# A Simulation Model for the Combustion Process of Natural Gas Engines with Pilot Diesel Fuel as an Ignition Source

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### A Simulation Model for the Combustion Process of Natural Gas Engines with Pilot Diesel Fuel as an Ignition Source

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### **ABSTRACT**

During the last years a great deal of efforts have been made to reduce pollutant emissions from Direct Injection Diesel Engines. The use of gaseous fuel as a supplement for liquid diesel fuel seems to be one solution towards these efforts. One of the fuels used is natural gas, which has a relatively high auto – ignition temperature and moreover it is an economical and clean burning fuel. The high auto ignition temperature of natural gas is a serious advantage against other gaseous fuels since the compression ratio of most conventional diesel engines can be maintained. The main aspiration from the usage of dual fuel (liquid and gaseous one) combustion systems, is the reduction of particulate emissions. In the present work are given results of a theoretical investigation using a model developed for the simulation of gaseous fuel combustion processes in Dual Fuel Engines. The model is a two – zone combustion one, taking into account details of diesel fuel spray formation and mixing with the surrounding gas, which is a mixture of air and natural gas. The natural gas burning initiates after the ignition of the diesel fuel. The combustion rate of natural gas depends on the rate of entrainment of surrounding gas into the fuel jet formed and on the velocity of the flame front, which is formed around the area of the burning zone and spreads inside the combustion chamber. The flame front, which is used in the present work, takes into account the history of pressure and temperature values inside the chamber and the local composition to estimate the flame velocity. The model is applied on a single cylinder test engine located at the author's laboratory at various operating conditions. The engine performance under normal diesel operation is used as basis for evaluating engine performance and emissions when using gaseous fuel. The engine load is controlled by changing the amount of the primary gaseous fuel added to the intake air, while the quantity of the pilot liquid fuel per injection stroke is fixed for the given engine regardless of engine operating conditions. It is examined the effect of gaseous fuel quantity (load) on engine performance and emissions at various operating conditions. From the results it is revealed

a change of the heat release mechanism when compared to standard diesel operation, an increase of maximum combustion pressure and an increase of NO emissions especially at high engine load. On the other hand soot emissions are considerably reduced and become negligible.

### INTRODUCTION

The compression ignition engine of the dual fuel type has been employed in a worldwide range of applications to utilize various gaseous fuel resources to minimize particulate emissions without excessive increase in cost from that of conventional diesel engines. This has been prompted by the cleaner nature of the gaseous fuels combustion compared to conventional liquid fuels as well as their relative increased availability at attractive prices [1-41\*

The dual fuel combustion system features essentially a homogeneous gas – air mixture compressed rapidly below its autoignition conditions and ignited by the injection of pilot liquid fuel around top dead centre position. The primary fuel is generally a gaseous one at atmospheric conditions. The pilot liquid fuel, which is injected through the conventional diesel injection equipment, normally contributes only a small fraction of the maximum power output. Power output is controlled by varying the amount of primary gaseous fuel added to the air during the induction stroke, whilst the quantity of the pilot fuel per injection stroke is fixed.

A mathematical model can provide an adequate way for describing details of the complicated mixing, combustion and pollutants emission processes in dual fuel engines. The present contribution describes a model that simulates dual fuel combustion using a two – zone approach to simulate the combustion process for the liquid pilot fuel and also for the primary gaseous fuel.

<sup>\*</sup>Numbers in brackets designate references at the end of the paper

The basic purpose of the present model is to provide an adequate way for describing the complicated combustion process, taking place inside dual fuel engines with pilot liquid fuel [5-7].

The main purpose of the present model is to estimate, apart from power and efficiency, the concentration of soot emissions and nitrogen oxides at the engine exhaust. For this reason preliminary results from the modeling are provided for various engine operation conditions. To validate the model and to compare with the findings under dual-fuel operation an experimental is conducted on a single cylinder test engine under normal diesel operation. From the analysis of results obtained it is revealed that the simulation model developed predicts adequately engine performance and pollutants under normal diesel engine operation. Furthermore comparing the findings for dual-fuel operation with the standard diesel one, a serious effect of the gaseous fuel is observed on engine performance, soot and NO emissions.

To validate the findings of the dual-fuel modeling an experimental investigation is currently under way and results will be presented in the near future [8].

### BRIEF DESCRIPTION OF THE MODEL

Once the gaseous fuel is admitted inside the cylinder and mixed with the intake air, the premixed gaseous fuel—air charge is subjected during compression to high temperatures and pressures as the TDC is approached. The cylinder charge at start of compression is a homogeneous mixture of gaseous fuel and air. At the time of pilot fuel injection, the homogeneous mixture has a different pressure and temperature from the air charge in normal diesel engines due to the different thermodynamic properties of the constituents. The entire charge of the homogeneously premixed gaseous fuel and air inside the cylinder is treated as a single zone up to pilot fuel injection [8-9].

When the pilot diesel fuel is injected into the combustion chamber, a two – zone model is considered. In each zone there is uniformity in space of pressure, temperature and composition at each instant of time, neglecting heat transfer between the zones. The first zone consists of air–gaseous fuel (unburned zone) and the second zone consists of combustion products, unburned gaseous fuel and unburned evaporated liquid fuel (burning zone)

The present model assumes that the ignition of the charge takes place after the pilot fuel autoignites. The ignition delay is thus the one of the pilot diesel fuel and is calculated from the pressure and temperature of the charge and the equivalence ratio of the burning zone.

During ignition delay the two zones are separated by the outer boundary of the conical jet which is formed during injection of pilot fuel. The quantity of the gaseous fuel and air entrained into the burning zone is estimated from the volume change rate of the jet.

After ignition the two zones are separated by a thin flame front, which has the shape of the conical jet and covers the outer area of the jet. The flame front and consequently the burning zone spreads towards the

unburned zone having a flame speed, which is calculated taking into account the flame propagation mechanism. Therefore the heat release rate is affected by the interaction of the jet with the surrounding gas and from the laminar flame speed. It must be stated here that steady state jet theory, including wall impingement, is used to describe the fuel – air mixing process of the fuel jet formed [4-6,8].

For the heat transfer calculation between the cylinder charge and cylinder walls, the Annand formula is employed [11]. For prediction of soot emissions, the amount of net soot is calculated considering the difference between the rates of soot formation and soot oxidation inside the burning zone [12-15].

Dissociation of combustion products is taken into account by incorporating the Vickland et al [16,17] method including eleven species. For the formation of nitric oxides the extended Zeldovich chain reaction mechanism is considered [12,13,15,18].

The liquid fuel used is dodecane ( $C_{12}H_{26}$ ) representing adequately the commercial diesel fuel used in the present analysis and the gas fuel used is a mixture of methane (CH<sub>4</sub>), carbon dioxide and nitrogen in proportion (98%-1%-1%) in (v/v), which is a typical representative of natural gas fuels.

#### MATHEMATICAL TREATMENT

CONSERVATION AND STATE EQUATIONS. - As already stated inside the combustion chamber there are considered two zones, a burning one consisting of air, evaporated fuel, gaseous fuel plus burned products and an unburned one consisting of air and gaseous fuel. Each zone posses its own temperature and composition while the pressure is uniform. The first thermodynamic law for each zone may be written as [10,13]

$$\begin{split} dU_{b,u} &= dQ_{b,u} - P \times dV_{b,u} + \\ &\sum \left( dm_{b,u} \times h_{b,u} \right) + dm_{fb} \times h_f \end{split} \tag{1}$$

where " $dm_{fb}h_f$ " is the total enthalpy addition to the burning zone from the liquid diesel fuel and " $\acute{O}dm_{bu}h_{bu}$ " is the total enthalpy addition to the burning zone from the unburned zone due the entrainment rate of unburned mixture. The internal energies and enthalpies in the above equation are total ones, so that the heat release is taken into account implicitly. The temperature, pressure and volume of each zone is obtained from the integrating of a set of three ordinary first order differential equations with unknowns " $T_b$ ", " $T_u$ " and "P". These equations are derived after some mathematical elaboration from the first law and perfect gas state equations for both zones and the volume constraint. The system of the three equations has as follows

$$dT_{u} = \begin{pmatrix} dQ_{u} - R_{u}T_{u}dm_{u} + V_{u}dP + \\ h_{u}dm_{u} - u_{u}dm_{u} \end{pmatrix} / m_{u}C_{pu}$$
 (2)

$$dT_{b} = \begin{pmatrix} dQ_{b} - R_{b}T_{b}dm_{b} - m_{b}T_{b}dR_{b} \\ + V_{b}dP + h_{u}dm_{ub} + h_{fev}dm_{fev} \\ - u_{b}dm_{b} - m_{b} \left[ \sum_{k=\text{species}} dy_{k}u_{k} \right]_{b} \end{pmatrix} / m_{b}C_{pb}$$
(3)

$$dP = \begin{cases} \frac{R_{u}}{C_{pu}} \begin{bmatrix} dQ_{u} - R_{u}T_{u}dm_{u} + \\ h_{u}dm_{u} - u_{u}dm_{u} \end{bmatrix} + \\ \frac{R_{b}}{C_{pb}} \begin{bmatrix} dQ_{b} - R_{b}T_{b}dm_{b} - \\ m_{b}T_{b}dR_{b} + h_{u}dm_{ub} + \\ h_{fev}dm_{fev} - u_{b}dm_{b} - \\ m_{b} \left( \sum_{k=species} dy_{k}u_{k} \right)_{b} \end{bmatrix} \\ + R_{u}T_{u}dm_{u} + R_{b}T_{b}dm_{b} \\ + m_{b}T_{b}dR_{b} - PdV \end{cases}$$

$$(4)$$

Term (dR<sub>b</sub>) in EQ (4) expresses the specific gas constant variation due to the composition change of the burning zone, i.e.:

$$dR_b = R_{mol} \times \left( \sum_{j=\text{species}} \frac{dy_j}{MB_j} \right)_b$$
 (5)

HEAT TRANSFER MODEL. – The heat exchange rate is obtained by employing the Annand expression [11,19],

$$dQ = A_{tot} \times \begin{bmatrix} a \times \lambda \times \frac{Re^{b}}{D} \times (T_{g} - T_{w}) + \\ c \times (T_{\sigma}^{4} - T_{w}^{4}) \end{bmatrix}$$
 (6)

where  $(\dot{a},b,c)$  are constants and  $(\lambda)$  is the thermal conductivity. The only problem existing is the application of the above equation during the combustion stroke, since the burning zone is not entirely in contact with the cylinder wall surfaces. [12] For this reason a bulk average temperature of both zones is used as follows

$$T_{g} = \frac{\sum_{i=b,u} m_{i} \times C_{vi} \times T_{i}}{\sum_{i=b,u} m_{i} \times C_{vi}}$$
(7)

The total heat exchange rate is then distributed among the two zones according to their mass, temperature and specific heat capacity as follows

$$dQ_{b,u} = dQ \times \frac{m_i \times C_{vi} \times T_i}{\sum_{i=b,u} m_i \times C_{vi} \times T_i}$$
(8)

PILOT FUEL SPRAY DEVELOPMENT. – The rate of pilot fuel injection from a single hole is expressed as follows, assuming a constant value for the discharge coefficient ( $C_{Dini}$ ) at the nozzle orifice:

$$\frac{dm_{fp}}{dt} = \rho_f \times u_{inj} \times \left(\frac{\pi}{4} \times d_{ho}\right)$$
 (9)

where the injection velocity is:

$$u_{inj} = C_{D_{inj}} \times \sqrt{\frac{2 \times \Delta P}{\rho_f}}$$
 (10)

and (ÄP) is the pressure difference across the injector hole as

$$\Delta P = P_{\rm ini} - P_{\rm cvl} \tag{11}$$

The liquid fuel density  $(\tilde{n}_f)$ , the diameter of the nozzle  $(d_{ho})$ , the nozzle discharge coefficient  $(C_{Dinj})$ , the fuel line pressure  $(P_{inj})$  are input values to the program together with the dynamic injection timing. Since the injected fuel velocity is critical for the model, the history of injection pressure difference  $(\Delta P)$  is checked against experimental data [20,21].

MECHANISM OF FLAME PROPAGATION – An important intricic property of a combustible fuel air, burned gas mixture is its laminar burning velocity. The laminar burning velocity is defined as the velocity, relative to the flame front, with which unburned gas moves into the flame front and is transformed to products. Because the laminar flame thickness under engine conditions is around 0.2mm and is therefore much less than the characteristic vessel dimensions, the flame is treated as negligibly thin. The laminar burning (flame) velocity for several hydrocarbons premixed with air depends on the fuel—air equivalence ratio, the temperature of the unburned gas and on the cylinder pressure [5-6].

The present model assumes that a flame front of negligible thickness propagates into the unburned zone having a direction perpendicular to the outer surface of the conical jet formed after pilot fuel injection. The laminar flame speed is given by the following correlation:

$$u_1 = u_{1,0} \times \left[ \frac{T_u}{T_0} \right]^{a_T} \times \left[ \frac{P}{P_0} \right]^{b_T}$$
 (12)

where  $(u_{l,0})$  is the reference laminar flame (burning) velocity depending on the fuel – air equivalence ratio, (P) is the chamber pressure,  $(T_u)$  is the unburnt mixture temperature,  $(T_0,P_0)$  are reference temperature and pressure,  $(a_T,b_T)$  are constants depending on the fuel—air equivalence ratio. To allow for the effect of turbulence a correction factor is used [14,15,19]. The turbulence flame (burning) speed is estimated from the following equation:

$$\mathbf{u}_{t} = \mathbf{f}\mathbf{f} \times \mathbf{u}_{1} \tag{13}$$

where (ff) is a function of engine speed.

DEFINITION OF THE BURNING ZONE - After initiation of fuel injection the burning zone forms and penetrates inside the combustion chamber. The present model, while based on simplified relations, represents the above mechanism with reasonable accuracy. For jet penetration the proposal of Hiroyasu has been adopted [14,15,19,21].

Inside the jet we assume uniformity of density, temperature and composition. The resulting fuel jet is considered to have the shape of a cone.

During the ignition delay period the unburned mixture entrainment rate with respect to time is obtained from:

$$\frac{dm_b}{dt} = \rho_u \times \frac{dV_b}{dt}$$
 (14)

where the volume change of the burning zone due to its penetration into the combustion chamber is given by:

$$\frac{dV_b}{dt} = \frac{\pi}{3} \times \tan^2\theta \times \frac{dS}{dt}$$
 where (S) is the penetration length of the jet given by:

$$S = 2.95 \times \left(\frac{\Delta P}{\rho_u}\right)^{0.25} \times \sqrt{d_{ho} \times t}$$
 (16)

and (è) is the jet cone angle estimated from the following correlation:

$$\theta = \left[ \frac{d_{\text{ho}}^2 \times \rho_{\text{u}} \times \Delta P}{\mu_{\text{u}}} \right]^{0.25}$$
 (17)

After initiation of combustion the unburned mixture entrainment rate is given by:

$$\frac{dm_b}{dt} = \rho_u \times \left[ \frac{dV_b}{dt} + \frac{dV_{b,flame}}{dt} \right]$$
 (18)

where  $(dV_b/dt)$  is the volume change due to the penetration of the jet whilst (dV<sub>b.flame</sub>/dt) is the volume entrained due to the existence of the flame front which spreads. If (A) is the area of the jet periphery the volume entrainment rate due to the existence of the flame front is given by:

$$\frac{dV_{b,flame}}{dt} = u_t \times \frac{dA}{dt}$$
 (19)

In most models the assumption is made that the burning zone after impingement follows a path parallel to the cylinders walls. In the present work the existing well-tested wall jet theory of "Glauert" [22] is used to determine the burning zone history after wall impingement upon the cylinder walls. After this point the unburned mixture is entrained from the wall jet front and from the spreading of the flame inside the combustion chamber.

IGNITION DELAY PERIOD - Before the injected liquid fuel ignites, it undergoes an ignition delay period. The ignition delay period is estimated from the following

$$S_{pr} = \int_{0}^{t} \frac{1}{a_{del} \times P^{-2.5} \times \phi^{-1.04} \times exp(5000/T_{b})} dt$$
 (20)

where  $(\phi)$  is the local equivalence ratio of the evaporated liquid fuel-air mixture inside the burning zone and (a<sub>del</sub>) is

Ignition initiates when the previous integral becomes equal to one, the integration having started from the initiation of pilot fuel injection. At this point we must state that due to the rather high cetane number of natural gas, auto-ignition of the gaseous fuel is avoided for the CR values used, since in the opposite case serious problems

would arise. Thus the liquid fuel is the ignition source for the gaseous fuel. This is an important advantage of natural gas over other gaseous fuels used in the past that required a serious reduction of CR, which has negative effects on engine efficiency.

COMBUSTION RATE OF THE LIQUID PILOT FUEL -The semi-empirical model of Whitehouse-Way is used to calculate the combustion rate of pilot liquid fuel. The preparation rate of injected fuel is given by [9,18]:

$$dm_{fpr} = k \times m_{fi}^{1-x} \times m_{fupr}^{x} \times P_{O_{2}}^{m}$$
 (21)

where (m<sub>fi</sub>) is the total amount of fuel injected up to the time considered,  $(m_{fupr})$  is the total unprepared fuel,  $(P_{O2})$  is the partial pressure of available oxygen and (x,m) are constants. Constant (k) depends on the total amount of the injected pilot fuel per injection stroke, on the duration of injection and on geometrical characteristics of the injection nozzle.

The burning rate of the diesel fuel follows the Arrhenious type reaction mechanism. The burning rate is thus given by

$$dm_{fb} = \begin{cases} \frac{k' \times P_{O_2}}{RPM \times T_b^{0.5}} \times exp\left(\frac{-ACT_{diesel}}{T_b}\right) \\ \times min(m_{fav}, m_{aav} \times \phi_{st}) \end{cases}$$
(22)

where  $(m_{fav})$  is the total amount of unburned fuel,  $(m_{aav})$  is the total amount of unburned air and  $(\phi_{\text{st}})$  is the stoichiometric equivalence ratio of the liquid fuel. The term, min  $(m_{fav}, m_{aav} * \phi_{st})$ , denotes the combustion rate dependence on fuel vapor or air availability inside the burning zone.

At the beginning of the combustion period, combustion is controlled from the reaction rate. After a short period, the fuel prepared during ignition delay is consumed and combustion is then controlled from the preparation rate.

COMBUSTION RATE OF THE GASEOUS FUEL - As already stated in the present work, we replace a major part of the liquid fuel with gaseous. The working media at the start of compression is a mixture of air and gaseous fuel. Thus the temperature level of the mixture during the compression stroke is very important for establishing whether auto-ignition takes place. Experiments in combustion bombs have shown that auto-ignition of natural diesel-like conditions requires higher under temperatures from those achieved during the compression stroke [1-3] of normal diesel engines. Thus auto-ignition is avoided in the present investigation.

During combustion phase, the mass of the gaseous fuel entrained inside the burning zone depends on the penetration of the jet inside the combustion chamber and on the propagation of the turbulent flame around the jet outer surface. The gaseous fuel entrained inside the burning zone, due to the flame front spread is transformed immediately into products. Thus this portion of combustion actually depends on the flame speed, which is a function of unburnt mixture, temperature, pressure and gaseous fuel - air equivalence ratio [4-7].

Inside the burning zone there is also an amount of unburnt gaseous fuel entrained due to the penetration of the liquid fuel jet inside the combustion chamber. The reaction rate of this gaseous fuel is determined using an Arrhenious type equation for each constituent as follows [14-16]:

$$\frac{dm_{gb,i}}{dt}_{i=\text{constituen. of Gaseous fuel}} = \begin{pmatrix} k_i^{"} \times [y_{i,av}]^{z_{1,i}} \times [y_{O_2,av}]^{z_{2,i}} \\ \times exp\left(\frac{-E_{g_1f}}{R_m \times T_b}\right) \end{pmatrix}$$
(23)

where ( $[y_{i,av}]$ ) is the mass fraction of the available mass of each constituent of the gaseous fuel, ( $[y_{O_2,av}]$ ) is the concentration of the available mass of oxygen inside the burning zone and ( $E_{gif}$ ) is the activation energy of each constituent of the gaseous fuel while ( $z_1,z_2$ ) are constants.

Thus the total heat release rate is the sum of two rates, the liquid fuel heat release rate and the gaseous one. The gaseous fuel heat release rate is the sum of the heat release rate caused by the spread of the flame front and from the Arrhenious type combustion of entrained unburnt gaseous fuel, inside the burning zone.

CHEMISTRY OF COMBUSTION – EQUILIBRIUM CONSIDERATIONS - Combustion products are defined by dissociation considerations. For the C-H-O system the complete chemical equilibrium scheme proposed by Vickland et al. (1962) is used [16]. For the combustion zone, given its volume, temperature, mass of fuel burned and mass of air entrained, the concentration of each one of the eleven species can be calculated by solving a system of 11 equations containing: 4 atom balance equations (one for each element C,H,O,N) and 7 equilibrium equations. Apart from soot, at any instant of time, the following gas species are considered to be present inside each burned region, all in chemical equilibrium,

### (9) CO (10) O<sub>2</sub> (11) O

where the species are referred to by the number in parenthesis, in front of their name, and expressed by means of "kmole" fraction "X". The equilibrium concentrations of the eleven species can be described by the following seven equilibrium reactions ( $B=X_1/X_2$ ):

$$\begin{split} &\frac{1}{2}\,H_{2} \leftrightarrow H, K_{P1} = \sqrt{P}X_{4}\big/\sqrt{X_{2}} \\ &\frac{1}{2}\,O_{2} \leftrightarrow O, K_{P2} = \sqrt{P}X_{11}\big/\sqrt{X_{10}} \\ &\frac{1}{2}\,N_{2} \leftrightarrow N, K_{P3} = \sqrt{P}X_{7}\big/\sqrt{X_{5}} \\ &2H_{2}O \leftrightarrow 2H_{2} + O_{2}, K_{P4} = PX_{10}\big/B^{2} \\ &H_{2}O \leftrightarrow OH + \frac{1}{2}\,H_{2}, K_{P5} = \sqrt{P}X_{3}\,\Big/\Big(B\sqrt{X_{2}}\Big) \\ &CO_{2} + H_{2} \leftrightarrow H_{2}O + CO, K_{P6} = BX_{9}\big/X_{8} \\ &H_{2}O + \frac{1}{2}\,N_{2} \leftrightarrow H_{2} + NO, K_{P7} = \sqrt{P}X_{6}\,\Big/\Big(B\sqrt{X_{5}}\Big) \end{split}$$

where "K<sub>p</sub>" are the reactions equilibrium constants.

The solution of the above equations is obtained by incorporating the method proposed by Vickland et al (1962), with some slight modifications to ensure fast conversion [16,17].

NITRIC OXIDE FORMATION MODEL. - Since the formation of nitric oxides is a kinetically controlled mechanism, the extended Zeldovich chain reaction mechanism is used. The three following reactions are considered [18],

$$\begin{cases} N + NO \leftrightarrow N_2 + O, \\ k_{1f} = 1.6 \times 10^{10} \\ N + O_2 \leftrightarrow NO + O, \\ k_{2f} = 6.4 \times 10^6 \times T \times e^{(-3125/T)} \\ N + OH \leftrightarrow NO + H, \\ k_{3f} = 4.2 \times 10^{10} \end{cases}$$

$$(25)$$

After some transformations we obtain the following differential equation for NO formation:

$$\frac{1}{V} \times \frac{d[(NO)V]}{dt} = \frac{2 \times (1 - \beta^2) \times R_1}{\left(1 + \beta \times \frac{R_1}{R_2 + R_3}\right)}$$
(26)

where (NO) denotes concentration,  $\beta = (NO)/(NO)_e$  and subscript "e" denotes equilibrium. "V" is the burned gas volume and  $R_I$  (i=1,2,3) is the one way equilibrium rate, for the "i" reaction, defined as follows:

$$R_1 = k_{1f} \times (NO)_e \times (NO)_e$$

$$R_2 = k_{2f} \times (N)_e \times (O_2)_e$$

$$R_3 = k_{3f} \times (N)_e \times (OH)_e$$
(27)

and " $k_{if}$ " is the forward reaction rate constant for the "i" reaction.

SOOT FORMATION MODEL. - The modeling of soot formation is a difficult task in common internal combustion engine simulation models. For this reason researchers usually use semi-empirical models that have been derived from the analysis of experimental data. In the present work a semi-empirical model, that has been widely tested, is used to predict the rate of soot formation. [10,12-14,20]

The soot formation and oxidation rates are given respectively by,

$$dm_{sf} = A_f \times m_{fav} \times P^{0.5} \times exp \left( \frac{-E_{sf}}{R_m T_b} \right)$$
 (28)

$$dm_{sb} = A_b \times m_s \times \frac{P_{O_2}}{P} \times P^{1.8} \times exp \left(\frac{-E_{sb}}{R_m T_b}\right) (29)$$

where " $m_s$ " is the net soot formed, " $P_{O2}$ " is the partial pressure of oxygen and " $A_f$ " and " $A_b$ " are constants.

The net soot formation rate is then obtained from the expression:

$$dm_s = dm_{sf} - dm_{sh} \tag{30}$$

## ENGINE DESCRIPTION AND EXPERIMENTAL FACILITIES

To calibrate the present model an experimental investigation has been conducted on a single cylinder, Lister LV1, direct injection diesel engine located at the authors' laboratory. The results of this investigation are used to calibrate and evaluate the model under normal diesel fuel operation. These results are also used as basis to evaluate the findings when the engine operates with pilot fuel injection. The technical data of the engine are given in Table 1. It is a naturally aspirated, air-cooled, four-stroke engine, with a bowl-in-piston combustion chamber and a normal speed range of 1000-3000 rpm. A three-hole injector nozzle (each hole having a diameter of 0.24mm) is located in the middle of the combustion chamber head. The injector nozzle opening pressure is 190 bar. The main parts of the test installation used are:

- Lister LV1 diesel engine.
- Heenan & Froude hydraulic dynamometer.
- Tank and flow meter for diesel fuel.
- TDC marker (magnetic pick-up) and rpm indicator.
- K-type thermocouples for measuring the temperatures of the exhaust gas and engine oil.
- 'Kistler' 6001 miniature piezoelectric transducer for measuring the pressure in the cylinder, flush mounted to the cylinder head and carefully calibrated.
- 'Kistler' 7063 piezoelectric transducer for measuring fuel-line pressure before the injector.
- 'Kistler' 5007 charge amplifiers.

Table 1: Engine basic design data, Lister LV1-Diesel high speed engine

Bore	85.73mm
Stroke	82.55mm
Connecting Rod Length	148.59mm
Compression Ratio	18
Cylinder Dead Volume	28.03cm <sup>3</sup>
Inlet Valve Opening	15°CA before TDC
Inlet Valve Closure	41°CA after BDC
Exhaust Valve Opening	41°CA before BDC
Exhaust Valve Closure	15°CA after TDC
Inlet Valve Diameter	34.5mm
Exhaust Valve Diameter	31.5mm
Static Injection Timing	28°CA before TDC

The output signals from the magnetic pick-up and piezoelectric transducers are connected to the input of a 'KEITHLEY' DAS-1801ST A/D board, installed on a IBM compatible Pentium II PC.

The exhaust gas analysis system consists of a group of analyzers for measuring the main gaseous pollutants together with soot concentration. The nitric oxide concentration (NO) is measured using a "Signal" chemiluminiscent analyzer having a NO<sub>2</sub> to NO converter switch and fitted with a heated line, while the soot concentration is measured using a Bosch RTT100 analyzer.

The series of experiments conducted for this preliminary study, involved as already mentioned only the diesel fuel (no gas was added) in a variety of engine operating conditions. The following discussion refers to the results for 1500, 2000 and 2500 rpm engine speed and four different loads. Currently efforts are given to modify the existing engine and conduct experiments using gaseous fuel as supplement for liquid fuel taking into account the observations obtained from the modeling. These results will be used to evaluate the findings of the newly developed dual-fuel model.

### RESULTS AND DISCUSSION

PRESSURE DATA UNDER NORMAL OPERATION - Figures 1-6 present the comparison between theoretical and experimental pressure and heat release traces in the case of pure Diesel operation, for 1500, 2000 and 2500 rpm engine speed and two different loads namely 40 and 80% of full load. As observed the agreement in all cases is good, which is promising for the utilization of the model to predict engine performance for dual fuel engines. It must be stated here that the values of the present model's constants are held the same for the entire range of operating parameter variation considered in the present study. Results for the experimental heat release rate curves in the following figures were obtained from the analysis of the corresponding experimental cylinder pressure traces using a diagnostic code [24]. At this point it must be stated that the results provided in Figures 1-6 are considerably improved compared to an earlier version of the present model [8].

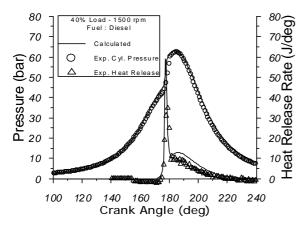


Fig.1 Comparison between experimental and calculated pressures and heat release traces at 1500 rpm engine speed and 40% load under 100% diesel fuel operation

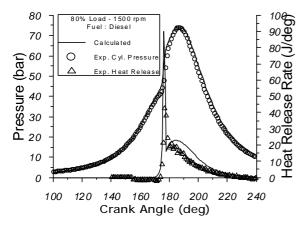


Fig.2 Comparison between experimental and calculated pressures and heat release traces at 1500 rpm engine speed and 80% load under 100% diesel fuel operation

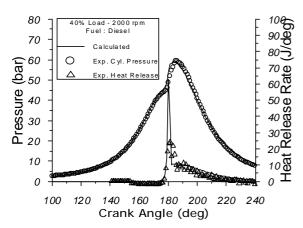


Fig.3 Comparison between experimental and calculated pressures and heat release traces at 2000 rpm engine speed and 40% load under 100% diesel fuel operation

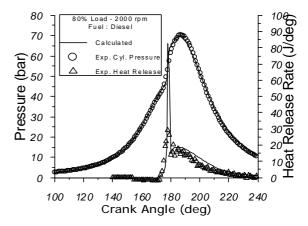


Fig.4 Comparison between experimental and calculated pressures and heat release traces at 2000 rpm engine speed and 80% load under 100% diesel fuel operation

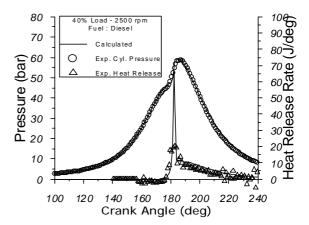


Fig.5 Comparison between experimental and calculated pressures and heat release traces at 2500 rpm engine speed and 40% load under 100% diesel fuel operation

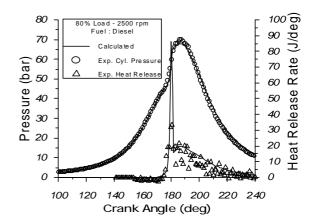


Fig.6 Comparison between experimental and calculated pressures and heat release traces at 2500 rpm engine speed and 80% load under 100% diesel fuel operation

CYLINDER PRESSURE AND HEAT RELEASE UNDER DUAL FUEL OPERATION - Figures 7-12 present the comparison between calculated pressure and heat release traces under diesel and dual fuel operation for 1500, 2000 and 2500 rpm engine speed and two different loads namely 40 and 80% of full load respectively. It must be stated, that engine load is controlled by changing the amount of the primary gaseous fuel added to the air, whilst the quantity of the pilot liquid diesel fuel is fixed and contributes approximately 10% of the total heat release under pure diesel operation at full load. In Figures 7-12 we observe that for a fixed pilot diesel quantity, the cylinder pressure changes significantly when increasing the amount of gaseous fuel.

As observed under part load conditions the presence of gaseous fuel affects slightly the trace of the pressure during the premixed-controlled combustion phase. At part load condition the heat release rate values are lower to these observed under pure diesel engine operation.

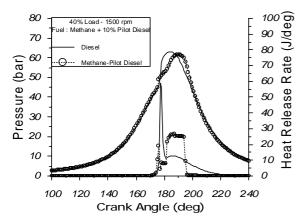


Fig.7 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 1500 rpm engine speed and 40% load.

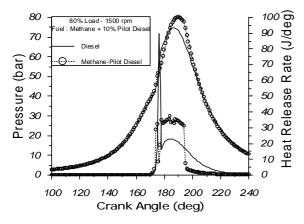


Fig.8 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 1500 rpm engine speed and 80% load.

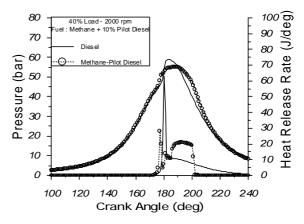


Fig.9 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 2000 rpm engine speed and 40% load.

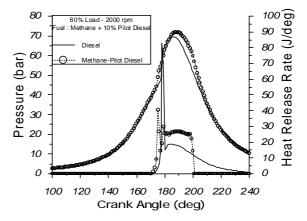


Fig.10 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 2000 rpm engine speed and 80% load.

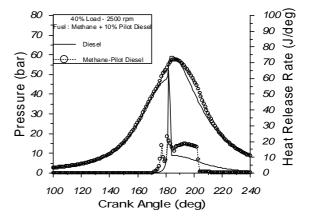


Fig.11 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 2500 rpm engine speed and 40% load.

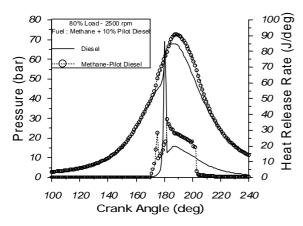


Fig.12 Comparison between calculated pressures and heat release traces under diesel and dual fuel operation respectively at 2500 rpm engine speed and 80% load.

On the other hand the combustion duration is shorter compared to normal diesel fuel operation since during the late part of combustion the flame spread results to a faster heat release.

At high load conditions the increase of gaseous fuel mass leads to a sharper rate of heat release during the initial stage of combustion. The high concentration of gaseous fuel in the charge combined with the high temperature and pressure results to a considerable increase of the flame propagation velocity compared to the one at part load. The above leads to an increase of the total heat release rate resulting to a faster pressure rise compared to operation using pure diesel fuel.

EFFECT OF DUAL FUEL OPERATION ON ENGINE PRESSURE - The variation of maximum cylinder pressure with total equivalence ratio is given in Figures 13-15. Comparing the calculated values of maximum engine pressure with the measured ones under pure diesel operation, it is revealed a good coincidence.

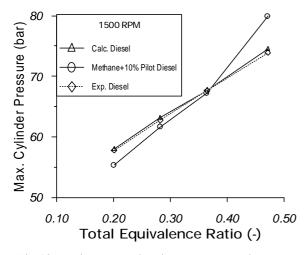


Fig.13 Maximum combustion pressure under pure diesel and dual fuel operation vs. total equivalence ratio at 1500 rpm engine speed

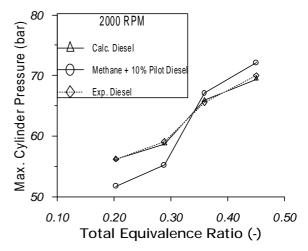


Fig.14 Maximum combustion pressure under pure diesel and dual fuel operation vs. total equivalence ratio at 2000 rpm engine speed

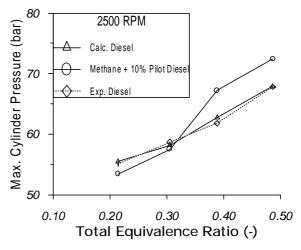


Fig.15 Maximum combustion pressure under pure diesel and dual fuel operation vs. total equivalence ratio at 2500 rpm engine speed

The utilization of a larger amount of gaseous fuel as the total equivalence ratio increases, improves combustion performance as a result of the higher rates of total heat release. This results to an increase of maximum cylinder pressure compared to the one under pure diesel operation at high engine loads while at part load the peak pressures under dual fuel operation are lower. But as revealed from the modeling the increase at high load is not so severe to cause problems on the engine structure.

EFFECT OF DUAL FUEL OPERATION ON ENGINE PERFORMANCE - The variation of indicated power output with equivalence ratio under diesel and dual fuel operation is shown in Figures 16-18. Examined these figures it is derived a good agreement between calculated and experimental indicated power output, a fact that is promising for the utilization of the present model to predict engine performance for dual fuel operation. It is observed

that dual fuel operation tends to increase indicated power available from normal diesel operation for the same equivalence ratio. At part load the presence of the gaseous fuel results to lower indicated power output compared to normal diesel operation.

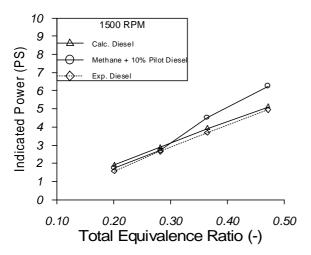


Fig.16 Variation of indicated power with total equivalence ratio under pure diesel and dual fuel operation at 1500 rpm engine speed

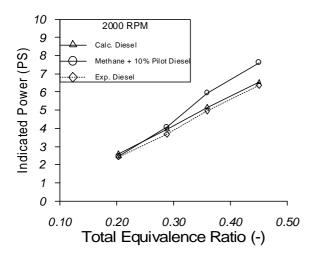


Fig.17 Variation of indicated power with total equivalence ratio under pure diesel and dual fuel operation at 2000 rpm engine speed

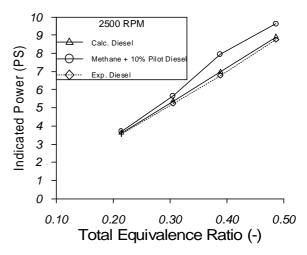


Fig.18 Variation of indicated power with total equivalence ratio under pure diesel and dual fuel operation at 2500 rpm engine speed

Figures 19-21 present the variation of brake specific fuel consumption with engine load. It is observed that in the case of pure diesel fuel operation the model predicts accurately the measured (b.s.f.c) values for all loads examined. As shown in these figures the total brake specific fuel consumption at part load under dual fuel operation is inferior to that under pure diesel operation. The increment of the gaseous fuel concentration in the charge (i.e. load) has as a result an increase of engine efficiency as the utilization of the fuel becomes more efficient. This is more obvious at higher engine speeds where the available time for combustion is less and gaseous fuel combustion is faster.

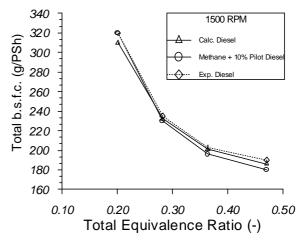


Fig.19 Variation of the total brake specific fuel consumption with total equivalence ratio under pure diesel and dual fuel operation at 1500 rpm engine speed

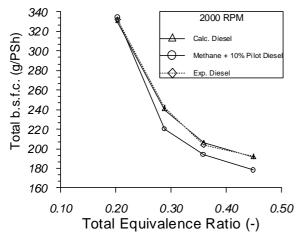


Fig.20 Variation of the total brake specific fuel consumption with total equivalence ratio under pure diesel and dual fuel operation at 2000 rpm engine speed

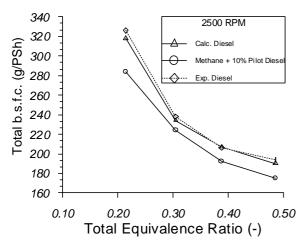


Fig.21 Variation of the total brake specific fuel consumption with total equivalence ratio under pure diesel and dual fuel operation at 2500 rpm engine speed

EFFECT OF DUAL FUEL OPERATION ON POLLUTANT EMISSIONS - The variation of Nitric Oxide concentration with the total equivalence ratio under pure diesel and dual fuel operation is presented in Figures 22-24. Comparing the calculated values of NO with the measured ones under pure diesel operation, it is revealed a good coincidence.

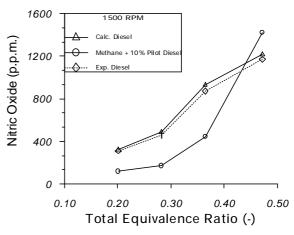


Fig.22 Nitric Oxides emissions at 1500 rpm engine speed vs. total equivalence ratio under pure diesel and dual fuel operation

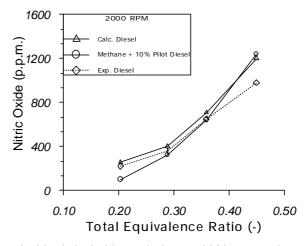


Fig.23 Nitric Oxides emissions at 2000 rpm engine speed vs. total equivalence ratio under pure diesel and dual fuel operation

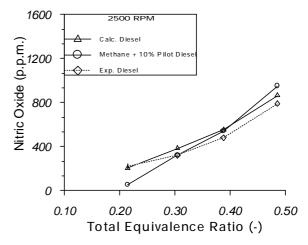


Fig.24 Nitric Oxides emissions at 2500 rpm engine speed vs. total equivalence ratio under pure diesel and dual fuel operation

The model over-predicts slightly absolute values, which is normal for a two-zone model, but it manages to predict the trend as equivalence ratio changes. This enables us to use it for NO prediction under dual fuel operation. The formation of nitrogen oxides is favored in general by oxygen concentration and high gas temperature. At part load conditions under dual fuel operation the NO concentrations are inferior to that when using pure diesel since the gas temperatures at the initial stages of combustion are lower due to the lower heat release rate compared to normal diesel operation.

At high load, NO concentration exceeds the values observed under normal diesel operation because mainly of the increased gas temperature due to the higher heat release rates at the early stages of combustion and at the range of equivalence ratios examined.

Finally as shown in Figures 25-27, dual fuel operation could be a potential way of reducing soot emissions. Examined these figures we can see that the current model predicts adequately the experimentally measured soot emissions under pure diesel operation. This is encouraging and makes the results obtained under dual fuel operation more reliable. A difference is observed at 60% load, which is due to different behavior of the engine fuel injection system, as observed from the measured values of fuel injection pressure. Observing these figures, as the total equivalence ratio increases, the soot concentration is decreased sharply since less liquid fuel is injected on a percentage basis and thus less soot is formed. Also due to the higher temperatures observed at high equivalence ratios the soot oxidation rate is higher contributing to a further decrease of soot emissions. Moreover, gaseous fuels such as methane being the lower member in the paraffin family have very little tendency of pyrolysis to liberate soot. Thus practically the gaseous fuel produces no soot, while it contributes to the oxidation of the one formed from the combustion of the pilot liquid fuel.

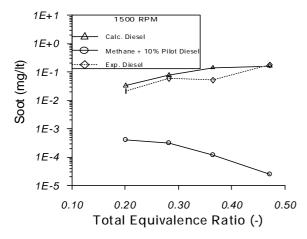


Fig.25 Soot emissions at 1500 rpm engine speed vs total equivalence ratio under pure diesel and dual fuel operation

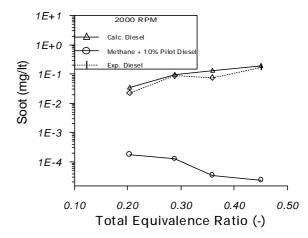


Fig.26 Soot emissions at 2000 rpm engine speed vs total equivalence ratio under pure diesel and dual fuel operation

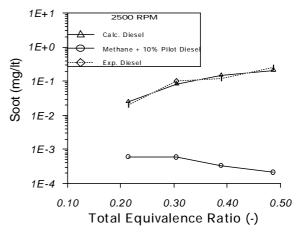


Fig.27 Soot emissions at 2500 rpm engine speed vs total equivalence ratio under pure diesel and dual fuel operation

### **CONCLUSIONS**

Under the present work a new model has been developed to simulate the operation of dual-fuel diesel engines using pilot injection, for the prediction of performance and pollutant emissions. This preliminary investigation focuses on diesel engines where engine load is controlled by changing the amount of primary gaseous fuel added through the intake air, while the quantity of the pilot liquid fuel per injection stroke is fixed. The main purpose is to provide an adequate way to describe the complicated combustion process of the primary gaseous fuel to estimate apart from power and efficiency, the concentration of soot emissions and nitrogen oxides at the engine exhaust.

For this reason a two-zone model has been developed taking into account details of diesel fuel spray formation and mixing with the surrounding gas. Combustion is initiated by the ignition of the liquid fuel. The burning rate of gaseous fuel is controlled by its entrainment rate into the burning zone and also from the velocity of the flame front, which is formed around the area of the burning zone and spreads inside the combustion chamber. To validate the

model before using it to predict engine performance and pollutants emissions under dual-fuel operation an extended experimental investigation has been conducted on a high speed DI simple cylinder test engine located at our laboratory. Measurements have been taken for both performance and emissions at various operating conditions using diesel fuel only. These are used for model validation and mainly serve as comparison between normal diesel fuel operation and dual fuel operation.

Comparing calculated and measured values under normal diesel operation a good coincidence is observed for both performance and pollutant emissions. This enables us to use the model to predict engine behavior under dual-fuel operation. From the analysis of computational data it is revealed that dual-fuel operation results to higher combustion pressures at high load and slightly lower ones at part load. The effect at higher engine speeds is more intense. Concerning engine efficiency it is revealed in general that as the concentration of gaseous fuel increases thus results to an improvement of engine efficiency.

As far as pollutant emissions are concerned the use of gaseous fuel has a negative effect on NO emissions and a positive one on soot. Specifically an increase of NO emissions is observed at high engine loads, which is not severe and a slight decrease at part load. The increase of NO is more intense at higher engine speeds. On the other hand soot is seriously decreased when using gaseous fuel. The effect is stronger at higher engine loads and higher concentrations of gaseous fuel. But the most important is that when using gaseous fuel we always have a considerable reduction of soot emission regardless of the engine operating conditions.

The results of this preliminary investigation are encouraging and urge us to conduct an experimental investigation to verify the findings. This is currently under progress and results will be given in the near future. Even though it is difficult to generalize the findings of the current preliminary investigation, we believe that they are important since the reduction of soot emissions on existing DI diesel engines is extremely important.

### **NOMENCLATURE**

a, b, c = constants  $a_{del}$  = constant A = area  $m^2$ 

A = area,  $m^2$  $A_f$  = constant in soot formation mechanism

 $A_b$  = constant in soot oxidation mechanism

C<sub>v</sub> = specific heat capacity under constant volume, J/kgK

C<sub>p</sub> = specific heat capacity under constant pressure,

 $C_{Dinj}$  = injector hole discharge coefficient

 $d_{ho}$  = injector hole diameter, m

D = cylinder bore, m

E = activation energy, J/Kmole

k = constant for liquid fuel preparation rate k' = constant for liquid fuel reaction rate k" = constant for gaseous fuel reaction rate m = mass, kg, or constant for the liquid fuel

P =pressure, Pa

P<sub>O2</sub> = partial pressure of oxygen, bar O = heat transfer to walls, J

R<sub>m</sub> = universal gas constant, J/kmoleK

S = penetration length, m

t = time, sec

T = absolute temperature, K u = specific internal energy, J/kg u<sub>t</sub> = turbulent flame velocity, m/sec

 $\vec{V}$  = volume,  $\vec{m}^3$ 

X = kmole fraction on species y = mass fraction on species

 $z_1, z_2 = constants$ 

### Greek

 $\begin{array}{ll} \theta & = \text{initial jet angle, rad} \\ \Delta P & = \text{pressure difference, Pa} \\ \lambda & = \text{thermal conductivity, W/mK} \\ \mu & = \text{dynamic viscosity, kg/ms} \\ \nu & = \text{kinematic viscosity, m}^2/\text{sec} \end{array}$ 

 $\rho$  = density, kg/m<sup>3</sup>  $\phi$  = equivalence ratio

### **Subscripts**

a = air

av = available quantity
b = burned zone
del = delay
e = equilibrium

f = fuel

fpr = liquid fuel prepared fi = liquid fuel injected fupr = liquid fuel unprepared

fb = fuel burned

g = gaseous fuel or gas mixture

= index denoting control volume or the kind of

gaseous fuel

k = index denoting the species of the gaseous

 $\begin{array}{ccc} & & mixture \\ o & = initial \ value \\ tot & = total \\ s & = soot \\ sf & = soot \ formed \end{array}$ 

sb = soot formed sb = soot oxidized st = stoichiometric u = unburned zone

 $\mathbf{w} = \mathbf{wall}$ 

### **Dimensionless number**

Re = Reynolds

### **Abbreviations**

CR = Compression Ratio DI = Direct Injection

bsfc = Brake specific fuel consumption

NO = Nitric oxide

ppm = parts per million (volume)

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