CHAPTER 3

DUAL FUEL ENGINE COMBUSTION MODELLING

3.1 INTRODUCTION

It has been realised that of the three different approaches of the design available, such as design by experience or thumb rule, rational method of design utilising the fundamental laws of engineering sciences like Thermodynamics, Fluid Mechanics and Heat Transfer and experimental methods of design, the one combining the rational and experimental methods is becoming more attractive especially in the present context of large scale computer application. Basically for an I.C. Engine, this method envisages the development of a mathematical model of the combustion process using physico-chemical laws and relevant engine parameters by using a comprehensive computer programme. The results of such an analytical exercise are compared with the data obtained from a well planned and neatly executed experimental programme. An attempt has been made to develop such a mathematical model for the combustion process in a dual fuel combustion system in a C.I. engine. A review of C.I. engine modelling, the details of dual fuel combustion model developed and the computer programming technique adopted are presented and discussed in the following sections.
3.2 REVIEW OF DIESEL COMBUSTION ENGINE MODELLING

It is a well established fact that the power, efficiency and stresses developed in an I.C. engine depend upon the way by which the pressure and temperature change during combustion with respect to time or crank angle. This cylinder pressure-time history is primarily influenced by factors like combustion chamber geometry, rate of fuel burning and the rate of heat loss to the engine parts. Rate of fuel burning or heat release in turn depends upon the type of fuel, overall air-fuel ratio, time of ignition and the rate of fuel-air mixing or preparation.

In the process of understanding the effects of various parameters on the performance and combustion characteristics and fuel economy, which are complex functions of many interrelated variables, engine cycle analysis, referred to as simulation, has been recognized as a powerful tool. The completeness and accuracy of such cycle simulation largely depend on the prediction of the rate of fuel burning and the validity and closeness of the assumptions and approximations included in the formulation of the analytical expressions representing the physical and chemical processes.

The rate of burning of a homogeneous air-fuel mixture in a S.I. engine where the combustion is initiated by a spark, is varying according to some established reaction rates as well as the overall air-fuel ratio. This mode of combustion
seems to be more amenable to analysis and various theoretical models have been proposed, which exhibit good agreement between the calculated and experimental results.

However, the combustion in a compression ignition engine is extremely complicated due to the heterogeneous nature of combustion involving different rate controlling mechanisms for different parts of combustion period. Development of diesel spray, droplets distribution, evaporation, mixing with air, ignition delay and the formation of multiple ignition nuclei are factors that are involved in the process, all of which are unsteady in time and also not separate but tend to overlap. Determination of spatial and temporal variations of temperature, composition and the air motion has not been amenable in obtaining some useful analytical correlations between various design and operating factors and the rate of fuel burning. Besides, in compression ignition combustion systems, the burning rates are far from uniform and are believed to be controlled to a large extent by physical processes rather than chemical reactions. These difficulties have led to the development of methods which predict an apparent heat release rate from the experimentally measured pressure-crank angle diagrams. This is achieved, ignoring the real phenomena like fuel injection, vaporization and pre-flame reactions, by the assumption of a homogeneous or uniform heat source with instantaneous equilibrium products as dictated by the measured cylinder pressure changes. In
some cases the model has been made more complex by considering the way in which fuel and air mix inside the cylinder and expressing the result as if the cylinder contents consisted of a volume of air, fuel and combustion products at any particular instant, called a two-zone model.

Lyn [43] has analytically investigated the cylinder pressure development, cycle efficiency and the rate of pressure rise for various assumed patterns of heat release rates. He showed that power output and efficiency are closely related to the development of pressure course which in turn depend on the heat release pattern. The triangular heat addition having its peak at the beginning and 40 crank angle of heat release period is found to give the best results in respect of maximum efficiency and optimum values of peak pressure and rate of pressure rise. Reduction in the period of heat release results in the abnormal increase in peak pressure and rate of pressure rise with a marginal increase in efficiency. No attempt was made to link any parameter like ignition delay, equivalence ratio and speed that governs combustion with the shape of heat release rate.

Austin and Lyn [44] proposed a method of predicting the heat release rates from the fuel injection diagrams. The basic idea of this model is to keep track of the injected fuel, during the delay period, which for each element can be estimated from empirical equations. The fuel which has been injected prior to ignition of the first element burns rapidly
causing a sharply rising triangular heat release diagram. Subsequent burning is essentially proportional to the rate of injection. Though this approach is highly empirical, it predicts the peak pressure and rate of pressure rise quite reasonably.

Wiebe [45] developed a semi-empirical burning law in a non-dimensional form giving the ratio of fuel burned at any instant to the total fuel injected into the combustion chamber, as an exponential function. The model employed two coefficients, namely combustion efficiency coefficient, related to the total quantity of fuel burnt to that present and an adjustable shape factor and a dimensionless time function related to the duration of combustion. From the experimentally obtained time averaged fuel/cycle and the derivative of Wiebe's equation, the heat release rate can be determined. However, this model fails to predict the distinct initial spike that is typical of diesel combustion.

Krieger and Borman [46] reported a method of calculating the heat release curve from an analysis of experimentally obtained, accurate and well averaged pressure-crank angle diagrams. This model takes into account both the effects of heat transfer and dissociation of the products of combustion. It is assumed that the entire cylinder contains a homogeneous mixture of air and products of combustion at each instant and thus acts as a uniform heat source. Suitable mathematical expressions for the internal energy and gas constant as a
function of pressure, temperature and equivalence ratio were developed and used in the model. They showed that the effect of dissociation of the products of combustion was found to be negligible. Though the resulting heat release diagram does not provide a clear understanding of the combustion phenomenon, it does give some quantitative information over a wide range of operating conditions.

Following the concept of Borman, Shipinski [47] reported a detailed experimental and analytical investigation on the relationship between the rate of fuel injection and the rate of heat release. From the results of the investigation he has postulated a model for heat release studies based on a spray droplet size distribution and single droplet burning.

The model for transient spray mixing and combustion for diesel engine, developed by Shahed [48] et.al, is based on the growth of a spray plume and mixing theory. This model uses both semi-empirical equations describing the time variant spray geometry and mass conservation equation. Computing the mixing rate of fuel and air from the known pattern of diesel spray distribution and ignition delay through some already established equations, instantaneous pressure, temperature and the rate of heat release are obtained by applying the law of conservation of energy and thermodynamic property equations.
Whitehouse and Sareen [49] proposed a more realistic two-zone model by which heat release rate is calculated from the volume growth of the jet and air entrainment. Maguerdichian and Watson [50] developed a multi-zone model for the mixture formation and rate of heat release based on jet mixing processes and temperature dependent reaction rates. This model helps the study of spatial and temporal history of burning rates, temperature and air-fuel ratio and also enables the prediction of the various pollutants formed during the process of combustion. A reasonably good agreement between the predicted and experimentally observed results over a wide range of operating conditions has been noticed.

However, in dual fuel combustion systems, the total energy is divided into two and each is admitted at different times of the cycle characterizing a particular approach. In the dual fuel combustion technique of the author's interest, a fraction of the total energy is introduced along with the intake air through ethanol and the nearly homogeneous air-ethanol mixture, compressed below the autoignition temperature of ethanol, is ignited by the injection of a diesel spray.

Compared with the straight diesel operation, diesel is injected in a different atmosphere where the oxidizer is diluted by ethanol vapour and the presence of ethanol vapour acts in a complex manner before and during the process of combustion.
Though it can be stated that the four stages of compression ignition combustion, as proposed by RICARDO could not be applied to a dual fuel combustion, it is still believed that premixed and diffusion modes of combustion are possible. From experimental and analytical investigations, Karim et. al [51] have reported that two distinct phases of combustion phenomena exist in the case of dual fuel combustion. The first is associated with the combustion of diesel spray and some inducted fuel present in the vicinity of the multiple ignition centres. In the second phase of normal knock-free combustion, the multiple ignition centres developed earlier further develop into a macro flame fronts and move through the rest of the charge. They have indicated that under relatively weak mixtures of the inducted fuel, the heat release in the first phase has been found to correspond approximately to the heating value of diesel spray.

Govinda Mallan [52] had attempted to model the dual fuel combustion process following Lyn's approach. He assumed the combustion of inducted fuel-air mixture to follow the pattern of S.I. engine combustion, where the propagation of a thin walled turbulent flame front was considered. The injected diesel mass was divided into two equal parts, one part undergoing premixed combustion and the other in diffusion combustion. Further, right angled triangular heat release shapes with a duration of combustion of 160°crank angle for the diffusion part and a combustion duration ratio of 1:6 between premixed to diffusion were also assumed.
However, no closer agreement between the computed and measured cylinder pressure Vs crank-angle traces was noticed. During the whole closed period the computed pressures were greater than the measured pressures and the computed peak pressures were about 30 percent higher than the measured values.

From the foregoing it is evident that sufficient background material is available for developing a straight diesel combustion engine modelling which will reasonably predict the pressure-time history and heat release rates which can be used for designing new engine systems. However only limited attempts seem to have been made for developing a dual fuel engine combustion modelling for a compression ignition engine. Hence an attempt has been made for developing a mathematical model to understand the complex behaviour of the dual combustion process and to study the effects of some influencing parameters on the engine performance.

3.3 ETHANOL-DIESEL DUAL FUEL ENGINE COMBUSTION MODELLING

Dual fuel combustion in compression ignition engines adopting the carburetion technique can be visualised as the most complex version of the combustion systems available today. Admission of ethanol along with the intake air introduces significant complexities in the initiation and subsequent combustion processes and offers some distinct
variations with regard to thermal efficiency, peak pressure, rate of pressure rise, noise, smoke and exhaust emissions compared with straight diesel operation. The extent of these variations depends upon the operating conditions such as speed, load and the relative proportions of ethanol and diesel fuel.

Though extensive combustion modelling capable of predicting the mass burning rate of fuel or rate of heat release in respect of straight diesel operation are available as mentioned earlier, ethanol and diesel dual fuel combustion model enabling the prediction of the rate of burning of inducted and injected fuels and the resulting combustion parameters has not been reported so far. In order to have a better understanding of the dual fuel combustion process as a first step, a single zone model following Watson's [53] approach has been proposed and presented in the following sections.

3.3.1 FORMULATION OF DUAL FUEL COMBUSTION MODEL

Among the number of events taking place in the working of any internal combustion engine, significant importance is attached to the closed period of the cycle since the important events such as compression, heat release and power development are concentrated in this period with no exchange of gases between the system and the surroundings. As it is highly desirable to understand the influence of inducting
ethanol along with the intake air in the processes of compression, combustion and expansion, the present studies are directed to the closed period only.

Among the number of factors which control the autoignition of the injected fuel and the subsequent combustion of air-ethanol mixture, the developments of pressure and temperature during the process of compression are considered to play the most important roles. The high latent heat of evaporation of ethanol (904 kJ/kg) significantly lowers the charge temperature at the start of the compression stroke due to the partial evaporation of ethanol. Further the pressure and temperature histories during the compression process are hampered by the increase in the specific heat values of the charge due to the presence of ethanol and water vapours and the continuing evaporation of ethanol and water droplets. The understanding of the development of compression pressure and temperature with regard to the quantity and quality of ethanol is considered to be the first step in developing the dual fuel combustion model. In order to acquire the necessary knowledge, a mathematical model for compression process has been developed through reasonable assumptions in the first instance.

The engine with usual boundary conditions is reduced to a thermodynamic system consisting of a homogeneous mixture of air, ethanol and water vapour and residual gas. The boundaries of the system are the cylinder walls, cylinder
head and the top of the piston. Work is added or taken from the system through the motion of the piston and heat is transferred to or from the system through any and all of the boundary surfaces.

For simplicity, the inducted hydrated ethanol is divided into water and neat ethanol from the known value of the proof of ethanol. In dual fuel operations not involving any preheating of air or air-ethanol mixture, owing to the high latent heat of evaporation and the inadequate heat transfer taking place in the inlet passage, complete evaporation of ethanol and water is not ensured. Though the complete evaporation of ethanol, equivalent to 25 percent of energy input could cause a drop in the mixture temperature to about 20°C, the temperature of air-ethanol mixture measured close to the inlet port did not indicate this drop. Further, the measured mixture temperature for different flow rates of ethanol indicated that only less than 50 percent of ethanol could have been vaporized prior to the entry to the inlet port. Under these circumstances it is assumed that only a portion of inducted ethanol evaporates in the process of induction and subsequent mixing with the residual gas, and the remaining ethanol and the contained water evaporate linearly during the compression process. For simplicity it is further assumed that evaporation of ethanol and water is complete by 20°crank angle before TDC, i.e., before the start of injection of diesel fuel.
The system is really a heterogeneous mixture of air, ethanol and water vapour, droplets of diesel and products of partial and complete combustion. Thus, there are extreme gradients in composition, velocity and the temperature of the charge. However, for simplicity and as a first step, the system is assumed to be a homogeneous one and hence at any instant the pressure and temperature are uniform throughout the charge behaving like an ideal gas and obeying the equations of state. Further the following assumptions have also been made in order to simplify the computation.

(a) The droplets of ethanol and their vapour remain in phase equilibrium during the compression process.

(b) Kinetic and potential energies of the charge and injected fuel are assumed to be zero.

(c) The heat transfer surfaces of the system consist of the following five different surfaces namely,

(i) Area of the cylinder head less valve areas
(ii) Area of the piston top
(iii) Area of the inlet valve and
(iv) Area of the exhaust valve
(v) Instantaneous area of the sleeve

(d) The residual gas fraction in the clearance volume corresponds to the fraction which is frozen at a temperature of 800°K and pressure of 1.12 bar and this fraction is treated as air.
(e) The properties of the commercial diesel fuel are considered to be equal to that of dodecane ($C_{12}H_{26}$).

(f) Every increment of injected fuel as soon as it enters the combustion chamber vaporises immediately.

(g) Rate of injection of pilot fuel is assumed to be constant.

(h) Dissociation of the products of combustion is not considered.

(i) Blow-by and valve leakage losses are ignored.

(j) Surface temperature of each of the heat transferring surface is constant throughout the cycle.

(k) The instantaneous heat transfer coefficient computed from the bulk mean temperature of the system is assumed to be equal for all the boundary surfaces through which heat transfer occurs.

(l) Preflame reactions and self ignition of ethanol vapour are assumed to be absent.

With the foregoing assumptions, the first law of thermodynamics as applied to the closed period of cycle for the compression process can be written as:

\[ \dot{U} = -P\dot{V} + \sum \dot{Q}_i - \dot{M}_B\dot{L}_B - \dot{M}_W\dot{L}_W \quad \ldots (3.1) \]
In the absence of any dissociation it is assumed that the total internal energy $U$ is a function of mass averaged temperature and the constituents of the charge, thus

$$U = f(T, M_B, M_W) \quad \ldots \quad (3.2)$$

Differentiating Equation 3.2 and on rearranging to evaluate the rate of change of temperature in terms of known variables, the resulting equation becomes

$$\dot{T} = (\dot{U} - \frac{\Delta U}{M_B} \dot{M}_B - \frac{\Delta U}{M_W} \dot{M}_W) / \frac{\partial U}{\partial T} \quad \ldots \quad (3.3)$$

Thermodynamic properties like internal energy and gas constant $R$ during compression and subsequent combustion processes are computed at each instant from the known mass of each constituent and its specific heat. Though the assumption of constant specific heat enables the combustion studies to be carried out with ease, owing to its limited accuracy, variable specific heat as a function of temperature, as shown in Table 3.1, is used.

At each instant, gas constant $R$ is computed from

$$R = \frac{R_0}{\text{Molecular weight of the charge}}$$

where

$$R_0 = \frac{\text{Total wt. of the charge}}{\text{Molecular Weight}}$$

The detailed derivations are shown in the Appendix 1.
TABLE 3.1

Specific heat constants for the constituents of the charge.

a) For Ethanol and Diesel \( CP = 0.999 (C_1 + C_2T + C_3T^2 + C_4T^3) \) - \( T \) in °K

b) \( CO_2 \) and \( N_2 \) \( CP = C_1 + C_2/T + C_3/T^2 + C_4/T^3 \) - \( T \) in °R

c) \( H_2O \) and \( O_2 \) \( CP = C_1 + C_2/\sqrt{T} + C_3/T \) - \( T \) in °R

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Constituents</th>
<th>Mol.</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
<th>( C_3 )</th>
<th>( C_4 )</th>
<th>Units</th>
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<tbody>
<tr>
<td>1</td>
<td>( C_2H_5OH )</td>
<td>46</td>
<td>0.1311</td>
<td>9.186x10^-4</td>
<td>-2.36x10^-7</td>
<td>-7.190x10^-11</td>
<td>kEaLS/Kg°C</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>( C_{12}H_{26} )</td>
<td>170</td>
<td>0.051</td>
<td>1.28x10^-3</td>
<td>-2.818x10^-7</td>
<td>+1.66x10^-10</td>
<td>&quot;</td>
</tr>
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<td></td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>( CO_2 )</td>
<td>44</td>
<td>16.20</td>
<td>-6.53x10^-3</td>
<td>1.41x10^-6</td>
<td>&quot;</td>
<td>Btu/mol °R</td>
</tr>
<tr>
<td>4</td>
<td>( N_2 )</td>
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<td>9.47</td>
<td>-3.47x10^-3</td>
<td>1.16x10^-6</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>( H_2O )</td>
<td>18</td>
<td>19.86</td>
<td>-597</td>
<td>7500</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>( O_2 )</td>
<td>32</td>
<td>11.515</td>
<td>-172</td>
<td>1530</td>
<td>&quot;</td>
<td></td>
</tr>
</tbody>
</table>

* Specific Heat - Non metallic Liquids and gases
  - Y.S.Touloukian and Tadashi Makita

** Internal Combustion Engines - Edward F. Obert
The total internal energy $U$ of the charge can be expressed from the known composition of the charge, as:

$$U = U_A \cdot T$$  \[ (3.4) \]

Where,

$$U_A = \sum m_j C V_j$$

where $j$ represents the different constituents present in the charge.

Therefore

$$\frac{\partial U}{\partial T} = U_A + T \frac{\partial U_A}{\partial T}$$  \[ (3.5) \]

Hence

$$\dot{T} = \left( \dot{U} - \frac{\partial U}{\partial M_B} \dot{M}_B - \frac{\partial U}{\partial M_W} \dot{M}_W \right)/(U_A + T \frac{\partial U_A}{\partial T})$$  \[ (3.6) \]

The above differential equation representing the rate of change of temperature of the system can be integrated suitably to predict the temperature and other properties at each instant during the compression process.

As indicated earlier, the modelling of dual combustion process is highly involved due to the significant differences in the physico-chemical properties of the two fuels and the insufficient knowledge on the sharing of the available oxygen by the fuels and the influence of ethanol vapour on the
evaporation and the formation of multiple ignition nuclei of the injected diesel fuel. Besides, owing to the complexity of the reaction mechanism, no precise kinetic equations could be written for the combustion process. Nevertheless, the gross energy release rate depends upon the individual energy release pattern of the injected and inducted fuels. Several major assumptions are required due to the lack of understanding of the simultaneous and sequential processes characterising the dual fuel combustion systems.

Details of instantaneous values of thermodynamic properties and the various constituents of the cylinder content are the essential prerequisites for the solution of the energy equations already developed for the compression process and combustion process to be developed later. Internal energy equations, in terms of pressure, temperature and equivalence ratio, reported by Borman [54] are not applicable for the dual fuel combustion systems because of the difficulty in defining an equivalence ratio having the same meaning and sense as defined for a single hydrocarbon fuel.

In view of what has been stated, it is assumed that at any instant the constituents are considered to be air, unburned fuels and products of complete combustion, namely $\text{CO}_2$ and $\text{H}_2\text{O}$. Further it is assumed that the reactants are transferred into products of complete combustion as step changes which are defined by the apparent mass burning rates
of fuels. Thus with the progress in burning of the fuels, the proportions of oxidant and reactant in the charge decrease and correspondingly the products of combustion increase.

The properties of the cylinder content at any instant are computed on the assumption that the constituents behave both individually and collectively as ideal gases and expressed as functions of temperature and composition with temperature dependent specific heats.

This assumption leads to express the total internal energy during the process of combustion and expansion as:

\[ U = f(T, W_B, W_D) \quad \ldots (3.7) \]

where \( W_B \) and \( W_D \) being the cumulative masses of ethanol and diesel burnt respectively, which take into account, the products of combustion and unused oxygen present in the system at any instant.

The energy equation as applied to the system during combustion can be written as:

\[ \dot{U} = -PV + \sum \dot{Q}_i + \dot{Q}_B + \dot{Q}_D - D.L_D \quad \ldots (3.8) \]

Differentiating the Equation 3.7 with respect to crank angle and re-arranging with Equation 3.8, the rate of change of temperature of the system can be given as:
The basic Equations 3.6 and 3.9 are solved numerically by fourth order Runge-Kutta Scheme in a step by step method, starting from inlet valve closing and ending at the point of exhaust valve opening, the closed period of the system. A time step of one degree crank angle during combustion and two degrees crank angle during the rest of the period of investigation were used.

3.3.2 MODEL FOR HEAT TRANSFER

The rate of heat transfer through any surface at any instant can be expressed as

\[ \dot{Q}_1 = h_1 A_1 (T - T_w) \]  \( \ldots (3.10) \)

Where \( h_1 \), \( A_1 \) and \( T \) are the instantaneous values of heat transfer coefficient, area of heat transfer and bulk mean temperature of the charge respectively and \( T_w \) is the time averaged mean temperature of the heat transfer surface. The mean cylinder wall temperature is taken from the measurements made on similar engines by other workers [55] who had reported that a mean surface temperature of 550 K enabled the estimation of the heat transfer rates within an accuracy of ±5 percent.
The available information on the heat transfer coefficient of cylinder boundary surfaces is inadequate. Theoretical and experimental studies made by several authors like Eichelberg, Annand, Woschni, Nusselt and Hohenberg had resulted in a number of empirical correlations for the determination of the instantaneous heat transfer coefficient $h_i$. The mode of heat transfer between the working fluid and the walls is mainly by forced convection and the value of $h_i$ depends, among other things, on the flow conditions of the gas close to the surface of the wall. Not much is known about the gas motion adjacent to the walls, so all authors considered the gas velocity to be proportional to the mean piston speed.

As the choice of a suitable correlation for the gas side heat transfer coefficient in the cylinder is still a matter of considerable importance, a preliminary exercise was carried out in choosing a suitable correlation for the heat transfer coefficient. This analysis has shown that while Nusselt's correlation indicated in higher values of $h_i$, other expressions proposed by Eichelberg, Woschni, Annand and Hohenberg gave comparable values.

Moreover, looking into the physical aspect of combustion, the dual fuel combustion can be visualised as predominantly a premixed type of combustion accompanied by multiple macroscopic flame fronts. Besides, factors like lower flame temperature and C/H ratio of ethanol fuel reduce the flame
radiation component of heat transfer. In the light of the above, it is proposed to use the expression developed by Hohenberg [56], well suited for the operation of compression ignition engines, for the determination of the instantaneous heat transfer coefficient, given as:

\[ h_1 = 130 p^{0.8}(v_p + 1.4)^{0.8}v^{-0.06}T^{-0.4} \text{ W/m}^2\text{°K.} \quad \ldots (3.11) \]

The heat transfer coefficient calculated from the above relation has been assumed to be constant for all the surfaces. Assuming a steady state one dimensional heat transfer, the total heat transfer rate \( \Sigma Q_1 \) through all the boundary surfaces is computed at each instant.

3.3.3 BURNING RATES OF DIESEL

Instantaneous values of individual fuel burning rates and the proportions of constituent species along with their properties are required for the solution of the energy equation developed in the previous section.

In the proposed model, the combustion of diesel is assumed to follow the two part burning concept as proposed by Watson et.al [53]. The salient feature of this approach is that it apportions the total injected fuel into the mass undergoing the premixed mode of combustion and the mass undergoing diffusion type combustion. The proportion of fuel consumed in either mechanism is weighted by a phase
proportionality factor which may be related to appropriate combustion parameters such as ignition delay and the trapped equivalence ratio of the diesel fuel. Watson has also claimed that operations with prolonged ignition delay periods, where the delay period is longer than the duration of injection, certain quantity of diesel is likely to remain in the liquid form and later undergo the diffusion type of combustion. The adoption of this principle in the dual fuel combustion seems to be more reasonable and successful.

Thus, the total instantaneous burning rate of diesel is given by the sum of two cumulative components which can reasonably predict the well established sharp spike of the initial premixed combustion and a slower diffusion controlled combustion - a typical combustion characteristic of a direct injection combustion system. From the above, the total instantaneous diesel burning rate at any instant is given by

\[
\dot{W}_D = \dot{W}_{PD} + \dot{W}_{DD} \quad \text{... (3.12)}
\]

Or in terms of normalized burning rates

\[
\dot{W}_D = \left[ \beta \dot{W}_{PD} + (1 - \beta) \dot{W}_{DD} \right] \frac{\dot{W}_{TD}}{6} \quad \text{... (3.13)}
\]

Where

\[
\dot{W}_{PD} = \text{Normalized premixed burning rate of diesel}
\]

\[
= \frac{\dot{W}_{PD}}{\dot{W}_{PD/6}} \quad \text{... (3.14)}
\]
\[ \dot{W}_{DD} = C_{p1} C_{p2} \tau_{p1} (1 - \tau_{p1}) C_{p2} \] ...

(3.15)

\[ \dot{W}_{DD} = \frac{\dot{W}_{DD}}{\dot{W}_{DD}/\delta} \] ...

(3.16)

\[ W_{TD} = C_{d1} C_{d2} \tau_{d2}^{-1} \exp(-C_{d1} \tau_{d2}) \] ...

(3.17)

\[ W_{TD} = \text{Total mass of diesel injected/cycle} \]

\[ \delta = \text{duration of combustion of} \quad \Delta \text{CA} \]

\[ \tau = \text{dimensionless time factor} \]

\[ \tau = (\theta_i - \theta_{ign})/\delta \] ...

(3.18)

\[ \beta = \text{Phase proportionality factor} \]

\[ \beta = \frac{\dot{W}_{PD}}{\dot{W}_{TD}} \] ...

(3.19)

Following an extensive series of tests, Shape factors \( C_{p1}, C_{p2}, C_{d1} \) and \( C_{d2} \) and the phase proportionality factor \( \beta \) are evaluated in terms of ignition delay, trapped equivalence ratio \( F_{tr} \) of diesel fuel, and engine speed so that the computed pressure - crank angle diagram of straight diesel operation compares well with that of the measured one, over a wide range of speed and load. The resulting expressions of the shape factors are as given below:

\[ C_{p1} = 2.6 + 1.25 \times 10^{-8} [\text{DELAY (MS)} \times \text{RPM}]^{2.2} \] ...

(3.20)
\[ C_{p2} = 1500 \ C_{p1} \] ... (3.21)

\[ C_{d1} = 14.2 \ (F_{tr})^{-0.644} \] ... (3.22)

\[ C_{d2} = 0.85 \ (C_{dl})^{0.25} \] ... (3.23)

\[ \beta = 1 - 0.926 \ (F_{tr})^{0.35} \text{ [DELAY (MS)]}^{-0.26} \] ... (3.24)

\( F_{tr} \), trapped equivalence ratio of diesel, is determined from the amount of diesel injected during the delay period, mass of air and stoichiometric fuel-air ratio of diesel. From the computed instantaneous burning rate of diesel, the heat release rate is determined as

\[ \dot{Q}_D = \dot{W}_D \cdot LCV_D \] ... (3.25)

Where

\( LCV_D \) = the lower heating value of diesel.

3.3.4 BURNING RATE OF ETHANOL

Compared with straight diesel operation, the magnitudes of temperature and pressure during the dual fuel compression process are significantly lowered due to

(a) the reduction in the inlet temperature of the mixture as a result of partial evaporation of ethanol in the carburettor,
(b) continued evaporation of remaining ethanol and water droplets during the process of induction and compression and

(c) the increase in the specific heat values of air-ethanol mixture.

The reduction in temperature and pressure depend on the amount of ethanol induction and the proof of ethanol.

In the absence of any preflame reactions due to ethanol fuel, which may produce aldehydes, peroxides, ketones and other partially burnt products to trigger the combustion mechanism and for ethanol to take part in the combustion, the temperature of air-ethanol mixture has to be raised to chemical reaction conditions and this is possible only when sufficient energy through the combustion of diesel is released and transferred. The charge surrounding the evaporating droplets at the envelop of the diesel spray in a dual fuel engine, is a mixture of diesel liquid and vapour with different proportions of air and ethanol vapour. The diesel vapour concentration decreases with an increase in distance from the diesel jet. Ignition will generally take place in the region where the overall reaction rate is greatest and is governed mainly by the relative concentration of the diesel vapour and ethanol vapour with air as well as the temperature and their variations with time. Besides, the continuing evaporation of ethanol droplets during the
processes of induction and compression and the intake swirl are likely to introduce variations in the local air-ethanol ratio of the mixture resulting in the formation of zones where the air-ethanol ratio is within the flammable limit.

Hence, it is reasonable to assume that dual fuel operations involving rich mixtures of air-ethanol, subsequent to the start of diesel combustion at multiple centres, small independent flame fronts might propagate through the charge wherever the air-ethanol ratio is favourable for the flame propagation. When the air-ethanol mixture is too lean to support the propagation of the small independent flames, it is probable that molecules of ethanol, enveloped by the diesel spray or entrained into the spray volume as a result of air swirl or present very close to the ignition centres can only take part in the combustion. Hence it can be surmised that if any air-ethanol mixture is to take part in the process of combustion, it might be due to the energy released by the burning of diesel fuel and so the cause of ignition and combustion of ethanol should be attributed to diesel combustion.

In order to predict the apparent mass burning rate of ethanol, the supplied ethanol mass is also divided into two parts. One part is assumed to burn along with the premixed combustion of diesel and the other part is assumed to burn during the diffusion mode of diesel combustion. From the hypothesis, where, the combustion of ethanol is dependent upon
the burning of diesel, it can be further assumed that the parts of ethanol which burn along with the premixed and diffusion combustion of diesel, burn at rates equal to the normalized premixed and diffusion mass burning rates of diesel combustion.

For convenience a term RATIO, defined as the fraction of mass of ethanol that burns along with the premixed combustion of diesel to the total mass of ethanol supplied, is introduced and used in subsequent computation. From the foregoing, it follows that the apparent mass burning rate equation for ethanol can be written in terms of normalized premixed and diffusion burning rates of diesel as:

\[
\dot{W}_E = [\text{RATIO} \dot{W}_{ED} + (1-\text{RATIO}) \dot{W}_{DD}] \frac{W_{EB}}{\delta} \quad \ldots (3.26)
\]

Therefore,

\[
\dot{Q}_E = \dot{W}_E \cdot LCV_E \quad \ldots (3.27)
\]

From the Equation 3.26, it is seen that the value of RATIO controls the quantum of ethanol taking part in either premixed or diffusion type combustion and is believed to be governed by factors like air-ethanol ratio, ignition delay, swirl ratio, inlet temperature of the charge and the spray characteristics of diesel. In the absence of any detailed information with regard to their influence on the combustion pattern of ethanol, the effects of all the factors are lumped
into the value of RATIO. At lower percentages of diesel substitution, where the delay period is shorter than the duration of injection, compared with straight diesel operation, the extended delay period influences the diesel spray development and penetration. This enhanced delay will increase the premixed combustion of diesel as well as enable a higher volume of air-ethanol taking part in the premixed combustion.

However, at higher percentages of diesel substitution, the long delay period not only allows the entire quantity of diesel to be injected in a short time but also provide adequate time for the evaporation and mixing of diesel and air-ethanol mixture. Though the penetration is proportional to the square root of injection time, at reduced injection duration it is compensated by the prolonged ignition delay which allows the mixing of large quantities of diesel with air-ethanol mixture. However, the smaller temperature difference between the charge and diesel droplets reduces the heat transfer rate and hence the complete evaporation of all the diesel droplets is not ensured at the time of the start of ignition. These unevaporated diesel droplets later may undergo diffusion type combustion. Thus, it seems probable that prolonged delay associated with short duration of diesel injection can also increase the amount of ethanol undergoing combustion during the premixed mode of combustion.
The combined effects of swirl and spray pattern may also have some significant influence on the mass of ethanol burnt in the premixed or diffusion modes. Mixing of diesel with air-ethanol charge depends on the kinetic energies of both air and diesel spray. The quantity of diesel droplets carried away by the swirling air depends on the intensity of the swirl as well as the spray characteristics. Increasing the swirl ratio may remove more diesel particles from the spray core and these particles on evaporation can form more zones with favourable environment serving as ignition centres for the combustion of the surrounding air-ethanol mixture. It is thus believed that intense swirl can promote high rate of mixing of diesel and ethanol, in addition to carrying the unburnt mixture of air-ethanol into the combustion zones. Increasing the injection pressure of diesel results in a decrease in the mean droplet diameter and higher surface area to volume ratio, the result of which might provide a higher heat transfer coefficient. However, fine droplets have a smaller store of kinetic energy and are stopped faster resulting in a smaller dispersion.

Thus, owing to the influence of numerous complex and interrelated factors, it may be concluded that the precise evaluation of the term RATIO in terms of some of the operating and design variables is certainly much more involved. In the absence of any detailed information in respect of their influence on the combustion of ethanol and
to simplify the task to some manageable proportion, the effects of all these factors are lumped into the value of RATIO. Values of RATIO, 0.5 up to 40 percent of energy share and 0.4 above 40 percent seem to yield fairly good results.

The computation of the apparent mass burning rates of diesel and ethanol enables the quantitative determination of the products of complete combustion as dictated by stoichiometry. The total internal energy $U$ for the combustion and expansion processes can be written as:

$$U = U_A \cdot T \quad \ldots (3.28)$$

Where

$$U = (W_T - W_E) CV_B + (W_D - W_D) CV_D$$

$$+ (W_B E_3 + W_D D_3) CV_3 + (W_B E_4 + W_D D_4) CV_4$$

$$+ (W_T E_5 - W_D D_5) CV_5 + W_T \cdot CV_6 \quad \ldots (3.29)$$

From Equation 3.29 the values of $\frac{\partial U}{\partial W_E}$ and $\frac{\partial U}{\partial W_D}$ are calculated and from all the known values in the RHS of Equation 3.9 corresponding to the $i$ instant, the temperature at $(i + 1)$ instant is computed using fourth order RUNGE-KUTTA method of numerical integration.

3.4 COMPUTER PROGRAMMING AND FLOW CHART

The computer program is built on FORTRAN IV language and run on an IBM 370 system. It consists of a main program and
seven subroutines and a total number of about 700 statements.
The flow chart of the main program is shown in Fig. 3.1.

The program analyses and prints out the results of
motoring and firing runs separately. The subroutine EQNI
computes the temperature derivative with respect to crank
angle, heat transfer coefficient, sum of heat transfer
through the boundary surfaces and the gas constant R at
every step for the motoring run. Subroutine EQN2 shown in
Fig.3.2, computes the above, in addition to the mass burning
rates of ethanol and diesel for the firing run. Subroutine
FUELTR computes the mass of diesel injected during the
delay period as computed by the subroutine COMB.
Subroutines CVA, CVB and CVC compute the temperature
dependent specific heats and the rate of change in specific
heat with respect to temperature.

In the subroutine EQN2 two checks are made to test
whether (a) the sum of each increment of injected diesel mass
equals or exceeds the total diesel mass injected per cycle
and if so the injection is set to zero and (b) the values of
\( C_P \) and \( \tau \) are equal to or greater than 0.03 and 1.0
respectively and if so the normalized premixed and diffusion
burning rates are made equal to zero, thus avoiding the
computation with zero as a parameter which is out of computer
range.
FIG. 3.1. FLOW CHART OF COMPUTER PROGRAM - MAIN

START

READ ALL INPUT VARIABLES

CALCULATE TRAPPED CONDITIONS, T, P, R, MASS OF O2 & N2

COMPUTE HEAT TRANSFER AREAS

SET ALL SUM TO ZERO

CALL SUB-Routine EQU 1

COMPUTE RUNGE-KUTTA ESTIMATES

A

compute t at the next cr-angle

increment crank angle

compute incremental work, heat transfer etc

is ca > caeqvo

NO

print the required values at each increment

call sub-routine comb

compute delay and fix caign

set all variables of firing run to zero

B

call sub-routine fuel tr

compute trapped equivalence ratio

compute cp1, cp2, c41, c42 and β

CALL 'EQU 2'. COMPUTE MASS BURNING RATES, NORMIALIZED BURNING RATE, R, U ETC.

compute runge-kutta estimates

estimate temp., pres., and other parameters

C

is ca > caexp

NO

REDEFINE STEP SIZE

YES

is ca > caeqvo

NO

yes

print all the required variables

stop

FIG. 3.1. FLOW CHART OF COMPUTER PROGRAM - MAIN
FIG. 3.2. FLOW CHART FOR SUB-Routine ‘EQN 2’
The program starts at IVC by reading in those design and operating parameters required for the analysis and terminates at EVO. Computed values of cylinder volume, pressure, temperature, total work, heat transfer coefficient, sum of heat transfer, internal energy, mass burning rates of ethanol and diesel, cumulative heat release rate and rate of pressure rise are printed out at each instant. For each run a CPU time of 25 seconds were required.

The results of the computation are presented and discussed elsewhere in the present report.

3.5 ESTIMATION OF TRAPPED CONDITIONS

The trapped charge at the start of compression stroke consists of a mixture of inducted air, ethanol vapour, droplets of ethanol and some quantity of exhaust residual of the previous cycle. During the induction process, the temperature of the mixture is believed to increase above that of inlet manifold as a result of mixing with hot residual gases, heat transfer from the port and cylinder walls and compression during the final stages of induction stroke. Owing to the complexities and uncertainties faced in the estimation of heat transfer coefficient, temperature difference between the charge and cylinder components and the process of ethanol evaporation in the gas exchange process, any mathematical representation of the induction process
accounting all these factors is highly involved. This justifies the use of less accurate method of calculation based on number of simplifying assumptions.

Assuming no back flow of combustion products for a zero overlap, Whitehouse et. al [57] had reported that the maximum possible quantity of residual gas is equal to that contained in the clearance volume at the pressure in the cylinder at TDC on the suction stroke. Despite the high temperature of the residual gas, compared with the incoming charge, its effect is considered to be quite low because of the high compression ratio employed for compression ignition engines. Lyn and Valdmanis [58] had pointed out that an error of 10°C in the trapped temperature of the charge could result in an error of 30°C in the compression temperature and 5 percent in the value of heat loss.

The theoretical temperature drop computed for the complete evaporation of 190 proof ethanol using the relation

\[ \Delta T = \frac{L_B}{(A/B)(C_P_A + C_P_B)} \]  

works out to be 16°C, 32°C and 48°C for the diesel substitutions of 20, 40 and 60 percent respectively. A comparison of the measured temperature of the air-ethanol mixture corresponding to various percentages of energy share, at the point of entry to the intake port with the values of theoretical drop has revealed that only about 30 to 40
percent of inducted ethanol might have evaporated before entering the intake port. Any further heat addition to the mixture from the walls of the intake port and the cylinder might probably help in vaporizing the ethanol droplets rather than increasing the temperature of the mixture.

In the light of the above, it appears to be reasonable to assume that only about 50 percent of inducted ethanol evaporates at the instant of inlet valve closing. Though this assumption might be more justifiable at higher flow rates of ethanol, the error that could be introduced in the estimation of the trapped conditions at lower flow rates is expected to be small. Hence from the known rates of air and ethanol flow and a reasonable assumption on the parameters of the residual gas, which result in a coefficient of residual gas of 0.045, the trapped conditions of the charge was computed by making use of an enthalpy balance. The trapped temperature thus computed also showed a fair agreement with the values evaluated from the expression given in reference [59].

\[
T_{IVC} = T_{IN} \frac{Y}{(Y-1)+T_{IN}/T_{RBS}} \tag{3.31}
\]

which has been derived from the assumption that no heat transfer takes place and the cylinder pressure remains constant during the process of induction.
3.6 DURATION OF COMBUSTION

In addition to the shape factors, the slope of the fuel burning rate curve will also be governed by the duration of combustion. Generally, the combustion duration of straight diesel operation in terms of crank degrees increases with an increase in the equivalence ratio (fuelling) or speed. However, the combustion duration of dual fuel system is believed to be influenced by the percentage of diesel substitution.

The results of earlier investigators and the author's own work indicate that generally ignition occurs before TDC during the admission of ethanol amounting to less than 40 percent of diesel substitution. The faster burning rate of ethanol and the increase in the delay period are expected to cause a higher fraction of both injected and inducted fuels to take part in the premixed or constant volume combustion. This might probably result in the reduction of the relative amount of fuel burnt by diffusion or after-burning thereby resulting in a shorter duration of combustion, compared with straight diesel operation. However, at higher percentages of diesel substitution, the combustion starting after TDC, the duration of combustion, compared with the earlier situation, is likely to be increased as a result of the prevailing lower temperature and pressure.
As the assumption of a combustion duration of 100° CA for straight diesel operation resulted in a good comparison between the computed and measured pressure-crank angle diagrams, it follows from the foregoing that the assumption of a shorter duration of combustion of 80° CA upto 40 percent energy share and 90° CA for higher percentages are reasonable.

3.7 IGNITION DELAY STUDIES

It is known that the smooth operation of a compression ignition engine is highly dependent on the ignition delay due to its influence on the development of the rate of pressure rise, peak pressure, combustion induced noise and exhaust emissions. Ignition delay is controlled by many factors, like charge temperature and pressure at the point of injection, oxygen concentration and the type of fuel. Very little is known about the detailed reaction mechanisms of the chemical reactions leading to the self ignition of the complex hydrocarbon fuels.

Ignition delay is commonly divided into two parts, namely physical and chemical delay and it is rather difficult to draw a distinct line separating these two processes since they generally overlap. However, physical delay is defined as the time required for the formation of droplets, evaporation and diffusion of the vapour forming a combustible mixture of fuel and air, preparatory to chemical reactions at the self ignition temperature. Chemical delay refers to the time taken
for the decomposition of the fuel molecules into lighter components and the processes of preflame reactions between the decomposed components and oxidant resulting in the formation of multiple ignition centres.

A study of the self ignition of liquid hydrocarbon fuels in C.I. engines indicates that ignition is possible only when the concentration of some leading intermediate compounds like peroxides and aldehydes formed during the ignition delay reach a critical value. Any failure in reaching the above requirement, which is highly dependent on the temperature of the charge, results in the ignition failure with the formation of products of partial oxidation. It has been well established that the rate of formation of the intermediate compounds depends on the temperature, concentrations of the fuel vapour and the oxidant and the reaction velocity constant which is related to the activation energy of the fuel, defined as the minimum energy that the reactant must acquire before the chemical change takes place. From the global reaction kinetics, the reaction rate per unit volume of the charge can be had from reference [60].

\[
m = K m_f^a m_o^b \rho^{(a+b)} e^{-E_a/RT}
\]  

(3.32)

The importance of temperature, concentrations of fuel and oxidant are evident from the above equation.
In the light of the above and from the kinetic theory consideration, the ignition delay expressions assume a general form as:

\[ I.D(\text{ms}) = A e^{E_a/R T} / P^n \]  \hspace{1cm} (3.33)

where the constants \( A \) and \( n \) depend on the type of combustion chamber and \( E_a \), the activation energy which increases with a decrease in the cetane number of the fuel. Correlations for ignition delay, proposed by engine researchers, are given in Table 3.2. It is seen from the table that all correlations, except the one proposed by Tsao, use the mean temperature and pressure of the charge as independent variables. Tsao's correlation includes the engine speed as a factor affecting the delay period and considers the pressure and temperature at the point of diesel injection.

From the studies made in bombs, Wolfer [61] had reported that the shape of combustion chamber, air-fuel ratio, spray characteristics and temperature of the fuel had only little influence on the ignition delay. Small [62] who attempted to demonstrate the effect of turbulence reported that the turbulence introduced no appreciable change in the ignition delay.

### 3.7.1 IGNITION DELAY IN DUAL FUEL COMBUSTION SYSTEMS

The author has not come across any ignition delay expression for dual fuel combustion systems. Compared with
## TABLE 3.2

Ignition Delay Correlations

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Investigator</th>
<th>Correlation proposed</th>
<th>Notation and units</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ilmari</td>
<td>I.D. = $0.156 \times 10^8 \left( \frac{T}{10000} \right)^{11} e^{1000/T}$</td>
<td>I.D. in ms.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$R=\text{Universal gas constant} = 8.314 \text{ kJ/Emol}^\circ\text{K}$</td>
<td>$T$ and $P$ are mean Temp. and Pr. in $^\circ\text{K}$ &amp; bar</td>
</tr>
<tr>
<td>2</td>
<td>Sitkei</td>
<td>I.D. = $0.5 + 0.133 \left( \frac{T}{60} \right)^{0.7} e^{37564.8/RT} + 4.63 \left( \frac{T}{1.8} \right) e^{37564.8/RT}$</td>
<td>'' ''</td>
</tr>
<tr>
<td>3</td>
<td>Schmidt</td>
<td>I.D. = $0.0646 \left( \frac{T}{1.08} \right)$</td>
<td>'' ''</td>
</tr>
<tr>
<td>4</td>
<td>Wolfer</td>
<td>I.D. = $0.429 \left( \frac{T}{1.19} \right)$</td>
<td>'' ''</td>
</tr>
<tr>
<td>5</td>
<td>Tsao</td>
<td>I.D. = $\left( \frac{8.48}{T^<em>} + 0.415 \right) \left( \frac{20.17}{T^</em>} - 0.0222 \right) N^+$</td>
<td>$P^<em>$, $T^</em>$ are pressure and Temp. at the start of injection.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$R=\text{Universal gas constant} = 8.314 \text{ kJ/Kmol}^\circ\text{K}$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Hirogasu</td>
<td>I.D. = $A P^n \frac{\varnothing_1 e^D}{T}$ where $\varnothing_1 = P_{O_2}/(0.21 \times P \text{ total})$</td>
<td>N=Engine speed in rev/mt.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$P$ in Atmospheres $^\circ\text{K}$ $T$ Temp. in $^\circ\text{K}$ $n,c,D$ are constants</td>
<td></td>
</tr>
</tbody>
</table>
air only compression, compression of air-ethanol mixture depresses the temperature and pressure of the charge to varying degrees depending upon the quantity and quality of ethanol. Goodwine [63] had reported that the induction of low cetane fuels like iso-octane and n-octane results in some preflame reactions referred to as cool flame, which increases the temperature and pressure of the charge and results in a reduction of ignition delay of the injected fuel. However, Lewis [64] had showed the absence of such cool flames in fuels like methane, benzene and alcohols.

The analysis of the variations in precombustion reaction with octane number for various hydrocarbon fuels have shown that an increase in the octane number of the carburetted fuel results in a smaller heat of precombustion reaction and a decrease in the magnitude of precombustion reactions. Moreover increasing the octane number of the fuel also increases the temperature at which the cool flame reactions are detectable.

From the foregoing, it can be concluded that the combined effects of the lower temperature of the charge as a result of the high latent heat of evaporation, the high octane rating of ethanol and the lower number of carbon atoms present in ethanol fuel inhibit the occurrence of any preflame reactions, the products of which are capable of triggering the ignition of the injected fuel at a lower temperature.
On the other hand, preheating of the air-ethanol mixture altogether presents a different environment in the formation of ignition nuclei. Though the volume occupied by vaporized ethanol would dilute the oxygen concentration and consequently increase the ignition delay, the rapid formation of the intermediate products of oxidation probably exert an accelerating action on the formation of ignition nuclei. This is evident from the test results presented by Alperstein et.al [4] who demonstrated that the admission of vaporized ethanol caused no change or even a slight decrease in the ignition delay compared with straight diesel operation. The results of Foster et.al [40] are also in close conformity with that of Alperstein et.al. No plausible explanations were reported by the above authors for the decrease in the delay period caused by the admission of vaporized ethanol.

The present investigation enabled the author to develop a correlation for the ignition delay in diesel-ethanol dual fuel combustion system based on several experimental observations. The use of the correlation in the mathematical model and the close agreement between predicted and measured pressure values validates the expression proposed.