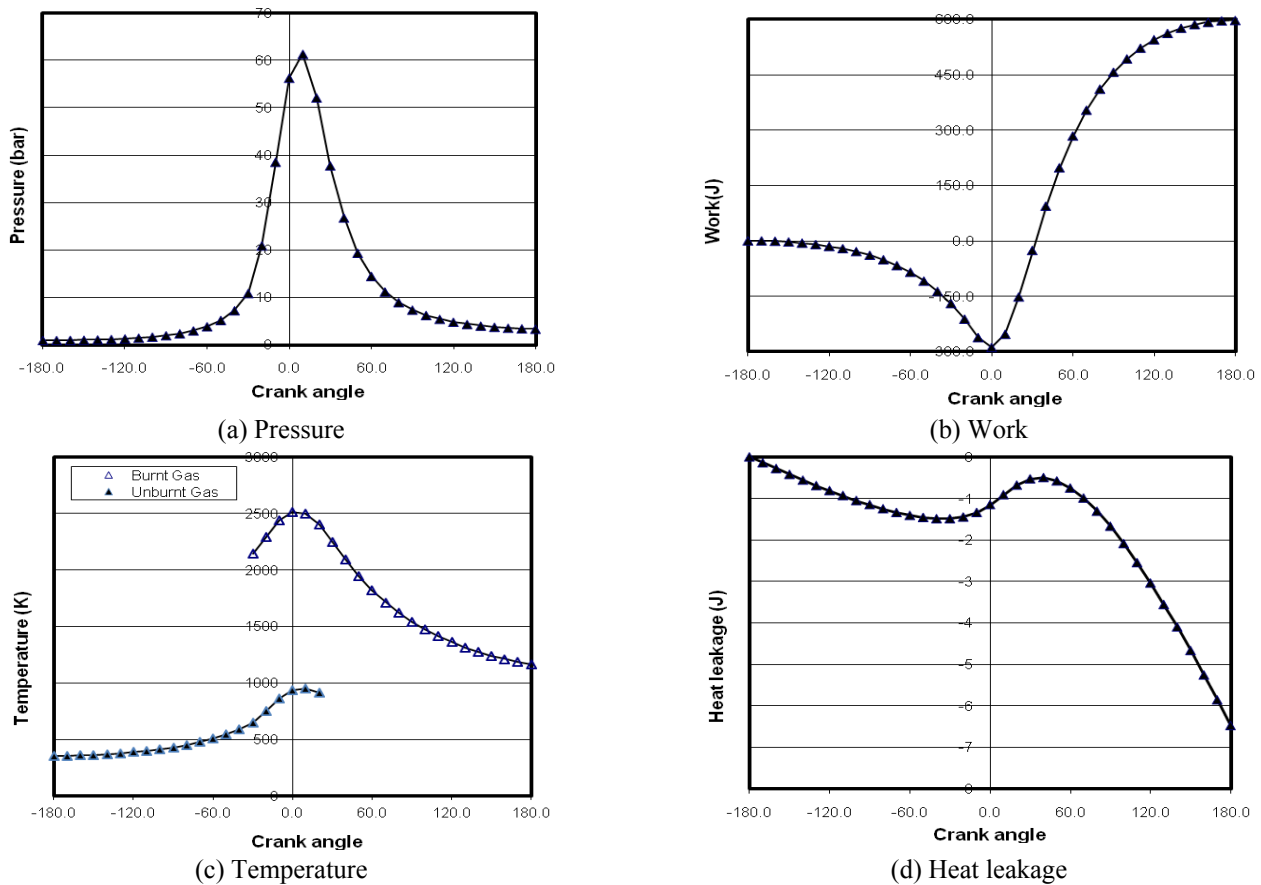


Fig. 3. Comparison of the results by the present model (symbols) to those of Ferguson [11] (solid line)

Table 1. Values of the Overall Performance Parameters compared to those given by Ferguson [11] and Buttsworth [12]

	η	IMEP	Error 1	Error 2
Ferguson [11]	0.38821	0.95102	-5.2238E-04	1.0633E-04
Buttsworth [12]	0.38890	0.95278	3.8258E-04	4.3581E-04
Present model	0.38807	0.95067	-5.3095E-04	8.8986E-04

The "Edit Fuel" option allows the model to deal with fuel blends. The blend can be added as a new fuel to the model's library after the respective values of its coefficient are calculated independently. This has the advantage that the model can deal with fuel blends without any modification to the model's formulation and computer code.

4. PERFORMANCE ANALYSIS OF GASOLINE MIXTURES

In order to use the air-fuel model for analysing the performance of internal combustion engines with fuel mixtures, the values of the different fuel coefficients have to be determined. The following relation is used for deriving the properties of a gasoline-ethanol fuel mixture with ξ referring to the property and x to the mass fraction of the fuel components [17].

$$\xi_{mixture} = \sum_{k=1}^N x_k \cdot \xi_k \quad (6)$$

Eq. (6) is applied to determine the values of the coefficients α , β , γ and δ for a gasoline-ethanol fuel mixture with different percentages of ethanol. According to Grill *et al.* [17], Eq. (6) can also be used to determine the values of the coefficients a_0 - e_0 in Eq. (5) for the mixture. Tables 2 and 3 give the values of the different coefficients for gasoline-ethanol blends with 0- 100% ethanol.

Gasoline-ethanol blends with different ethanol concentrations were added as new fuels to the model's fuel library. The model was then used to analyse the performance of the engine with the specifications shown in Fig. 2 with these fuel mixtures. Fig. 4 shows the variation of the indicated thermal efficiency and mean effective pressure with engine speed. The figure compares the results obtained with gasoline, ethanol, and gasoline-ethanol blend with 80% ethanol concentration (E80). Fig. 4a indicates that the thermal efficiency with ethanol and E80 slightly exceeds that with gasoline and the difference increases with the speed. The thermal efficiency with E80 lies between those of gasoline and ethanol. A similar pattern is exhibited by the variation of the mean effective pressure with engine speed as shown on Fig. 4b. Fig. 4 indicates that the optimum values of the thermal efficiency and IMEP occur at about 6000 RPM. Fig. 5 shows the effect of compression ratio on the engine's efficiency and mean effective pressure. Similar to the effect of engine speed, both parameters increase with compression ratio, with the values of ethanol and E80 being slightly higher than the corresponding values of gasoline. However, Fig. 5 shows that the optimum value of the compression ratio is approached at a much slower rate than that of optimum speed. Within practical limitations, the higher the compression ratio the higher the thermal efficiency and mean effective pressure.

Table 2. The Coefficients α - δ for Gasoline-Ethanol Blends with Different percentages of Ethanol

	0%	20%	40%	60%	80%	100%
α	7	6	5	4	3	2
β	17	14.8	12.6	10.4	8.2	6
γ	0	0.2	0.4	0.6	0.8	1
δ	0	0	0	0	0	0

Table 3. The Coefficients a_1 - a_7 for Gasoline-Ethanol Blends with Different percentages of Ethanol

	0%	20%	40%	60%	80%	100%
a_1	4.0652	3.95567128	3.84614257	3.73661385	3.62708513	3.51756
a_2	0.060977	0.05278135	0.0445857	0.03639005	0.02819439	0.0199987
a_3	-1.8801E-05	-1.6241E-05	-1.3681E-05	-1.1121E-05	-8.5614E-06	-6.0015E-06
a_6	-35880.0	-34764.262	-33648.5231	-32532.785	-31417.046	-30301.3
a_7	15.45	13.963246	12.476492	10.989738	9.502984	8.01623

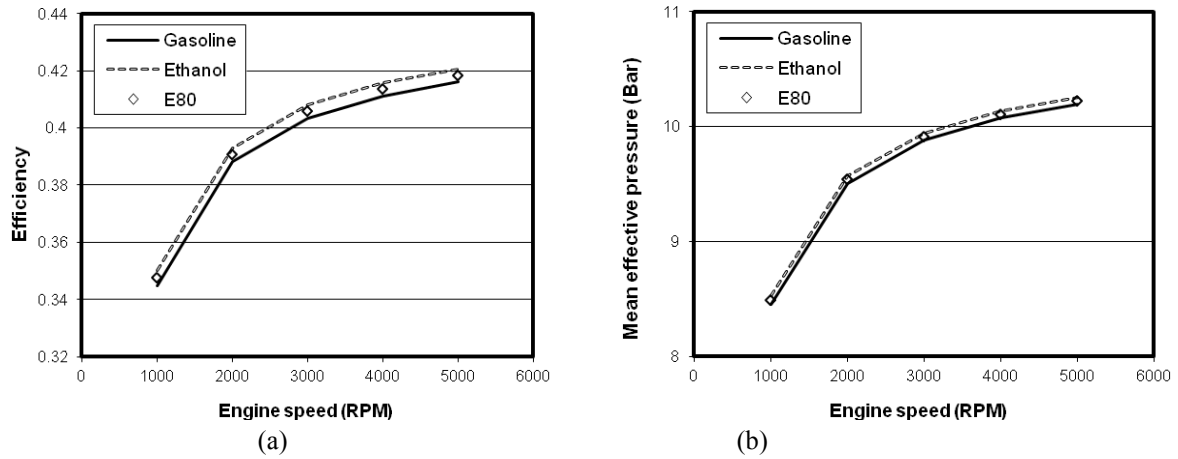


Fig. 4. Effect of engine speed on indicated thermal efficiency and mean effective pressure

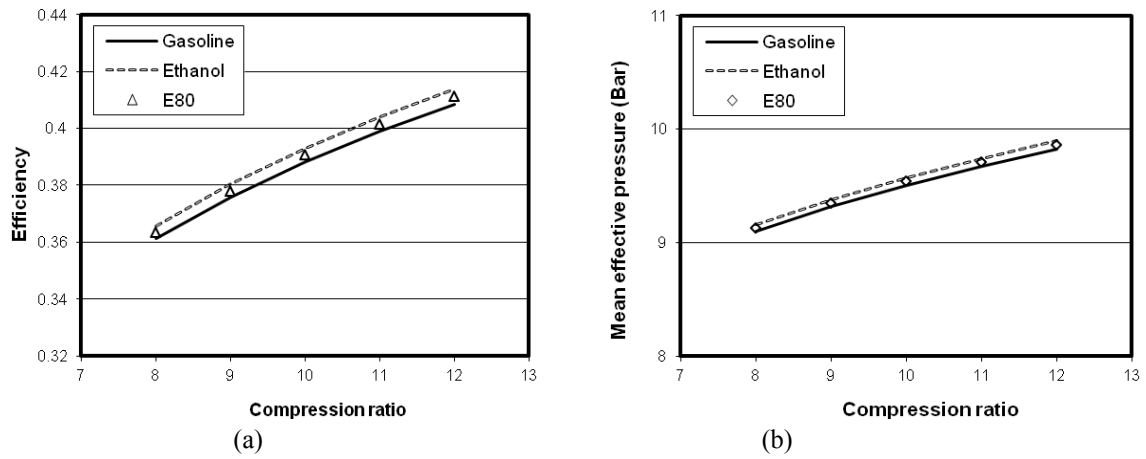


Fig. 5. Effect of compression ratio on indicated thermal efficiency and mean effective pressure

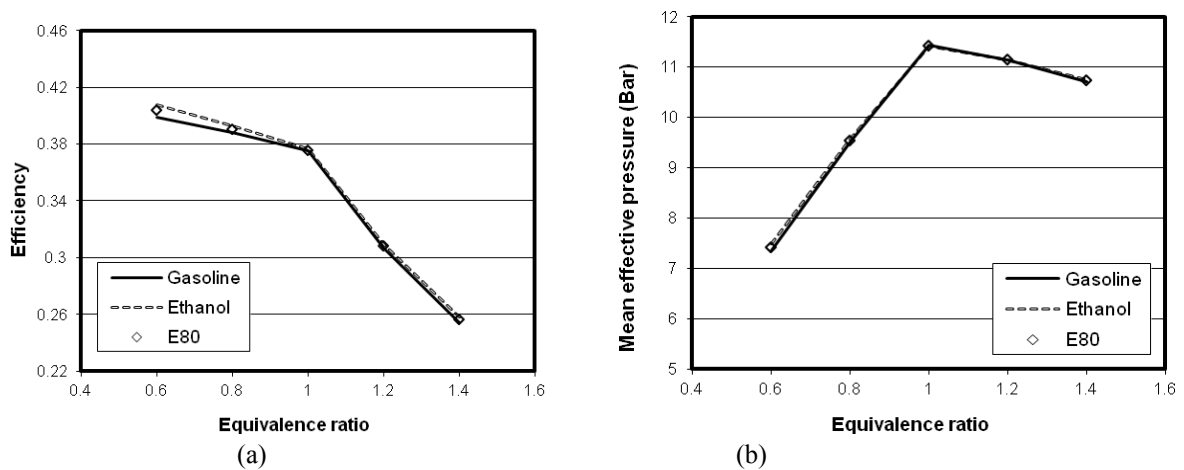


Fig. 6. Effect of equivalence ratio on indicated thermal efficiency and mean effective pressure

Fig. 6 shows the effect of equivalence ratio on the two engine parameters. The figure shows that the highest thermal efficiency is achieved at a much lower value of the

equivalence ratio than the highest mean effective pressure. The maximum value of the IMEP occurs at the stoichiometric combustion for all fuels.

5. CONCLUSIOMS

A computer-based air-fuel model has been presented to be used in analysing the performance of spark-ignition internal combustion engines with conventional and alternative fuels. Comparisons between the model's results and those provided by Ferguson [11] and Buttsworth [12] confirm that the model accurately produces the required results. Alternative fuels and their blends with gasoline can be added as new fuels to the model's library. The paper also analyses the performance of a SI engine fuelled with ethanol and ethanol-gasoline mixture. Performance parameters of the engine were evaluated at different engine speeds, compression ratios, and equivalence ratios.

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