PREDICTION OF MAJOR POLLUTANTS EMISSION IN DIRECT-INJECTION DUAL-FUEL DIESEL AND NATURAL-GAS ENGINES

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Abstract The dual-fuel diesel engine (D.F.D.E) is a conventional diesel engine in which much of the energy released, hence power, comes from the combustion of gaseous fuel such as natural gas. The exhaust emission characteristics of the D.F.D.E needs further refinements, particularly in terms of reduction of Unburnt Hydrocarbons (UHC) and Carbon Monoxide (CO) emission, because the concentration of these pollutants are higher than that of the baseline diesel engine. Furthermore, the combustion process in a typical D.F.D.E tends to be complex, showing combination of the problems encountered both in diesel and spark ignition (S.I.) engines. In this work, a computer code has been modified for simulation of D.F.D.E combustion process. This model simulates D.F.D.E combustion by using a Multi-Zone Combustion Model (MZCM) for diesel pilot jet combustion and a conventional S.I. combustion model for modelling of combustion of premixed gas-air charge. Also, in this model, there are four submodels for prediction of major emission pollutants such as UHC, NO, CO and soot which are emitted from D.F.D.E. For prediction of formation and oxidation rates of pollutants, relevant conventional kinetically-controlled mechanisms and mass balances are used. The model has been verified by experimental data obtained from a heavy-duty truck and bus diesel engines. The comparison shows that, there exist good agreements between the experimental and predicted results from the D.F.D.E.

Key Words Pollutants Emission, Dual-Fuel, Natural-Gas, Prediction, Diesel

INTRODUCTION

The compression-ignition type of D.F.D.E has been employed in a wide range of applications to utilize various gaseous fuels without excessive increase in cost compared with the baseline diesel engine. However, the combustion process in a D.F.D.E...
tends to display a complex combination of features of both diesel and Otto engines operation.

Introducing a gaseous fuel along with the inlet air in the cylinder during suction stroke enhances greatly the mixing and combustion processes of the pilot jet, which is usually retained to provide a reliable and strong source of ignition. Flames from the various ignition centers originating from the pilot fuel droplets can propagate to varying degrees and rates throughout the surrounding gaseous fuel-air mixtures.

Exhaust emissions from D.F.D.E vary largely from the baseline diesel engine at different conditions of engine speed and load. Due to heterogeneity nature of the cylinder charge, formation of the pollutants in the diesel engines is a complex process. In D.F.D.E, by introducing gaseous fuel, the heterogeneity nature of the cylinder charge increases tremendously.

A suitable computer based mathematical modelling can provide an adequate mean for describing details of the complicated mixing, combustion and pollutants emission processes in these engines. The development of such models for D.F.D.E operation has been so far very limited, mainly due to the complex combustion and emission formation processes. Most of these models are based on Single-Zone Combustion Model (SZCM), hence their accuracy for predicting the performance and pollutants characteristics of D.F.D.E are limited. For example, many SZCM based codes developed by Pirouzpanah, et al[1,2] and Rainie,[3] could only be used to predict the general combustion performance of the D.F.D.E such as cylinder pressure, temperature and power output. Recently Pirouzpanah, et al[4] and Karim, et al[5-7] developed a SZCM code which simulates pollutants emission in D.F.D.E.

The limited accuracy of SZCM in predicting of pollutants emission concentration and performance characteristics of D.F.D.E is mainly due to absence of measures for considering temporal and spatial variations of temperature and mixture strength within the cylinder. The formation and elimination processes of pollutants are strong functions of the distribution of the charge temperature and fuel concentration within the cylinder. Suitable approaches need to be developed involving multi-zone computational models for better simulation of the complex nature of the combustion and pollutants emission processes in D.F.D.E.

Since such models can predict in-cylinder temporal and spatial distribution of temperature and composition, they would lead to a better prediction of performance and pollutants emission. These models also require significantly less computing resources than the so-called, Computational Fluid Dynamics (CFD) models which can not offer, as yet, a realistic representation of the complex transient turbulent combustion processes in D.F.D.E.

The present contribution describes a model that simulates dual-fuel combustion by using a quasi-dimensional entrainment model (MZCM) for pilot jet combustion and a conventional S.I. combustion model for modelling the combustion of premixed gas/air charge. The thermodynamics parameters for cylinder charge are calculated during a complete closed cycle from the start of inlet valve closes (IVC) till the exhaust valve opens (EVO). Also, four submodels have been developed
for predicting the formation and oxidation rates of major in-cylinder pollutants (CO, UHC, NOx and soot) from D.F.D.E.

DESCRIPTION OF THE PRESENT MODEL

The inlet cylinder charge in D.F.D.E. is homogeneously premixed of gaseous fuel and air that has different thermodynamics properties (Cp, Cv and γ) from the charge (i.e. pure air) in baseline diesel engine. In this work, the model can predict these properties for various proportions of diesel and gaseous fuels. Also, by calculating the whole period of compression stroke, the actual condition at the injection timing is evaluated. On the basis of the work of Annand, W.J.D.[8], this model is also able to calculate heat transfer between charge and cylinder walls during the complete closed cycle.

The D.F.D.E model assumes that the ignition of the charge occurs as a result of the pilot jet auto-ignition and uses the ignition delay model[9] for the ignition delay period calculation. It should be noted, however, that the cylinder pressure and temperature during the ignition delay period will be affected by the presence of the premixed natural gas-air charge. More specifically, the high specific heat of natural gas compared with air, will extend the delay period in the D.F.D.E. For modelling the pilot jet combustion, the Multi-Zone Combustion Model[10] (MZCM) is modified and used in the present work. Furthermore, it is assumed that the quantity of air that is utilized for combustion of gaseous and pilot jet fuels is proportional to the mass ratio of those fuels that are supplied to the engine simultaneously.

A simple Wiebe Function burning pattern, which has previously been used in S.I. engines combustion models, has been employed here to determine the rate of gaseous fuel combustion[11]. For combustion of homogeneous gaseous-air mixture a two zone model (TZM) was considered. The first zone consists of the reactant mixture (unburnt zone-U) and the second zone contains the products of combustion (burnt zone-B). These zones are separated by a thin flame front. The laminar flame speed is calculated from an empirical correlation[3]. The combustion duration of the gaseous fuel is then calculated from the laminar flame speed by considering turbulence factor. It is also assumed that a) the unburnt zone(U) burns by passing the flame front, with a constant equivalence ratio during the period of combustion of gaseous fuel, b) the gas burning zones have a uniform and similar temperature and pressure and thus these properties are different from the properties of pilot jet burning zones, and c) in modelling the pilot jet combustion by MZCM, there is a uniform pressure in all zones, but there exists zonal temperature distribution within the pilot jet.

The overall structure of the present computational model is shown in Figure 1. The proposed Wiebe combustion function that characterizes the premixed combustion of gaseous fuel-air mixture is employed to describe the rates of burning and hence the heat released of the gaseous fuel-air mixtures.

On the other hand, the MZCM can predict only heat released rate of the pilot jet combustion[10]. Then total rate of the heat released in combustion chamber is the sum of the above rates. Also, the heat transferred from the pilot jet zones to the cylinder walls can be predicted by utilizing suitable correlation, whereas the heat
transferred from the gaseous burning zones can be predicted by solving the conservation of the energy equation.

The variations of thermodynamics parameters such as pressure and temperature can be calculated from the energy conservation, volume constraint and state equations. Then from the above data, the pollutants formation rate can be ultimately predicted. In the emission model, the concentration of major pollutants in D.F.D.E., such as Unburnt Hydrocarbon (UHC), Carbon Monoxide (CO), Nitrogen Oxide (NO) and soot particles are calculated.

For calculating the UHC mass, it is assumed that the difference between masses of input fuel and burnt fuel in each time step composes masses of UHC, soot and CO. Then by using the mass and energy balances the UHC mass can be obtained[12].

For the calculation of CO concentration, relevant kinetically-controlled mechanism for CO formation and its oxidation are used [12]. For the calculation of NO concentration, the famous extended Zeldovich mechanism has been used[13]. For the prediction of soot particles concentration, the amount of net soot is calculated by considering the differences between the rates of soot formation and soot oxidation inside different zones of pilot jet[14]. In this work, it is assumed that UHC, NO and CO concentrations are originated from both combustion regions (pilot jet and gaseous burning zones), but soot emission is attributed only to the pilot jet region.

**MATHEMATICAL TREATMENT**

**Modelling Performance and Combustion** One of the basic simplified assumptions made is that the injection of the diesel pilot jet can be represented by the characteristic of a steady state gas jet and calculated from momentum theory and supplemented by experimental data[10]. Molecular formula for the Iranian produced diesel and natural gas fuels are taken as: \(16(C_1H_{12})\) and \((C_1266H_{3765}O_{103}N_{101})\), respectively. At the end of the diesel fuel ignition delay period, both of the fuels start to burn. In each calculation time step, by utilizing the MZCM code for simulating the pilot jet combustion process, the heat released rate \(\left(\dot{q}_{\text{in}}\right)\), the heat transfer rate \(\left(\dot{q}_{\text{cond}}\right)\) and temperature and pressure of diesel combustion region \((T_{\text{as}}, P_{\text{as}})\) are predicted. In the combustion region of gaseous fuel, the laminar flame speed is calculated as[3]:

\[
u_l = \frac{1.08}{-A} \frac{\psi e}{1 + 0.45 - 0.015d} \]  

(1-1)

where: \(\psi\) = equivalence ratio of gaseous fuel

and, \(d\) = residual fraction (%)

The constant \(A\) affects the flame speed versus equivalence ratio characteristics and has a strong effect on the flammability limit at which \(u_l = 0.1 \text{ m/sec}[15]\). From the work of Raine, R.R [3] values of \(A=0.64\) and 2.59 are chosen which correspond to lean flammability limits of 0.54 and 0.0, respectively. In order to deal with the strong
effect of turbulence on the fuel burning rate, a combustion duration time in crank angle degree is calculated as:

$$\Delta \theta_{\text{comb}} = \frac{K}{n_1} \times 6 \pi a n$$  \hspace{1cm} (1-2)

Where $K$ is a semi-empirical constant which includes turbulence factor (i.e. Taylor microscale turbulence)\cite{11} and $n$ is the engine speed. Mass fraction of burnt gaseous fuel can be obtained as\cite{11}:

$$x_{\text{sg}}(\theta) = \frac{m_{\text{sg}}}{m_{\text{gas}}} = 1 - \exp\left[ -a \left( \frac{\theta - \theta_{\text{comb}}}{\Lambda_{\theta_{\text{comb}}}^0} \right)^{b+1} \right]  \hspace{1cm} (2-1)$$

Where $m_{\text{sg}}$ and $m_{\text{gas}}$ are the instantaneous mass of burnt zone (of gaseous fuel-air mixture combustion region) and total mass of gaseous-air mixtures, respectively. Also, $a$ and $b$ are empirical constants\cite{11} offered for a and b, respectively\cite{11} and $\theta_{\text{ig}}$ is the crank angle at the start of ignition.

Then, by differentiating equation (2-1) a rate of gas/air mixture combustion can be obtained as:

$$\frac{dm_{\text{sg}}}{d\theta} = \frac{a(b+1)}{\Lambda_{\theta_{\text{comb}}}^0} \left( \frac{\theta - \theta_{\text{comb}}}{\Lambda_{\theta_{\text{comb}}}^0} \right)^b \exp\left[ -a \left( \frac{\theta - \theta_{\text{comb}}}{\Lambda_{\theta_{\text{comb}}}^0} \right)^{b+1} \right] \hspace{1cm} (2-2)$$

So, for each time step, the rate of heat released $d\dot{q}_{\text{gas}}$ of gaseous fuel can be obtained as:

$$d\dot{q}_{\text{gas}} = \frac{dm_{\text{sg}}}{d\theta} \times \text{LHV}_{\text{gas}}  \hspace{1cm} (3)$$

LHV$_{\text{gas}}$ is the lower heating value of gaseous fuel. Furthermore, in each time step the thermodynamics properties such as $C_p$, $C_v$ and $\gamma$ and the masses and moles of each zone can be obtained as:

$$C_p_{\text{av}} = \frac{C_p_{\text{dis}} \cdot N_{\text{dis}} + C_p_{U} \cdot N_{U} + C_p_{B} \cdot N_{B}}{(N_{\text{dis}} + N_{U} + N_{B})} \hspace{1cm} (4-1)$$

$$C_v_{\text{av}} = C_p_{av} \cdot \gamma - R \hspace{1cm} (4-2)$$

$$\gamma_{\text{av}} = \frac{C_p_{av}}{C_v_{av}}  \hspace{1cm} (4-3)$$

Then, total rate of heat released is calculated as:

$$d\dot{q}_{\text{tot}} = d\dot{q}_{\text{gas}} + d\dot{q}_{\text{wall}} = \Pi \cdot R \cdot \gamma_{\text{av}} \hspace{1cm} (5)$$

The application of the first law of thermodynamics to the total in-cylinder charge gives:

$$d\dot{q}_{\text{tot}} = \left( \frac{\gamma_{\text{av}} \cdot P_{\text{av}}}{\Pi (\gamma_{\text{av}} - 1) \frac{dV}{d\theta}} + \frac{\frac{dP_{\text{av}}}{d\theta}}{(\gamma_{\text{av}} - 1) \frac{dV}{d\theta}} \right) + d\dot{q}_{\text{wall}} \hspace{1cm} (6)$$

where $d\dot{q}_{\text{wall}}$ is the total rate of heat transfer between cylinder walls and charge, then it can be written as:

$$d\dot{q}_{\text{wall}} = d\dot{q}_{\text{wall}} \gamma_{\text{av}} + d\dot{q}_{\text{wall}} \gamma_{\text{gas}} \hspace{1cm} (7)$$

As seen before, $d\dot{q}_{\text{wall}} \gamma_{\text{gas}}$ and $\gamma_{\text{av}}$ depend on the $T_{\text{gas}}$. Therefore, by means of the equation (6), $T_{\text{gas}}$ and $P_{\text{av}}$ are related together. Then by solving equation (6), $P_{\text{av}}$ can be obtained (by iteration method). Once the pressure of combustion chamber ($P_{av}$) is determined, the temperature of combustion chamber can be calculated from state equation:

$$T_{\text{av}} = \frac{P_{av} \cdot V}{N_{\text{tot}} \cdot R} \hspace{1cm} (8)$$

$$N_{\text{tot}} = N_{\text{dis}} + N_{U} + N_{\text{B}}$$

where $N_{\text{tot}}$ is the total moles of the charge in the cylinder. Then the actual value of $T_{\text{gas}}$ can be found from following relations:

$$m_{\text{tot}} = m_{\text{dis}} + m_{\text{gas}} \hspace{1cm} (9)$$

$$T_{\text{gas}} = \frac{m_{\text{tot}} \cdot T_{av} - m_{\text{dis}} \cdot T_{dis}}{m_{\text{gas}}} \hspace{1cm} (10)$$

where $m_{\text{gas}}$ and $m_{\text{dis}}$ are the instantaneous masses of pilot jet combustion region and gaseous fuel-air mixture combustion region.

**Pollutants Emission Formulation** The pollutants such as UHC, NO and CO concern both regions (i.e. pilot jet and gaseous fuel combustion regions). The concentrations of these pollutants are
calculated in each combustion region. Then the sum of their concentrations is considered as the total pollutants in dual-fuel combustion. But it is assumed that concentration of soot concerns the pilot jet combustion region only.

Chemical equilibrium calculation is a prerequisite to detailed emission formation models based on kinetics of various species. In this work two methods are utilized to calculate the equilibrium products of combustion within each zone. One of the methods is outlined by Oikara and Borman[16] and the other method is based on the work done by Benson et al[17]. The calculations include all major chemical species comprising CO₂, CO, H₂, OH, H₂O, NO, N₂, O₂, O, H₂ and Ar.

**UHC Formation** It is assumed that the difference between total masses of input fuels per cycle (mₙ) and total masses of burnt fuels (mₙₑ) includes the masses of UHC, CO and soot. Heating values of UHC and soot are heating values of dual-fuel equivalence (LHV)ₑₑ and carbon particle (LHV)ₑ, respectively.

Then for calculating the mass of UHC (mₙₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑₑᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉᵉ=e
Soot Formation. Formation of soot is concerned to pilot jet combustion region only. The formulation of soot formation and oxidation are based on the work of Pirouzpanah, et al[14].

NO Formation. The kinetics of thermal NO formation is based on the extended Zeldovich mechanism. The principal reactions governing the formation of thermal NO are based on the work of Pirouzpanah, et al[13].

NUMERICAL METHOD

As seen before, in the energy equation (6) there are two unknown parameters, namely $T_{\text{gas}}$ and $P_{\text{ad}}$, which are interdependent. In initial conditions (first step), it is assumed that $T_{\text{gas}}$ equals $T_{\text{ad}}$ and $P_{\text{gas}}$ equals $P_{\text{ad}}$. Then, this equation is solved by a fourth-order Runge-Kutta iteration method. Flow charts of the combustion and emission subroutines are given in Figures 2 and 3. The present code is written in FORTRAN 95 and executed on the PC 486 66.

RESULTS AND DISCUSSION

Figure 4 is a schematic representation of the engine test set-up. In this work, exhaust gas pollutants such as CO, CO$_2$, UHC, O$_2$ are measured by an exhaust gas analyzer (Cussons P8333), NOx(NO,NO$_2$) by a Signal Analyzer (4000 VM), and black smoke by a Bosch Smoke meter. Table 1 lists the technical specifications of the engine under investigation. For Figures 5-7 and 9, the engine speed is constant ($N=1400$ rpm) and engine operation is at full load.

Figure 5-a compares variations of the calculated pressure in D.F.D.E versus crank angle with those of experimental results. Figure 5-b compares variations of the calculated pressure in baseline diesel engine versus crank angle with those of experimental results. It can be seen that the maximum pressure values in D.F.D.E occur later than those observed for diesel operation due to the longer ignition delay resulting from the addition of the gaseous fuel.

It should be noted that the underprediction of the cylinder pressure in the early part of the compression stroke is not related to the inaccuracy of the model. It is mainly due to the measuring limitation of our electronic indicator, which only shows combustion and expansion parts of P-V diagram. So this part of the pressure curve has been extrapolated from the available data.

In these Figures corresponding temperature curves are also superimposed. It can be seen that the peak of the cylinder temperature in D.F.D.E occurs later than in the diesel engine, and therefore it can be concluded that the period of combustion in D.F.D.E is longer than that of the diesel one. Also the peak of pressure in D.F.D.E is lower than that in diesel operation, so cylinder charge pressure in D.F.D.E is higher than that of diesel engine at the end of expansion stroke.

Figure 6 shows the variations of the concentration of CO in different combustion regions in D.F.D.E and also in the baseline diesel engine. The only available experimental data[17] for concentration of CO at one speed of the engine is given in Table 2. Since the period of combustion in D.F.D.E is longer than that in diesel one, and the charge does not have enough time for completing its combustion, even at the end of expansion stroke, therefore, oxidation of CO is not complete and emission of CO in D.F.D.E is higher than that in...
A. calculate \( m_{\text{dis}}, m_{\text{gas}}, u, \Delta \theta_{\text{comb}} \) and start of new time step

\[ \text{calculate } T_{\text{dis}}, P_{\text{dis}}, H.R.R_{\text{dis}}, dq_{\text{wall}}_{\text{dis}}, N_{\text{dis}} \text{ from MZCM in pilot Combustion} \]

The initial value of \( T_{\text{gas}}, P_{\text{gas}} \) are equalized with \( T_{\text{dis}}, P_{\text{dis}} \).

with \( T_{\text{gas}} \) and \( P_{\text{gas}} \) the chemical composition of the two zones in gaseous fuel-air mixture (U, B Zones) and \( \gamma_{\text{gas}} \) and \( N_{\text{gas}} \) and \( dq_{\text{wall}}_{\text{gas}} \) are obtained.

\( \gamma_{\text{av}} \) is calculated.

Equation (6) is solved then \( P_{\text{av}} \) is obtained (by using order 4 of Runge-Kutta iteration method).

\[ T'_{\text{gas}} \text{ (the new amount) is obtained with equation (10).} \]

\[ \Delta T_{\text{gas}} = | T_{\text{gas}} - T'_{\text{gas}} | \text{ is calculated.} \]

\[ \Delta T_{\text{gas}} > \text{ accuracy} \]

\[ \text{Go to B} \]

\[ \Delta T_{\text{gas}} < \text{ accuracy} \]

\[ P_{\text{av}} \] is calculated by equation (6) again.

\[ \Delta P_{\text{av}} = \left| P_{\text{av}} - P'_{\text{av}} \right| \text{ is calculated.} \]

\[ \Delta P_{\text{av}} > \text{ accuracy} \]

\[ \text{Go to B} \]

\[ \Delta P_{\text{av}} < \text{ accuracy} \]

Overall performance parameters are calculated (\( P_{\text{av}}, T_{\text{av}}, \delta W, H.R.R. \), and \( Q_{\text{wall}} \)).

Call Emission submodels

Start of new time step

Go to A

---

**Figure 2.** Flowchart of combustion model.

**Figure 3.** Flowchart of emission submodel.

**TABLE 1.** Engine Specifications.

<table>
<thead>
<tr>
<th>Engine: OM 355 D - CNG</th>
<th>Make and Model: Mercedes-Benz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type: Direct-Injection, Naturally-Aspirated, Heavy Duty Vehicle Diesel, 4-stroke</td>
<td>No. of Nozzles / Injector: 4</td>
</tr>
<tr>
<td>Cylinders: 6, In-line - Vertical</td>
<td>Nozzle opening Pressure: 175 Bar</td>
</tr>
<tr>
<td>Bore * Stroke: 128 * 150 (mm * mm)</td>
<td>Max. Power: 240 HP (2200 RPM)</td>
</tr>
<tr>
<td>Capacity: 11.58 (liter)</td>
<td>Max. Torque: 824 N.m (1400 RPM)</td>
</tr>
<tr>
<td>Compression Ratio: 16.1</td>
<td>Engine Speed: 1400 RPM</td>
</tr>
</tbody>
</table>

Diesel engine.

Figure 7 shows the variations of the theoretical concentration of kinetically thermal NO in different combustion regions in D.F.D.E and also in the baseline diesel engine. Since the combustion period in D.F.D.E is longer than that in pure diesel engine, so there is enough time for backward reactions in the Zeldovich mechanism to be carried out in this type of engine (compared with early freezing of reactions in the baseline diesel engine). Also it can be reasoned that, due to
higher pressure and temperature during early stages of expansion stroke in D.F.D.E, the freezing of NOx is retarded. Therefore, at lower speeds the NO concentration in this engine is lower than that of diesel engine.

Figure 8 compares the experimental and theoretical concentrations of exhaust NO versus engine speed for D.F.D.E at full load. The curves show that by increasing speed, the concentration of NO also increases. This is mainly due to increasing of flame temperature and also short resident time for backward reactions in the Zeldovich mechanism. It can be seen that, the present model underestimates the concentration of NO in the exhaust gases of D.F.D.E.

**Figure 4. Schematic representation of D.F.D.E set-up.**
The concentration difference between the two curves may be due to the assumptions which are made for simplifying the model. It could also be due to kinetic problems which arise firstly from inadequacy of the existing mechanism which underpredicts NOx for lean homogeneous mixtures[19] in S.I. engines, and secondly from pressure dependence of the relevant rate constants. However, in this stage, the trends of the curves are important and they are nearly the same.

Figure 9 compares the theoretical concentration of soot between D.F.D.E and diesel engine at constant speed (1400 rpm) and full load operation. Obviously, with using the clean burning CNG fuel and hence reducing the consumption of heavy diesel fuel in D.F.D.E, the density of soot will be lower than that in diesel engine. The soot concentration can be converted to other units such as the Bosch Smoke Number using known correlations[20].

![Figure 5-a](image1.png)

**Figure 5-a.** Comparison of calculated and experimental charge pressure and temperature for D.F.D.E at constant engine speed (1400 rpm) and full load operation.

![Figure 5-b](image2.png)

**Figure 5-b.** Comparison of calculated and experimental charge pressure and temperature for diesel engine at constant engine speed (1400 rpm) and full load operation.

![Figure 6](image3.png)

**Figure 6.** The theoretical production of CO in different combustion regions in D.F.D.E and diesel engines at constant engine speed (1400 rpm) and full load operation.
Figure 7. The theoretical production of thermal NO in different combustion regions in D.F.D.E and diesel engines at constant engine speed (1400 rpm) and full load operation.

Figure 8. Comparison of calculated and experimental concentration of NO for D.F.D.E operation at full load.

Figure 9. Comparison between theoretical soot concentration in D.F.D.E and diesel engines at constant engine speed (1400 rpm) and full load operation.

Also, the theoretical and experimental [18] concentrations of UHC for these engines are reported in Table 2. With the same reasoning as for CO, emission of UHC is higher in D.F.D.E. Here also some part of UHC emission is due to longer overlapping period of the D.F.D.E.

Table 2 compares some important pollutants emission parameters of both engines at full load and speed of maximum torque (1400 rpm). From Table 2, it can be seen that there are good agreements between experimental [18] and theoretical results of pollutants emission. But it must be remembered that, analyzer for measuring concentration of UHC, certainly had to be calibrated accurately.

CONCLUSIONS

A model of D.F.D.E has been developed from
an existing diesel engine model. Comparison with experimental results indicates that important exhaust pollutants parameters of the D.F.D.E at full load are being adequately modeled. Further refinement of the model appears justified in order to incorporate the part load condition and define a specified ignition delay period for D.F.D.E. operation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>D.F.D.E.</th>
<th>Diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Speed (RPM)</td>
<td>1400</td>
<td>1400</td>
</tr>
<tr>
<td>Air Fuel Ratio</td>
<td>21.7</td>
<td>17.5</td>
</tr>
<tr>
<td>CO (%Vol)</td>
<td>expt. 0.60</td>
<td>expt. 0.18</td>
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<tr>
<td></td>
<td>calc. 0.57</td>
<td>calc. 0.21</td>
</tr>
<tr>
<td>UHC (ppm)</td>
<td>expt. 15.0</td>
<td>expt. 3.0</td>
</tr>
<tr>
<td></td>
<td>calc. 235</td>
<td>calc. 141</td>
</tr>
<tr>
<td>NO (ppm)</td>
<td>expt. 2150</td>
<td>expt. 1067</td>
</tr>
<tr>
<td></td>
<td>calc. 1050</td>
<td>calc. 1250</td>
</tr>
<tr>
<td>soot (Bosch No.)</td>
<td>expt. 0.52</td>
<td>expt. 3.45</td>
</tr>
<tr>
<td></td>
<td>calc. 0.47</td>
<td>calc. 4.94</td>
</tr>
</tbody>
</table>

**ACKNOWLEDGMENTS**

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**NOMENCLATURE**

A \(\text{empirical constant}\)

a, b \(\text{empirical constants}\)

Cp, Cv \(\text{specific heat at constant pressure and constant volume}\)

d \(\text{residual fraction(\%)}\)

d_q \(\text{heat released rate}\)

d_q_{wall} \(\text{heat transfer rate}\)

H.R.R. \(\text{heat released rate}\)

J \(\text{Newton constant}\)

K \(\text{empirical constant}\)

LHV \(\text{lower heating value}\)

m \(\text{mass}\)

n \(\text{engine speed(rpm)}\)

N \(\text{number of moles}\)

P \(\text{pressure}\)

P' \(\text{calculated intermediate pressure in iteration method}\)

R \(\text{universal gas constant}\)

t \(\text{time}\)

T \(\text{temperature}\)

T' \(\text{calculated intermediate temperature in iteration method}\)

V \(\text{volume}\)

x \(\text{mass fraction}\)

**Greek letters**

\(\phi\) \(\text{equivalence ratio}\)

\(\theta\) \(\text{crank angle degree}\)

\(\Delta\) \(\text{period}\)

\(\gamma\) \(\text{ratio of } C_p / C_v\)

**Subscripts**

av \(\text{average of in-cylinder charge}\)

b \(\text{burnt}\)

B \(\text{burnt zone}\)

C \(\text{Carbon particle}\)

CO \(\text{Carbon monoxide}\)

comb \(\text{combustion}\)

dis \(\text{diesel combustion region}\)

d-f \(\text{dual-fuel}\)
REFERENCES


