

# Rapid Thermodynamic Simulation Model of an Internal Combustion Engine on Alternate Fuels

Sundeep Ramachandran

**Abstract**—A thermodynamic model for the simulation of a spark ignition engine running on alternate hydrocarbon fuel is presented. This paper aims to develop a simple, fast and accurate engine simulation model without the need for a great deal of computational power or knowledge of precise engine geometrical data. The model is based on the classical two-zone approach, wherein parameters like heat transfer from the cylinder, blowby energy loss and heat release rate are also considered. The general fuel is specified by way of its C-H-O-N values. Curve-fit coefficients are then employed to simulate air and fuel data along with frozen composition and practical chemical equilibrium routines. The calculated data is then used to plot the various thermodynamic parameters with respect to crank angle.

**Index Terms**—Internal Combustion Engines, SI Engine Simulation, Thermodynamic Modeling of Engines.

## I. INTRODUCTION

The present trend is towards the development of comprehensive 3-D models, which describes the functioning of engines at a very high level of detail and accuracy; however, these require substantial computational power. Also, the need for precise experimental input makes the process significantly complicated and time consuming. There are several instances where theoretical methods, which are based on a limited set of experimental data, are preferred. From these considerations, the need for a simple, fast and accurate engine simulation model is quite evident. Hence, this paper aims to combine the advantages of various known models to achieve this goal.

A two-zone, Zero-dimensional model was used to simulate the engine operations. The most important assumptions were that, a) The working medium was considered, in general, to be a mixture of 14 species ( $O_2$ ,  $N_2$ ,  $CO_2$ ,  $H_2O$ ,  $H_2$ ,  $OH$ ,  $NO$ ,  $CO$ ,  $O$ ,  $H$ ,  $N$ ,  $Ar$ ,  $NO_2$ ,  $HO_2$ ) and fuel vapor. b) All 14 species were considered as ideal gases. and c) The alternate fuels are limited to C-H-O-N species.

## II. THERMODYNAMIC MODEL

For the present study, a Zero-dimensional combustion model is employed. The combustion chamber is divided into two zones consisting of unburned gas (mixture of fuel, air and residuals) and burned gas (mixture of 14 product species), each under uniform composition. This model assumes that at any instant of time during the combustion,

the cylinder volume is divided into burned and unburned zones by an infinitesimally thin flame-front with a spherical shape. The burned gases are assumed to be in chemical equilibrium during combustion and for the main expansion stroke, while near the end of expansion stroke the mixture is assumed frozen [7], [10], [18]. A Wiebe function specifies the fuel burn rate and controls the rate at which mixtures from the unburned zone is converted to the burned zone [10]. Mass and energy conservation relations and equations of state form the principle governing equations. Also considering crank angle as the independent variable, we thus form the base of our thermodynamic model.

### A. Mass and Energy Balance

The equation of state for an ideal gas is

$$PV = mRT \quad (1)$$

The rate of change of mass within any open system is the net flux of mass across the system boundaries. Hence for a control volume enclosing the air-fuel mixture, we have

$$\dot{m} = \sum_k \dot{m}_k \quad (2)$$

The first law of thermodynamics to an open system yields the energy equation as

$$\dot{E} = \dot{Q} - \dot{W} + \sum_k \dot{m}_k h_k \quad (3)$$

Equations (2) and (3) can be written as

$$\frac{dm}{d\theta} = \sum_k \frac{dm_k}{d\theta} \quad (4)$$

$$\frac{d(mu)}{d\theta} = \frac{dQ}{d\theta} - p \frac{dV}{d\theta} + \sum_k h_k \frac{dm_k}{d\theta} \quad (5)$$

Equation (5) neglects changes of kinetic and potential energy in the control volume.

### B. Air and Combustion Products Data

Gordon and McBride [8], proposed the following expressions that were curve-fitted to the tabulated JANAF Thermchemical tables [11].

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (6)$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (7)$$

$$\frac{s}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (8)$$

where  $c_p$  is the specific heat at constant pressure,  $h$  is the specific enthalpy and  $s$  is the specific entropy.

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The coefficients  $a_1$  to  $a_7$  are calculated over two different temperature ranges: 1)  $300 < T < 1000$  K; and 2)  $1000 < T < 5000$  K and can be sourced from [8].

The most complete models are based on the assumption that the unburned mixture is frozen in composition and the burned mixture is in equilibrium [10]. The following are species of interest during combustion:  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{CO}$ ,  $\text{H}_2$ ,  $\text{H}$ ,  $\text{O}$ ,  $\text{OH}$  and  $\text{NO}$  [7].

### C. Fuel Data

Heywood [10] has represented the thermodynamic properties of fuels (in vapor phase) using curves that slightly differ from (6), (7), (8).

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 \frac{1}{T^2} \quad (9)$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 - a_5 \frac{1}{T^2} + \frac{a_6}{T} \quad (10)$$

$$\frac{s}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 - \frac{a_5}{2} \frac{1}{T^2} + a_7 \quad (11)$$

Data for calculating the coefficients can be obtained from [11], [5] or [8]. Reference [9], has discussed about the methods for calculating the thermodynamic properties of user-defined fuels.

The following relation is proposed for deriving the properties like specific heats and enthalpies for various species, with  $\xi$  referring to the property and  $x$  is the burnt mass fraction.

$$\xi_{\text{mixture}} = \sum_{k=1}^N x_k \cdot \xi_k \quad (12)$$

### D. Equivalence Ratio

When modeling with a single fuel, the equivalence ratio is given by [7]

$$\phi = \left( \frac{[F]}{[\text{Air}]_{\text{Act.}}} \right) / \left( \frac{[F]}{[\text{Air}]_{\text{St.}}} \right) \quad (13)$$

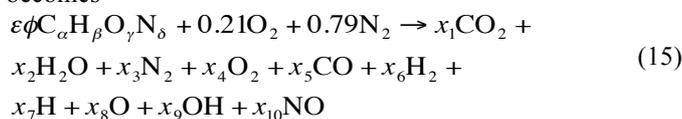
where subscript *Act.* refers to actual and *St.* refers to stoichiometric.

For blending of hydrocarbons and/or alcohol with hydrogen fuel, the equivalence ratio changes to [16]

$$\phi = \left( \frac{[F]}{[\text{Air}] - \frac{[H]}{([\text{H}]/[\text{Air}]_{\text{st.}})}} \right) / \left( \frac{[F]}{[\text{Air}]_{\text{st.}}} \right) \quad (14)$$

### E. Practical Chemical Equilibrium

Under the assumption of atmospheric air composition (21%<sub>v</sub> Oxygen and 79%<sub>v</sub> Nitrogen), and provided  $\phi < 3$ , the only species that are important because of dissociation are O, H, OH, and NO [7]. The combustion reaction thus becomes

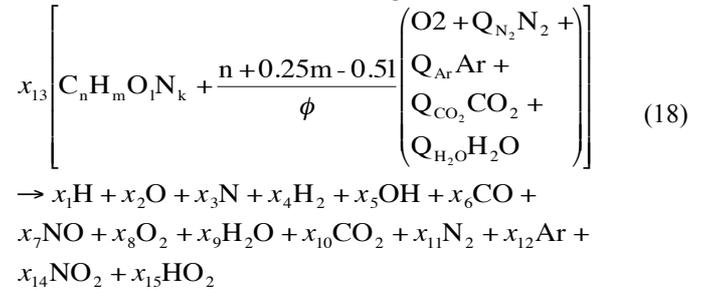


where  $x_1$  to  $x_{10}$  represents mole fractions of the products.

Olikara and Borman [14] included two additional mole fractions in the products: N and Ar. They also made provision to include user specified quality of air. Depcik [6] modified the Olikara and Borman [14] model by including the following two reactions



The combustion reaction now changes to



Here  $x$  and  $Q$  denote mole fraction and quality respectively.

For clarity, we define:  $\psi = \left( \frac{n+0.25m-0.5l}{\phi} \right)$

The atom balance for the various elements gives

$$C : x_6 + x_{10} = x_{13} (\psi Q_{CO_2} + n) \quad (19)$$

$$H : x_1 + 2x_4 + x_5 + 2x_9 + x_{15} = x_{13} (2\psi Q_{H_2O} + m) \quad (20)$$

$$O : x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10} + 2x_{14} + 2x_{15} = 2x_{13} (\psi (1 + Q_{CO_2} + 0.5Q_{H_2O}) + 0.5l) \quad (21)$$

$$N : x_3 + x_7 + 2x_{11} + x_{14} = 2x_{13} (\psi Q_{N_2} + 0.5k) \quad (22)$$

$$Ar : x_{12} = x_{13} \psi Q_{Ar} \quad (23)$$

The constraint that the mole fraction of all the products adds up to unity requires that

$$\sum_{k=1}^{12} x_k + x_{14} + x_{15} = 1 \quad (24)$$

To solve for the unknowns, we need equations that are provided by the criteria of equilibrium among the products, which are expressed by the following hypothetical relations

$$\frac{1}{2} \text{H}_2 \rightleftharpoons \text{H} \quad K_1 = \frac{x_1 \cdot p^{0.5}}{x_4^{0.5}} \quad (25a)$$

$$\frac{1}{2} \text{O}_2 \rightleftharpoons \text{O} \quad K_2 = \frac{x_2 \cdot p^{0.5}}{x_8^{0.5}} \quad (25b)$$

$$\frac{1}{2} \text{N}_2 \rightleftharpoons \text{N} \quad K_3 = \frac{x_3 \cdot p^{0.5}}{x_{11}^{0.5}} \quad (25c)$$

$$\frac{1}{2} \text{H}_2 + \frac{1}{2} \text{O}_2 \rightleftharpoons \text{OH} \quad K_5 = \frac{x_5}{x_4^{0.5} \cdot x_8^{0.5}} \quad (25d)$$

$$\frac{1}{2}\text{O}_2 + \frac{1}{2}\text{N}_2 \rightleftharpoons \text{NO} \quad K_7 = \frac{x_7}{x_8^{0.5} \cdot x_{11}^{0.5}} \quad (25e) \quad \text{O} : \phi\epsilon\gamma + 2W + 2Z = 2x_1 + x_2 \quad (34)$$

$$\text{H}_2 + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{H}_2\text{O} \quad K_9 = \frac{x_9}{x_4 \cdot x_8^{0.5} \cdot p^{0.5}} \quad (25f) \quad \text{N} : \phi\epsilon\delta + 2X = 2x_3 \quad \Rightarrow \quad x_3 = \frac{\phi\epsilon\delta + 2X}{2} \quad (35)$$

$$\text{CO} + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{CO}_2 \quad K_{10} = \frac{x_{10}}{x_6 \cdot x_8^{0.5} \cdot p^{0.5}} \quad (25g) \quad \text{Ar} : Y = x_7 \quad \Rightarrow \quad x_7 = Y \quad (36)$$

$$\text{NO} + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{NO}_2 \quad K_{14} = \frac{x_{14}}{x_7 \cdot x_8^{0.5} \cdot p^{0.5}} \quad (25h) \quad \epsilon = \frac{W}{\alpha + \frac{\beta}{4} - \frac{\gamma}{2}} \quad (37)$$

$$\text{O}_2 + \frac{1}{2}\text{H}_2 \rightleftharpoons \text{HO}_2 \quad K_{15} = \frac{x_{15}}{x_8 \cdot x_4^{0.5} \cdot p^{0.5}} \quad (25i) \quad \text{Hence the stoichiometric fuel-air ratio is} \quad \left(\frac{[F]}{[\text{Air}]_{\text{st}}}\right) = \frac{\epsilon(12.011\alpha + 1.008\beta + 16.0\gamma + 14.01\delta)}{31.998W + 28.012X + 38.948Y + 44.009Z} \quad (38)$$

The equilibrium constant K, for the above are determined from the Gibbs free energy as

$$-\frac{\Delta G^\circ}{RT} = \ln K_p \quad (26)$$

where  $\Delta G^\circ$  is the standard-state Gibbs free energy.

The values of the equilibrium constants can be obtained from [11]. Equations (25a) to (25i) reduces to the following which is then solved using Newton-Raphson iteration scheme.

$$x_1 + 2x_4 + x_5 + 2x_9 + x_{15} - \frac{(2\psi Q_{\text{H}_2\text{O}} + m)}{(\psi Q_{\text{CO}_2} + n)}(x_6 + x_{10}) = 0 \quad (27)$$

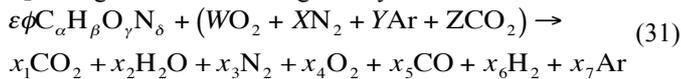
$$x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10} + 2x_{14} + x_{15} - \frac{2(\psi(1 + Q_{\text{CO}_2} + 0.5Q_{\text{H}_2\text{O}}) + 0.51)}{(\psi Q_{\text{CO}_2} + n)}(x_6 + x_{10}) = 0 \quad (28)$$

$$x_3 + x_7 + 2x_{11} + x_{14} - \frac{2(\psi Q_{\text{N}_2} + 0.5k)}{(\psi Q_{\text{CO}_2} + n)}(x_6 + x_{10}) = 0 \quad (29)$$

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 + x_9 + x_{10} + x_{11} + x_{14} + x_{15} + \frac{\psi Q_{\text{Ar}}}{(\psi Q_{\text{CO}_2} + n)}(x_6 + x_{10}) - 1 = 0 \quad (30)$$

#### F. Frozen Composition

Depcik model [6] is applicable only over the range of 600-4000 K. We use the Ferguson model [7] that calculates the species of combustion in the low ranges of temperature from 300-600 K. This model assumes that the only species prevalent in the exhaust are:  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$ , Ar, CO,  $\text{O}_2$  and  $\text{H}_2$ . The general reaction is given by



Equation (31) is formulated for stoichiometric case, i.e. ( $\phi = 1$ ) wherein  $x_4 = x_5 = x_6 = 0$ . For lean, i.e. ( $\phi \leq 1$ ),  $x_5 = x_6 = 0$  and for rich, i.e. ( $\phi > 1$ ),  $x_4 = 0$ . Performing atom balance for stoichiometric case and solving for the coefficients give

$$\text{C} : \phi\epsilon\alpha + Z = x_1 \quad \Rightarrow \quad x_1 = \phi\epsilon\alpha + Z \quad (32)$$

$$\text{H} : \phi\epsilon\beta = 2x_2 \quad \Rightarrow \quad x_2 = \frac{\phi\epsilon\beta}{2} \quad (33)$$

Equation (38) is used in (13) or (14) to calculate the equivalence ratio. Similar formulation can be used for lean and rich mixture cases.

#### G. Thermal Properties

We consider the unburned and burnt mixture zones as separate open systems. Therefore, the specific internal energy,  $u$  and specific volume,  $v$  is expressed as

$$u = \frac{U}{m} = xu_b + (1-x)u_u \quad (39)$$

$$v = \frac{V}{m} = xv_b + (1-x)v_u \quad (40)$$

subscripts  $b$  and  $u$  refers to burnt gas and unburned gas respectively.

Going by our assumption that the pressures of burnt and unburned gases are equal,  $v_b$  and  $v_u$  are functions of  $T_b$ ,  $T_u$  and  $p$ . Hence

$$\frac{dv_b}{d\theta} = \frac{\partial v_b}{\partial T_b} \frac{dT_b}{d\theta} + \frac{\partial v_b}{\partial p} \frac{dp}{d\theta} \quad (41)$$

$$\frac{dv_u}{d\theta} = \frac{\partial v_u}{\partial T_u} \frac{dT_u}{d\theta} + \frac{\partial v_u}{\partial p} \frac{dp}{d\theta} \quad (42)$$

Back substituting the logarithmic derivatives from Depcik model [6] on (41) and (42), we have

$$\frac{dv_b}{d\theta} = \frac{v_b}{T_b} \frac{\partial \ln v_b}{\partial \ln T_b} \frac{dT_b}{d\theta} + \frac{v_b}{p} \frac{\partial \ln v_b}{\partial \ln p} \frac{dp}{d\theta} \quad (43)$$

$$\frac{dv_u}{d\theta} = \frac{v_u}{T_u} \frac{\partial \ln v_u}{\partial \ln T_u} \frac{dT_u}{d\theta} + \frac{v_u}{p} \frac{\partial \ln v_u}{\partial \ln p} \frac{dp}{d\theta} \quad (44)$$

Similarly, the internal energies of both the burnt and unburned gases, under the same pressure condition and including the logarithmic derivatives can be written as

$$\frac{du_b}{d\theta} = \left( c_{p_b} - \frac{pv_b}{T_b} \frac{\partial \ln v_b}{\partial \ln T_b} \right) \frac{dT_b}{d\theta} - v_b \left( \frac{\partial \ln v_b}{\partial \ln T_b} + \frac{\partial \ln v_b}{\partial \ln p} \right) \frac{dp}{d\theta} \quad (45)$$

$$\frac{du_u}{d\theta} = \left( c_{p_u} - \frac{pv_u}{T_u} \frac{\partial \ln v_u}{\partial \ln T_u} \right) \frac{dT_u}{d\theta} - v_u \left( \frac{\partial \ln v_u}{\partial \ln T_u} + \frac{\partial \ln v_u}{\partial \ln p} \right) \frac{dp}{d\theta} \quad (46)$$

#### H. Trapped Mass in Control Volume

The trapped mass in control volume is defined at various

periods by [4]

for  $\theta_{IVC} \geq \theta \geq -360^\circ \text{CA}$  (intake)

$$m = \frac{V(\theta)}{v_u} \quad (47)$$

for  $\theta_{EVO} \geq \theta \geq \theta_{IVC}$  (valve - closed)

$$m = m_{IVC} e^{-C_b(\theta - \theta_{IVC})/\omega}$$

for  $360^\circ \text{CA} \geq \theta \geq \theta_{EVO}$  (blowdown and exhaust)

$$m = \frac{V(\theta)}{v_b} \quad (49)$$

IVC refers to intake valve open and EVO refers to exhaust valve open.

The volume of the cylinder at any crank angle instant is given by [7]

$$V(\theta) = V_c \left\{ 1 + \frac{r-1}{2} \left[ 1 - \cos\theta + \frac{1}{\varepsilon} \left[ 1 - (1 - \varepsilon^2 \sin^2\theta)^{0.5} \right] \right] \right\} \quad (50)$$

$V_c$  is clearance volume,  $r$  is the compression ratio and

$$\varepsilon = \frac{\text{stroke}}{2 \times \text{length of connecting rod}}$$

### I. Fuel Burning Rate Model

Many experiments show that the burning rate depends mostly on the combustion chamber shape and the position of the spark plug. The Wiebe function represents the mass fraction burned,  $x_b$  versus crank angle and defined as [10]

$$x_b(\theta) = 1 - \exp\left\{-a\left[\frac{\theta - \theta_0}{\Delta\theta}\right]^{m+1}\right\} \quad (51)$$

The present simulation uses  $a=5$  and  $m=2$  [10]. This model is capable of representing many combustion chamber shapes with different positions of spark plugs by adjusting  $a$  and  $m$ . The constant  $a$  is responsible for maximum value of  $x_b$  which is unity [12]. Hence  $a$  may represent the positions and/or number of spark plugs. By varying  $m$ , he observed the starting point and end point of  $x_b$  are independent of  $m$ . Hence even though, for a particular  $a$ , the amount of burned mass fraction  $x_b$  is independent of  $m$ , its rate closely depends on  $m$ . Hence as  $m$  increases,  $x_b$  is found to decrease and hence  $m$  may represent combustion chamber shape-factor.

### J. Heat Transfer Model

Heat transfer into a thermodynamic system is expressed in terms of heat loss

$$\frac{dQ}{d\theta} = \frac{-Q_1}{\omega} = \frac{-\dot{Q}_b - \dot{Q}_u}{\omega} \quad (52)$$

where

$$\dot{Q}_b = h \sum_{i=h,p,l} A_{bi}(T_b - T_{wi}) \quad (53)$$

$$\dot{Q}_u = h \sum_{i=h,p,l} A_{ui}(T_u - T_{wi}) \quad (54)$$

Here  $A_{bi}$  and  $A_{ui}$  are the areas of burnt and unburnt gases in contact with the combustion chamber component at temperature  $T_{wi}$ , and subscripts  $h, p, l$  refers to cylinder head, piston crown and liner, respectively. We have the following relations [7]

$$A_{bi} = A_r x^{0.5} \quad (55)$$

$$A_{ui} = A_i(1 - x^{0.5}) \quad (56)$$

$$A_h = \frac{\pi b^2}{2} \quad (\text{Hemispherical cylinder head}) \quad (57)$$

$$A_p = \frac{\pi b^2}{4} \quad (\text{Flat piston crown}) \quad (58)$$

$$A_l = \frac{4V(\theta)}{b} \quad (\text{Linear surface area exposed to gases}) \quad (59)$$

subscript  $i$  refers to intake.

### K. Heat Transfer Correlation

In (53) and (54),  $h$  is the instantaneous heat transfer coefficient. Woschni proposed a correlation of the form [18]

$$Nu = 0.035 Re^{0.8} \quad (60)$$

where  $Nu$  is Nusselt number and  $Re$  is Reynolds number. Now, assuming a local average gas velocity in the cylinder, becomes

$$h = 0.82b^{-0.2} (p \cdot 10^{-3} \cdot c)^{0.8} T^{-0.53} \quad (61)$$

where  $h$  is the heat transfer coefficient,  $p$  is pressure.  $c = 6.18$  cm (For gas exchange process)

$$T = xT_b + (1-x)T_u \quad (63)$$

### L. Blowby Energy Loss

Enthalpy loss due to blowby is expressed as [7]

$$h_1 = (1-x^2)h_u + x^2h_b \quad (64)$$

which indicates that more leaking is due to the unburned gas compared with the burnt gas in the early stage of combustion.

### M. Principle Governing Equations

Differentiating (40) with respect to crank angle and also considering (43) and (44), we have [7]

$$\frac{1}{m} \frac{dV}{d\theta} + \frac{VC_b}{m\omega} = x \frac{v_b}{T_b} \frac{\partial \ln v_b}{\partial \ln T_b} \frac{dT_b}{d\theta} + (1-x) \frac{v_u}{T_u} \frac{\partial \ln v_u}{\partial \ln T_u} \frac{dT_u}{d\theta} + \quad (65)$$

$$\left[ x \frac{v_b}{p} \frac{\partial \ln v_b}{\partial \ln p} + (1-x) \frac{v_u}{p} \frac{\partial \ln v_u}{\partial \ln p} \right] \frac{dp}{d\theta} + (v_b - v_u) \frac{dx}{d\theta}$$

here  $C_b$  is the blowby coefficient and given by  $C_b = \dot{m}_1/m$  and  $\dot{m}_1$  is the leakage due to blowby.

Expressing the heat loss of burnt and unburnt gases as a function of the rate of change of specific entropy gives

$$-\dot{Q}_b = m\omega x T_b \frac{ds_b}{d\theta} \quad (66)$$

$$-\dot{Q}_u = m\omega(1-x) T_u \frac{ds_u}{d\theta} \quad (67)$$

where

$$\frac{ds_b}{d\theta} = \left( \frac{c_{pb}}{T_b} \right) \frac{dT_b}{d\theta} - \frac{v_b}{T_b} \frac{\partial \ln v_b}{\partial \ln T_b} \frac{dp}{d\theta} \quad (68)$$

III. SIMULATION RESULTS

$$\frac{ds_u}{d\theta} = \left( \frac{c_{p_u}}{T_u} \right) \frac{dT_u}{d\theta} - \frac{v_u}{T_u} \frac{\partial \ln v_u}{\partial \ln T_u} \frac{dp}{d\theta} \quad (69)$$

Expressing the heat loss of burnt and unburnt gases as a function of the rate of change of specific entropy by combining (53)-(56) and (66)-(69)

$$c_{p_b} \frac{dT_b}{d\theta} - v_b \frac{\partial \ln v_b}{\partial \ln T_b} \frac{dp}{d\theta} = \frac{-h \sum_{i=h,p,l} A_{bi}(T_b - T_{wi})}{m\omega x} \quad (70)$$

$$c_{p_u} \frac{dT_u}{d\theta} - v_u \frac{\partial \ln v_u}{\partial \ln T_u} \frac{dp}{d\theta} = \frac{-h \sum_{i=h,p,l} A_{ui}(T_u - T_{wi})}{m\omega(1-x)} \quad (71)$$

Differentiating Equations (50) and (51) and incorporating with Equations (4), (39), (40), (43)-(46) and (52)-(64) into Equation (5), we have the following relations [7]

$$\frac{dp}{d\theta} = \frac{f_1 + f_2 + f_3}{f_4 + f_5} \quad (72)$$

$$\frac{dT_b}{d\theta} = \frac{-h \sum_{i=h,p,l} A_{bi}(T_b - T_{wi})}{m\omega c_{p_b} x} + \frac{v_b}{c_{p_b}} \frac{\partial \ln v_b}{\partial \ln T_b} \frac{dp}{d\theta} + \frac{h_u - h_b}{xc_{p_b}} \left[ \frac{dx}{d\theta} - (x - x^2) \frac{C_b}{\omega} \right] \quad (73)$$

$$\frac{dT_u}{d\theta} = \frac{-h \sum_{i=h,p,l} A_{ui}(T_u - T_{wi})}{m\omega c_{p_u} (1-x)} + \frac{v_u}{c_{p_u}} \frac{\partial \ln v_u}{\partial \ln T_u} \frac{dp}{d\theta} \quad (74)$$

where

$$f_1 = \frac{1}{m} \left( \frac{dV}{d\theta} + \frac{VC_b}{\omega} \right) \quad (75)$$

$$f_2 = \frac{h}{m\omega} \left[ \frac{v_b}{c_{p_b}} \frac{\partial \ln v_b}{\partial \ln T_b} \frac{\sum_{i=h,p,l} A_{bi}(T_b - T_{wi})}{T_b} + \frac{v_u}{c_{p_u}} \frac{\partial \ln v_u}{\partial \ln T_u} \frac{\sum_{i=h,p,l} A_{ui}(T_u - T_{wi})}{T_u} \right] \quad (76)$$

$$f_3 = -(v_b - v_u) \frac{dx}{d\theta} - v_b \frac{\partial \ln v_b}{\partial \ln T_b} \frac{h_u - h_b}{c_{p_b} T_b} \left[ \frac{dx}{d\theta} - (x - x^2) \frac{C_b}{\omega} \right] \quad (77)$$

$$f_4 = x \left[ \frac{v_b^2}{c_{p_b} T_b} \left( \frac{\partial \ln v_b}{\partial \ln T_b} \right)^2 + \frac{v_b}{p} \frac{\partial \ln v_b}{\partial \ln p} \right] \quad (78)$$

$$f_5 = (1-x) \left[ \frac{v_u^2}{c_{p_u} T_u} \left( \frac{\partial \ln v_u}{\partial \ln T_u} \right)^2 + \frac{v_u}{p} \frac{\partial \ln v_u}{\partial \ln p} \right] \quad (79)$$

Equations (75)-(79) are functions of  $\theta$ ,  $p$ ,  $T_b$  and  $T_u$  and are solved using the Runge-Kutta method.

Having formulated the mathematical framework, we simulate Pressure, Temperature, Work and Heat Transfer for an single cylinder, four stroke SI Engine running on Ethanol ( $CH_3CH_2OH$ ). We have assumed a bore of 0.1m, stroke of 0.08m and compression ratio of 10. The engine is assumed to operate at 2000 rpm, with an equivalence ratio of 0.8.

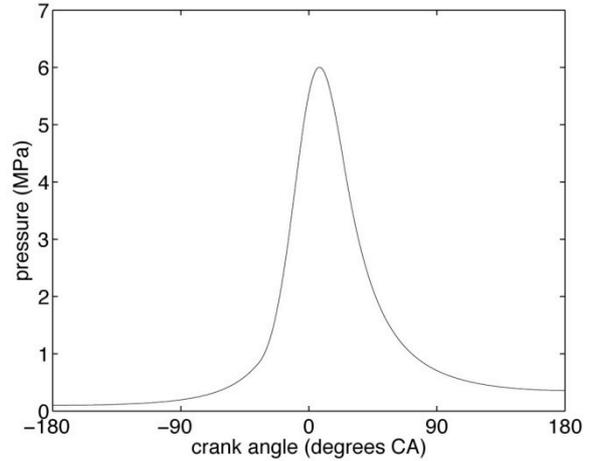


Figure 1: Pressure v/s Crank Angle

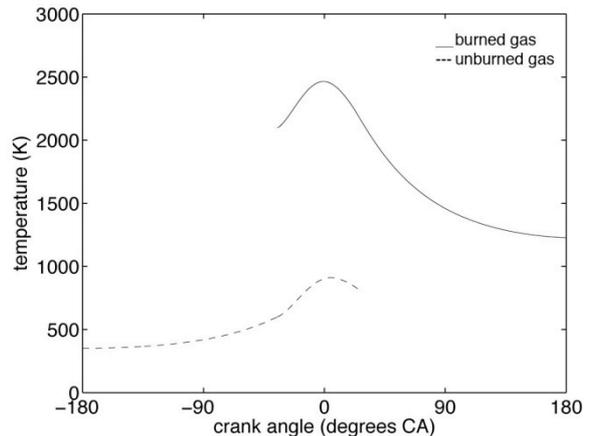


Figure 2: Temperature v/s Crank Angle

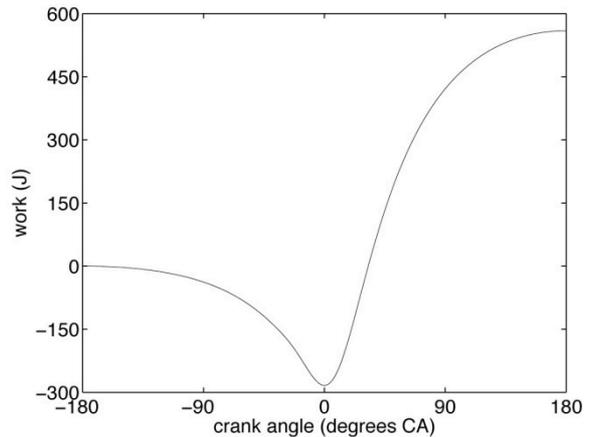


Figure 3: Work v/s Crank Angle

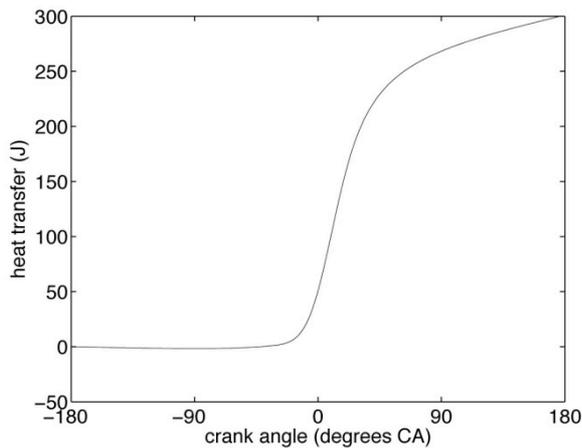


Figure 4: Heat Transfer v/s Crank Angle

#### IV. CONCLUSION

The present work achieves its goal by being a simple, fast and accurate engine simulation model. The results obtained can be used as a first-degree approximation and is useful in numerous engineering applications including general design predictions. The model can predict an array of thermodynamic and combustion parameters and easily adapt to any combustion chamber shape. Due to its simplicity and computational efficiency, the model can also be used as a preliminary test on a wide range of alternate hydrocarbon fuels.

#### NOMENCLATURE

$A$	area exposed to heat transfer ( $m^2$ )
$b$	bore of cylinder (m)
$c_p$	specific heat at constant pressure ( $kJ \cdot kg^{-1} \cdot K^{-1}$ )
$C_b$	blowby coefficient ( $s^{-1}$ )
$E$	total energy (kJ)
$\Delta G^\circ$	standard-state Gibbs free energy
$h$	specific enthalpy ( $kJ \cdot kg^{-1}$ ) or heat transfer coefficient ( $W \cdot m^{-2} \cdot K^{-1}$ )
$K$	equilibrium const.
$m$	mass (kg)
$Nu$	Nusselt number
$p$	pressure (Pa)
$Q$	heat transfer (kJ)
$r$	compression ratio
$R$	Gas constant
$Re$	Reynolds number
$s$	specific entropy ( $kJ \cdot kg^{-1} \cdot K^{-1}$ )
$T$	temperature (K)
$u$	specific internal energy ( $kJ \cdot kg^{-1}$ )
$U$	internal energy (kJ)
$v$	specific volume ( $m^3 \cdot kg^{-1}$ )
$V$	volume ( $m^3$ )
$W$	work done (kJ)
$x$	burnt mass fraction
$\theta$	crank angle ( $^\circ CA$ )
$\theta_0$	start of combustion ( $^\circ CA$ )
$\Delta\theta$	total combustion duration ( $^\circ CA$ )

$\omega$	angular velocity ( $rad \cdot s^{-1}$ )
$\phi$	equivalence ratio

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