# 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 air-fuel model that can be used to analyse the performance of spark-ignition (SI) internal combustion engines. Using the model, the performance characteristics of a real engine with conventional and alternative fuel mixtures can be estimated with lower cost and shorter time compared to experimental method. The paper describes the mathematical formulation of the model and outlines the main features of its computer code. The model is verified against published results of earlier fuel-inducted air-fuel models.

**Keywords:** *Alternative fuels; Air-fuel model; Fuel-induction engine*

## 1. INTRODUCTION

The depletion of the world oil reserves and the environmental pollution problems associated with fossil-fuels are deriving interest in alternative fuels for automotive engines. Therefore, numerous studies have been done to investigate the suitability of various alternative fuels for internal combustion (IC) 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 give 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 than in conventional liquid fuels [1]. 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], Abdalla and Abushousha [5], and Rodrigo et al [6] investigated the effects of ethanol or methanol–gasoline blends on the performance and exhaust emission of spark-ignition (SI) engines. Shahad and Abul Hadi [7] investigated the effect of hydrogen blending on the concentration of pollutants emitted from a four stroke diesel engine. Mahla et al [8] studied the effect of exhaust-gas recirculation (EGR) on the performance and emission characteristics of natural gas fueled diesel engines.

Experimental studies of alternative fuels require costly research engine test beds and well trained technicians to run them. Therefore, many researchers opted to develop computer-based theoretical models for internal combustion engines [9-16]. Realistic computer-based models of IC engines can be used to explore the effects of various operating parameters on the engine's performance while having the advantage of being more flexible and less costly. Ferguson [9] 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, etc. The models also apply the principles of thermodynamics to allow for the effects of suction and discharge of the fluids involved and takes account of the heat-transfer and mass transfer losses that take place. Apart from detailing the mathematical formulation, Ferguson [9] also provided FORTRAN computer codes for the air-fuel models. His air-fuel models have been adopted by other researchers, particularly in developing countries, to analyse the performance of IC engines with conventional and alternative fuels.

To avoid either major modifications to the engine or drastic degradations of its performance, the alternative fuels for IC engines are more commonly used as mixtures with conventional fossil fuels rather than in their neat form [3-7]. Pure alcohols for example require special materials to prevent corrosion of the engine parts and have problems with cold start. The addition of hydrogen, which has a high flame speed and a wide flammability limits, to gasoline and methane would improve the

combustion of these fuels which are disadvantaged with respect to these two properties [10]. However, most previous studies that used theoretical models considered only pure fuels [11-16]. To deal with fuel mixtures, the theoretical model needs a procedure to determine the thermodynamic properties of these mixtures. The present paper presents a theoretical model that can be used to analyse the performance of IC engines with fuel mixtures as well as pure fuels. The paper presents describes the mathematical formulation of the model and highlights the main features of its computer implementation. The model is validated by comparing its results for the main engine parameters with the respective results given by Ferguson [9] and Buttsworth [17]. The procedure used to determine the coefficients in the thermodynamic properties polynomials for fuel mixtures is outlined and values of the coefficients for gasoline-ethanol and methane-hydrogen blends at different concentrations are given. The model is also used to analyse the performance of an SI engine fuelled with gasoline-ethanol and methane-hydrogen blends at different engine speeds, pressure ratios, and equivalence ratios.

## 2. Mathematical Formulation of the Air-Fuel Model

The present model adopts a two-zone combustion model, whereby the combustion chamber is divided into two zones of unburned gases and burned gases [9,14,17,18]. The unburned gases are a mixture of fuel, air and residual gas while 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 expansion stroke the mixture is assumed frozen. A Wiebe function specifies the fuel burn rate and the rate at which the mixture from the unburned zone is converted to the burned zone [18]. The principle governing equations are the mass and energy conservation relations, the equations of state, and the second-law of thermodynamics. In the mathematical formulation of the principal governing equations the crank angle is taken as the independent variable. The differential form of the energy conservation equation (the first-law of thermo-dynamics) applied to an open system encasing the cylinder contents is [9]:

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

where, $\theta$ is crank-angle, $m$ mass, $u$ internal energy, $Q$ net heat added to the system, $P$ pressure, $V$ volume, and $\omega$ the rotational speed. In the last term of the equation ($m_l$) stands for the instantaneous leakage or blowby rate, which is assumed to be always out of the cylinder and taking with it gas characterised by the enthalpy ($h_l$) of the cylinder contents (which in turn depends on the temperature, pressure, and composition of the fluid).

Unlike standard gas cycles, the model also 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. Accordingly, the energy of the system ($u$) for spark-ignition engine is assumed to be given by:

$$u=\frac{U}{m}=xu_b+(1-x)u_u \tag{2}$$

where, $x$ is the mass fraction of the cylinder contents that have been burned, $u_b$ is the energy of the burnt gas that is at a temperature $T_b$ and $u_u$ is the energy of the unburnt gas at a temperature $T_u$ (the classical two-zone model). The mass fraction ($x$) burned is determined by an empirical burning law, such as:

$$x = \begin{cases} 0 & \theta < \theta_s \\ \frac{1}{2}\left\{1 - \cos\left[\frac{\pi(\theta - \theta_s)}{\theta_b}\right]\right\} & \theta_s < \theta < \theta_s + \theta_b \\ 1 & \theta > \theta_s + \theta_b \end{cases} \quad (3)$$

Likewise, the specific volume of the system ($v$) is expressed as:

$$v = \frac{V}{m} = x v_b + (1 - x) v_u \quad (4)$$

The enthalpy of the mass loss due to blowby: Early in the combustion process, unburned gas leaks past the rings. Late in the combustion process, burnt gas leaks past the rings it is assumed that:

$$h_l = (1 - x^2) h_u + x^2 h_b \quad (5)$$

Empirical relationships are also used to express the terms involving $dm/d\theta$ and $dQ/d\theta$ 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:

$$f\left(\theta, \frac{dP}{d\theta}, \frac{dT_b}{d\theta}, \frac{dT_u}{d\theta}, P, T_b, T_u\right) = 0 \quad (6)$$

Therefore, two more equations are needed to complete the mathematical formulation of model. One of the requisite equation is derived by differentiating Eq. (4) for the specific volume of the system. The second requisite equation comes from introduction of the un-burnt gas entropy into the analysis. Treating the unburned gas as an open system losing mass via leakage and combustion, leads to:

$$-\dot{Q}_u = \omega m (1 - x) T_u \frac{ds_u}{d\theta} \quad (7)$$

The three equations are then rearranged in the standard form used to numerically integrate a set of ordinary differential equations:

$$\frac{d\xi_i}{d\theta} = f_i(\theta, P, T_b, T_u) \quad (8)$$

where, $\xi_1$ , $\xi_2$ , $\xi_3$ 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 lost. 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 compression until the end of expansion, the indicated efficiency and the 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 model uses the formulae given by Heywood [18], which were obtained by curve-fitting the tabulated JANAF data [19]. For fuels (in vapour phase), the properties are obtained from the following polynomials:

$$\frac{c_p}{R} = a_0 + b_0 T + c_0 T^2 \quad (9a)$$

$$\frac{h}{RT} = a_0 + \frac{b_0}{2}T + \frac{c_0}{3}T^2 + d_0\frac{1}{T} \quad (9b)$$

$$\frac{s}{R} = a_0 \ln T + b_0 T + \frac{c_0}{2}T^2 + e_0 \quad (9c)$$

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 $d_0$ in the enthalpy equation and $e_0$ in entropy equation are constants resulting from the relevant integration of Eq. (9.a). Values of the different coefficients for gasoline, ethanol, methane and their blends are given in the following sections. For air components ($O_2$ and $N_2$) and the combustion products ($H_2O$, $CO_2$, etc), the following polynomial are used [9]:

$$\frac{c_p}{R} = a_1 + b_1 T + c_1 T^2 + d_1 T^3 + e_1 T^4 \quad (10a)$$

$$\frac{h}{RT} = a_1 + \frac{b_1}{2}T + \frac{c_1}{3}T^2 + \frac{d_1}{4}T^3 - \frac{e_1}{T^2} + f_1\frac{1}{T} \quad (10b)$$

$$\frac{s}{R} = a_1 \ln T + b_1 T + \frac{c_1}{2}T^2 + \frac{d_1}{3}T^3 - \frac{e_1}{2}\frac{1}{T^2} + g_1 \quad (10c)$$

## 3. The Computer Model

Ferguson [9] provided FORTRAN computer programs for air-fuel models of both fuel-inducted 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. Researchers who subsequently developed computer models based on those of Ferguson [9] attempted to make their models more user-friendly and self-contained. Buttsworth [17] developed his fuel-inducted model with Matlab in order to use its in-built function ODE45.m as the 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-inducted engine model of Ferguson [9], but the computer code has been developed in Visual Basic in order to make the model more user-friendly. Thus, the model has been developed with a graphical-user interface (GUI) that allows the fuel to be selected from a library of fuels as shown on Figure 1. After the fuel is selected, the GUI allows the user to specify the engine's specifications and operation parameters. Figure 2 shows that values of 14 parameters have to be specified. In order to make the present model self-contained, it has been developed with an in-built ODE solver that applies the classical fourth order Runge-Kutta method [20].

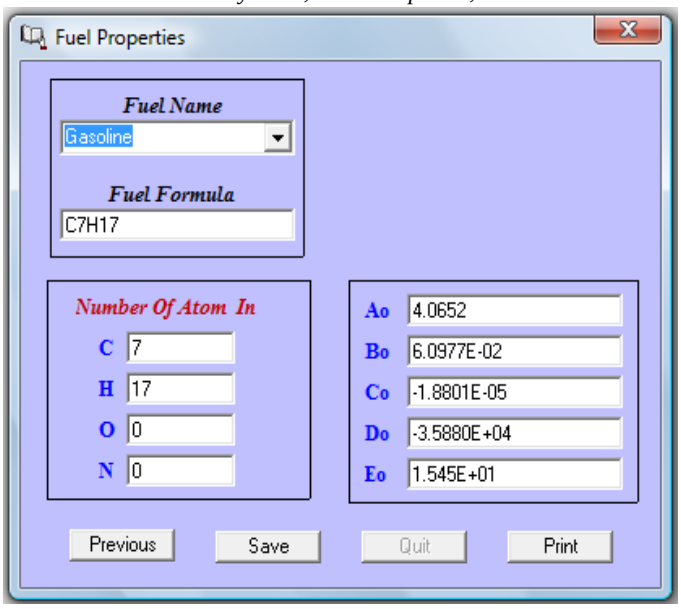



**Figure (1)**. Fuel properties.

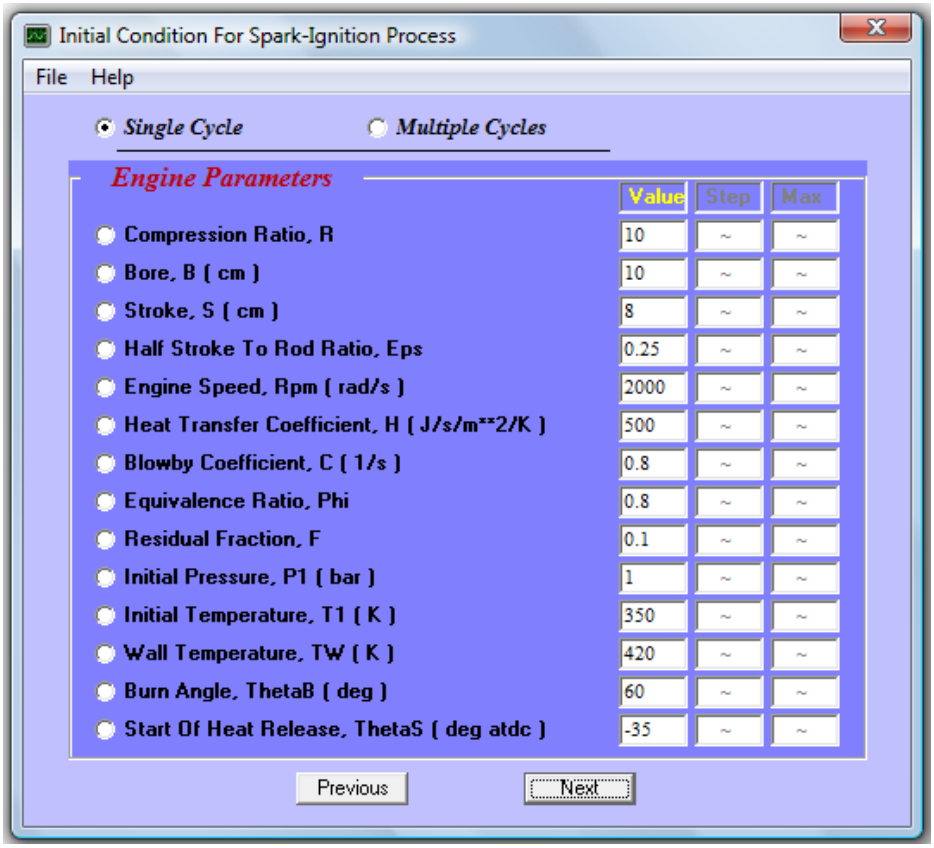



**Figure (2).** Engine specifications and operating conditions

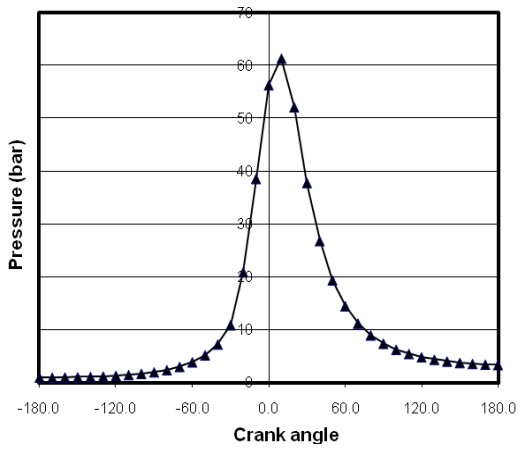
As shown on Figure 2, the model's GUI allows single or multi runs to be performed. If a single-cycle simulation is chosen, the model will proceed to integrate the ODEs starting from a crank angle of -180$^{o}$ until 180$^{o}$ to obtain the variation of the cycle parameters with crank-angle over the complete cycle. At the end of the cycle the simulation also gives the values of four overall parameters which are the indicated thermal efficiency ($\eta$), the indicated mean effective pressure (IMEP), the error in the conservation of mass (Error 1), and 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 ($\eta$, IMEP,

Error 1, and Error 2) with any of the 14 parameters shown on Figure 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.

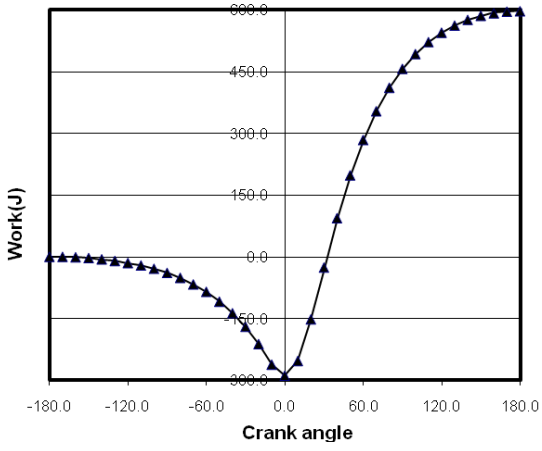
Following the specification of the fuel and engine properties, the model may be triggered to run the required simulation mode by pressing the "next" button shown on Figure 2. The results can then be plotted with Microsoft Excel. Figures 3 shows the results of a single-cycle simulation by the present model for the engine with the specifications shown on Figure 2 with gasoline as fuel. The figure shows the variation of the pressure, work, temperature, and heat leakage with the crank angle. The model results, which are compared with those provided by Ferguson [9] for the same case, confirm the close agreement between the two models. Table 1 compares the values obtained by the present model for the four overall parameters $\eta$, IMEP, Error 1, and Error 2 to the corresponding values given by Ferguson [9] and Buttsworth [17]. The figures show that the first three of the parameters are in good agreement with their corresponding values given by Ferguson [9]. Although the error in energy conservation (Error2) shows a significant difference from the corresponding value given by Ferguson [9] and Buttsworth [17], its absolute value is still insignificant.

**Table (1).** Values of the overall parameters compared to those given by Ferguson [9] and Buttsworth [17].

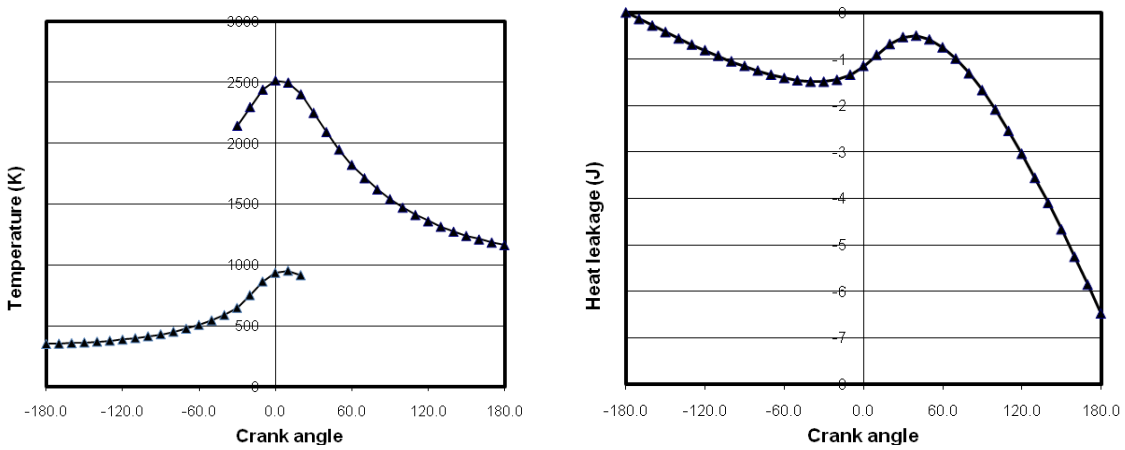
| | $\eta$ | IMEP | Error 1 | Error 2 |
|---|---|---|---|---|
| Ferguson [9] | 0.38821 | 0.95102 | -5.2238E-04 | 1.0633E-04 |
| Buttsworth [17] | 0.3889 | 0.95278 | 3.8258E-04 | 4.3581E-04 |
| Present model | 0.38807 | 0.95067 | -5.3095E-04 | 8.8986E-04 |




(a) Pressure




(b) Work




(c) Temperature (d) Heat leakage

**Figure (3).** Comparison of the results by the present model (symbols) to those of Ferguson [9] (solid line).

## 4. Concluding remarks

A new fuel can be added to the model's library by using the "Edit Fuel" option. The fuel properties that have to be provided for a new fuel include its content from carbon, hydrogen, oxygen and nitrogen. A general formula for fuels is $C_\alpha H_\beta O_\gamma N_\delta$. Figure 1 shows the respective values of these coefficients for gasoline ($C_7H_{17}$) [9]. The required fuel properties also include the values of five coefficients $a_0$ – $e_0$ used to determine the fuel's thermodynamic properties from Eq. (9). Figure 1 also shows the values of these coefficients for gasoline.

The "Edit Fuel" option also 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 [21,22]. This has the advantage of that the model can deal with fuel blends without any modification to the model itself. Using the model, parametric analyses can also be performed by choosing multiple cycles instead of a single cycle. The user selects one of the 14 parameters shown on Figure 2 and specifies its range.

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