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LAMINAR FLAME STRUCTURE AND HEAT RELEASE STUDY OF DIESEL FUEL

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ABSTRACT

A premixed diesel fuel-air laminar flame system propagating in a duct between parallel plates is modelled using the energy and mass species conservation equations. The chemical kinetics of the diesel fuel-air combustion is simulated by an Arrhenius reaction rate expression with overall order of 1.5. The flame structure and heat release rate as well as the various parameters characterizing the flame behavior are obtained at the stantard condition of atmospheric temperature and pressure, and stoichiometric mixture. The effect of high initial temperature and pressure, and lean mixture strengh on diesel flame structure, heat release rate and characteristic parameters is comprehensively investigated.

INTRODUCTION

Much of the work done in the area of laminar flame concerned itself with modelling an adiabatic one-dimensional laminar flame system,and devising various numerical techniques to tackle the resulting equations, e.g. references [1-3].

In contrast to the one-dimensional work, very few work was done in the area of multi-dimensional laminar flame propagation, e.g. von Karman and Millan [4] who studied the thermal behavior of the flame near a cold wall, Penner [5] in his flame stabilization investigation, and Aly et al [6] who provided a two-dimensional theory of laminar flame quenching.

Virtually no work was carried out to simulate and study the premixed laminar flame characteristics and reveal the internal structure of commercial fuels except that of Westbrook and Dryer [7], who provided a space one-dimensional numerical model to prodict the laminar flame proporties of methanol-air mixtures. Several factors may have contributed to such lack of work. These involve the requirement of two-dimensional formulation to model a flame system freely propagating between parallel plates or down

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a cylindrical tube and the difficulty involved in solving the resulting partial differential equations with their highly non-linear character and the eigenvalue feature of the laminar flame speed. In addition, there is a general lack of availability of Arrhenius global kinetic data which represent the oxidation of practical fuels.

The present work is concerned with providing a comprehensive study of the structure, heat release and characteristics of diesel fuel premixed laminar flame system propagating between parallel plates. This study involves the effect of burning diesel fuel under environmental and operating conditions comparable to those prevailing in many actual conditions.

GOVERNING EQUATIONS AND OUTLINE OF SOLUTION METHOD

Adopting a coordinate system travelling with the propagating laminar flame wave, the flame would be at rest relative to it, and the explosive mixture would be flowing by. Far upstream the mixture of diesel fuel and air is unburned, and appreaches the flame wave with the burning velocity (flame speed). Upon passing inside the flame region the mixture is heated and chemical reaction takes place between the fuel and oxygen in the mixture. The following global kinetic rate equation is used to simulate the oxidation of diesel fuel in air [8]

$$\frac{d[C_{16}H_{28}]}{dt} = - k\, p^{0.3}\, [O_2]\, [C_{16}H_{28}]^{0.5}\, T\, e^{-E/RT} \qquad (1)$$

where $[O_2]$ and $[C_{16}H_{28}]$ are the oxygen and diesel fuel concentrations, respectively, (mol per cm^3).

Neglecting the y component of the mixture velocity [9] the continuity equation yields the following relation

$$\rho u = G = \text{constant} \qquad (2)$$

Considering the usual approximation made in deflagration waves (laminar flame wave), namely $p \simeq$ constant, the system under study would be governed by the following energy and fuel mass species conservation equations

$$\lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - G c_p \frac{\partial T}{\partial x} = - H |w| \qquad (3)$$

$$G C_o \frac{\partial \bar{C}}{\partial x} = w \qquad (4)$$

Equation (4) ignores the diffusion of fuel species in accordance with the basic assumption of the thermal theory of laminar flame propagation. More details about the derivation of equations (3) and (4) and the underlying assumptions may be found in ref.[10].

6

The total heat release rate of the flame can be calculated using the following integral

$$THR = \int_0^L \int_{-\infty}^{\infty} | w(T,\bar{C}) | H \, dx \, dy \qquad (5)$$

The axial (x-direction) boundary conditions are of the Dirichlet type at the upstream boundary, namely, at $x=-\infty$, $T=T_o$ and $\bar{C}=1$, and of the Neumann type at the downstream boundary, namely, at $x=+\infty$, $\partial T/\partial x=0$ and $\partial \bar{C}/\partial x=0$. Regarding the boudary conditions in the transverse direction (y-direction), they reflect the symmetry of the duct centerline, namely, at $y=0$, $\partial T/\partial y=0$, and the fixed temperature at the wall, i.e. at $y=L/2$, $T=T_w$.

The solution method is based on linearizing the non-linear terms in the energy equation using Picard method [9]. The second and first derivatives are then discretized using central and upwind differencing, respectively. The resulting set of discretized equations are solved directly for the whole field to yield the first iterate of the temperature field. The concentration equation (4) is linearized relative to the concentration and solved by marching technique to obtain the first iterate of the concentration field. Iteration is then proceeded for the temperature and concentration equations until convergence is obtained. It is important to note that G in equation (2), which physically represents the mass flux burning rate, is not a priori known quantity, and is to be determined by the solution technique. This is done by tying G to the temperature and concentration fields as described in ref.[9].

Average values of c_p and λ are taken as 1.34 Kj/Kg K and 6.7×10^{-5} Kj/m K s, respectively. The activation energy, E, and heat of combustion, H, of diesel fuel are taken equal to [8], 114.723×10^{3} Kj/Kmol and 45.066 Mj/Kg, respectively. The pre-exponential factor k is adjusted so that the solution of flame equations yields a laminar flame speed equal to the experimentally measured value, about 0.4 m/s, for the stoichiometric mixture at atmospheric temperature and pressure. This value of k was found to be 0.6×10^{7} $cm^{3/2}/mol^{\frac{1}{2}}$ s $atm^{0.3}$ K. The wall temperature, T_w, is kept fixed at 300 K throughout the analysis.

RESULTS AND DISCUSSION

The solution of the governing equations outlined in the previous section along with their associated boundary conditions provide a complete picture of the characteristics, internal structure and heat release pattern of the diesel fuel-air premixed laminar flame for a certain set of initial (environmental) and operating conditions. The plate separation is fixed at 5 cm as commonly adopted in laminar flame experiments. The equations are first solved for normal environmental temperature and pressure equal to 300 K and 1 atm, respectively, and stoichiometric fuel air ratio, $\phi=1$. The flame structure and heat release results for this case, which will be referred to as the stantard case, are shown in Figs. (1) and (2).

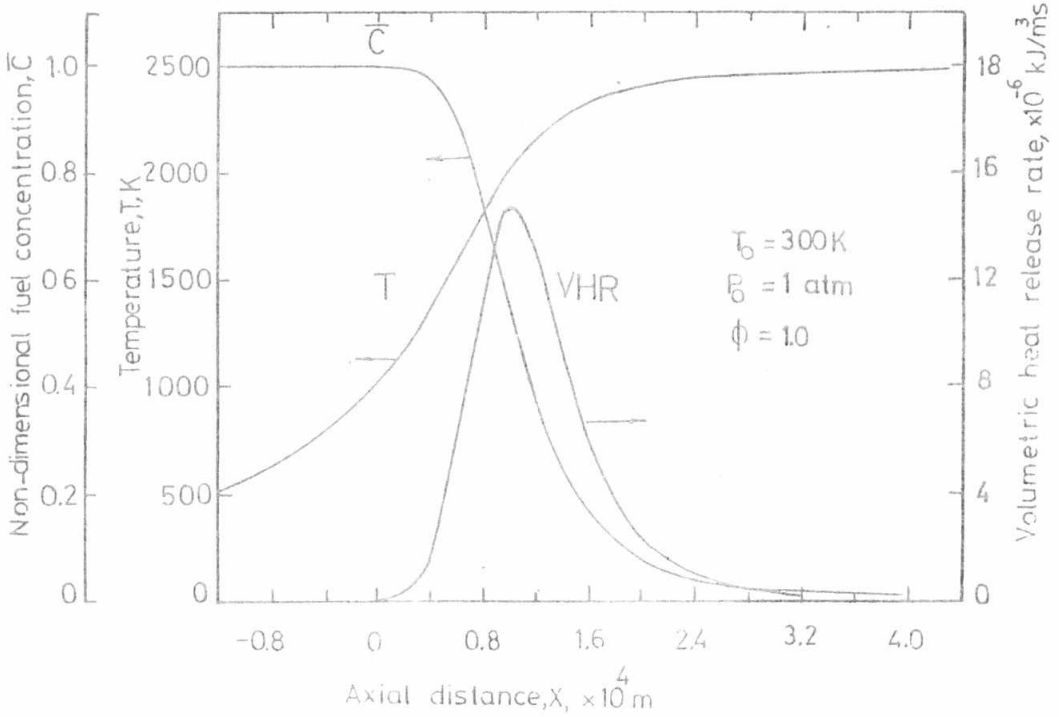

Fig.1. Axial Distribution of Temperature, Fuel Concentration and Volumetric Heat Release Rate

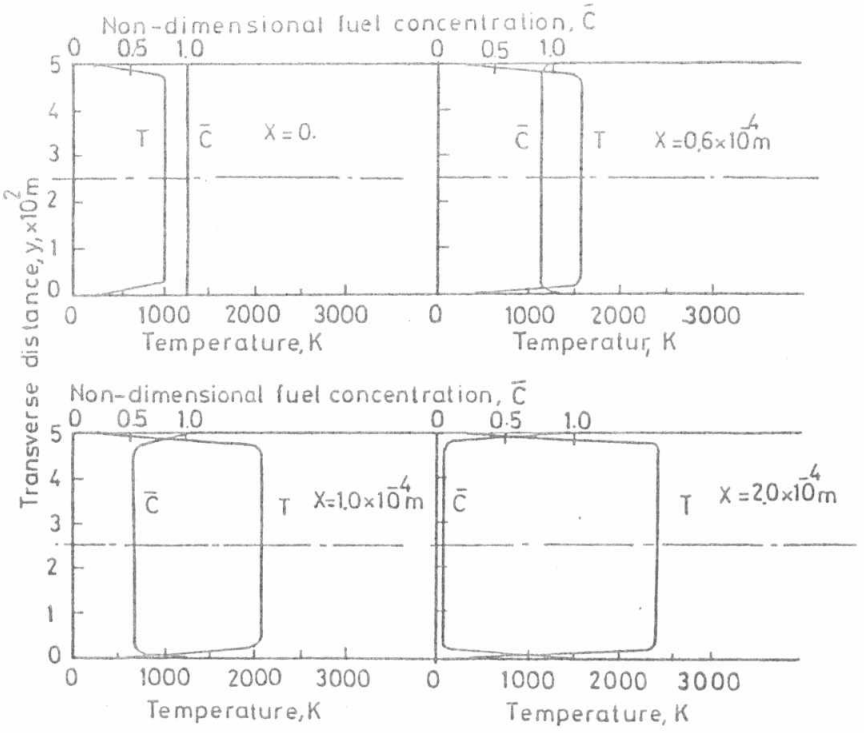

Fig.2. Transverse Distribution of Temperature and Fuel Concentration at Different Axial Locations

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The axial distribution of temperature, fuel concentration and volumetric heat release rate (VHR) are depicted in Fig.(1). It is to be noted that the VHR increases steeply up to its maximum value, which lies where only about 50% or less of the fuel is consumed. The temperature at this particular point is about 2000 K, which is about 80% of the maximum flame temperature. Beyond the point of maximum heat release, the temperature continues to increase, however, at a slower rate till it approaches its maximum value asymptotically.

It is important to note that the flame system of the present study is unattached, which physically corresponds to a system of premixed laminar flame freely propagating between parallel plates. Therefore, the flame is left free to locate itself anywhere along the axial distance in the integration domain. In the present study, the point of origin along the x-axis is selected to be where the first apparent consumption of fuel starts to occur, which physically coincides with the end of the preheat zone and the start of the reaction zone.

An important flame parameter which characterizes its behavior is the flame speed (burning velocity). It is to be recalled that the pre-exponential frequency factor was adjusted so that the solution of the flame equations yielded a flame speed equal to the experimental value of about 0.40 m/s under the same conditions. Another important parameter in laminar flame studies is the flame thickness. Although there is some level of arbitrariness in defining such parameter, as it is difficult to demarcate the flame end boundaries due to their asymptotic nature, it is usually defined in a way reflecting the extent of the reaction zone. In the present work, the flame thickness, δ, is defined as the distance along the duct centerline between the point at which the first apparent consumption of fuel occurs, the chosen origin of the x-axis, and the point where more than 95% of the fuel is depleted. This zone is basically the reaction zone where heat is released, more than 95% of the fuel is consumed and flame temperature approaches its maximum value. According to this definition, the flame thickness of diesel fuel flame at the aforementioned condition is calculated to be 0.26 mm. This small value of flame thickness explains why it has been difficult to carry out flame structure measurements under atmospheric conditions.

The temperature and fuel concentration distributions across the duct cross section are shown in Fig.(2) at different axial locations. All the shown profiles indicate clearly that the temperature and concentration profiles are uniform throughout most of the duct cross section at all the axial locations, and that the wall cooling effect is restricted to a very thin layer near the boundary. It follows that the bulk of the flame behaves essentially adiabatically. This explains why the laminar flame experiments in tubes or between parallel plates commonly adopted a dimension of 5 cm or more for the tube diameter or plate separation. It is to be noted that the transverse structure profiles will not be shown for the subsequent studied cases if they exhibit the same general distribution depicted in Fig.(2).

The effect of burning diesel fuel in a preheated mixture is shown in Fig.(3), where the axial distribution of flame temperature, fuel concentration and volumetric heat release rate are plotted for the case of preheated mixture temperature of 900 K. As shown in the figure, the maximum flame temperature increases to about 3090 K. It can also be noted that the point of maximum volumetric heat release rate inside the flame has the same position relative to the temperature and concentration fields as in the stantard case of Fig.(1). Its value has remarkably increased from 14.8×10^6 Kj/m^3 s, Fig.(1), to about 38.7×10^6 Kj/m^3 s, Fig.(3). The flame structure of the preheated mixture occupies almost the same axial spatial extension as the flame shown in Fig.(1), indicating that preheating the diesel fuel-air mixture has no effect on the thickness of the reaction zone. The numerical solution for this case yielded a flame speed equal to 2.69 m/s, which is considerably higher than the 0.4 m/s at 300 K.

In order to shed more light on the effect of initial temperature on diesel fuel flame, solutions of the flame equations were obtained for different T_o. The variation of the various parameters characterizing the flame behavior with T_o is shown in Figs.(4) and (5). As indicated in Fig.(4) the burning velocity and maximum flame temperature increase pronouncedly with T_o, and the variation of the latter is linear. Also, the maximum volumetric heat release rate shows a remarkable increase with T_o, so does the total heat release rate, which follows a trend very similar to that of maximum volumetric heat release rate. Regarding the flame thickness, it shows no variation with the initial mixture temperature.

To investigate the diesel flame structure and heat release at high environmental pressure, the solution of the flame equations was obtained for a value of pressure equal to 60 atm, with T_o and ϕ equal to 300 K and 1, respectively. Figure (6) depicts the axial distribution of flame structure at this high pressure. There is a striking increase in the maximum value of the volumetric heat release rate, which reaches a value of 18.4×10^9 Kj/m^3 s. Another pronounced feature of this flame is its thinness, as its thickness takes on the value of 0.007 mm, which is very small compared to the atmospheric flame. The figure also indicates that increasing the pressure does not affect the maximum flame temperature. The burning velocity (flame speed) at this pressure is calculated to be 0.24 m/s, which is much less than the atmospheric flame speed.

The variation of flame characteristics with pressure in the wide pressure range from 1 to 60 atm is shown in Figs.(7) and (8). The burning velocity is monotonically decreasing with pressure, and such decrease occurs at a rather high rate in the range from 1 to 10 atm. It is intriguing to note that despite the decrease in burning velocity the mass flux burning rate increases steeply with pressure. This is due to the increase in density which more than compensate the effect of decrease of burning velocity. The peak flame temperature shows no variation with pressure as illustrated in Fig.(7).

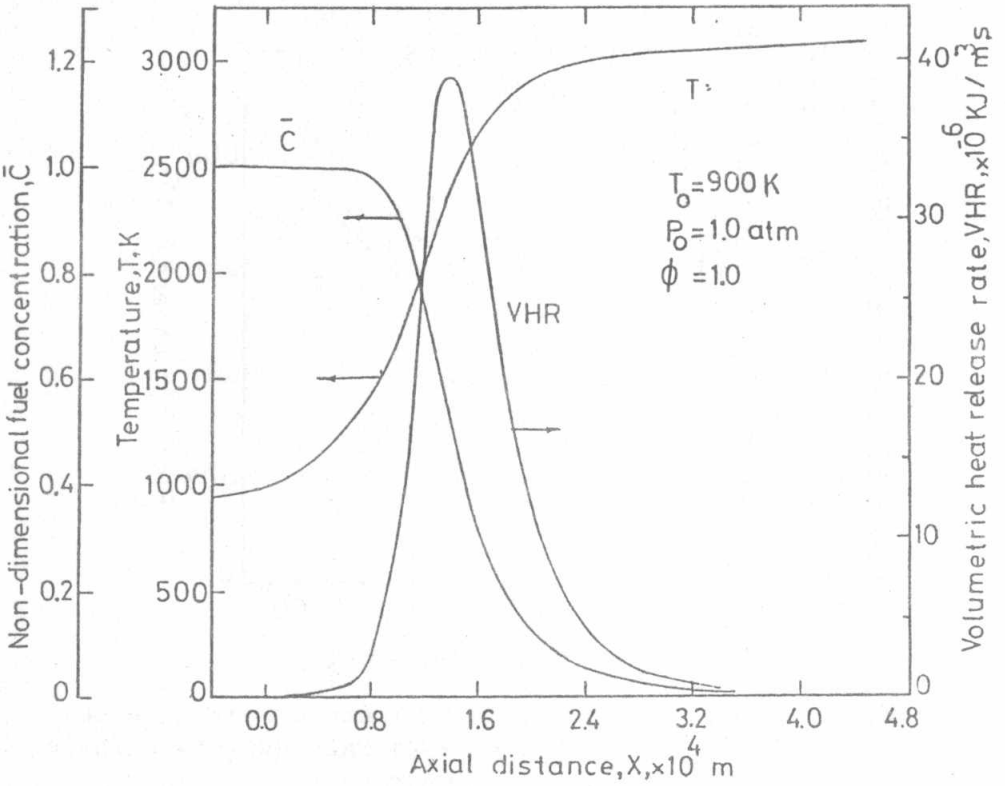

Fig.3. Axial Distribution of Temperature, Fuel Concentration and Volumetric Heat Release Rate at High Initial Temperature

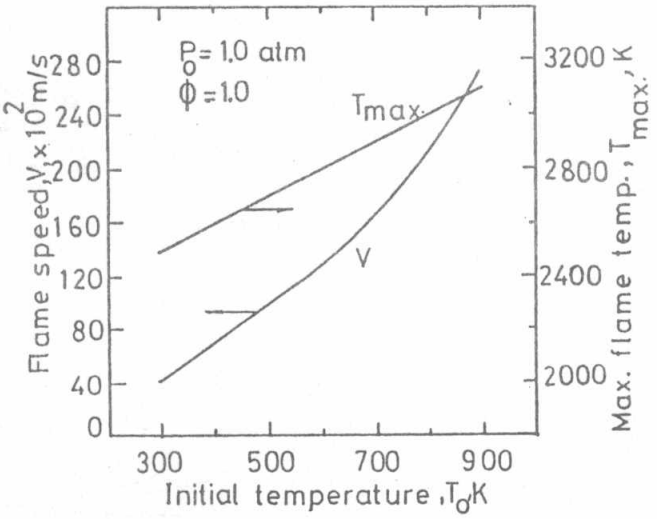

Fig.4. Variation of Flame Speed and Maximum Temperature with Initial Temperature

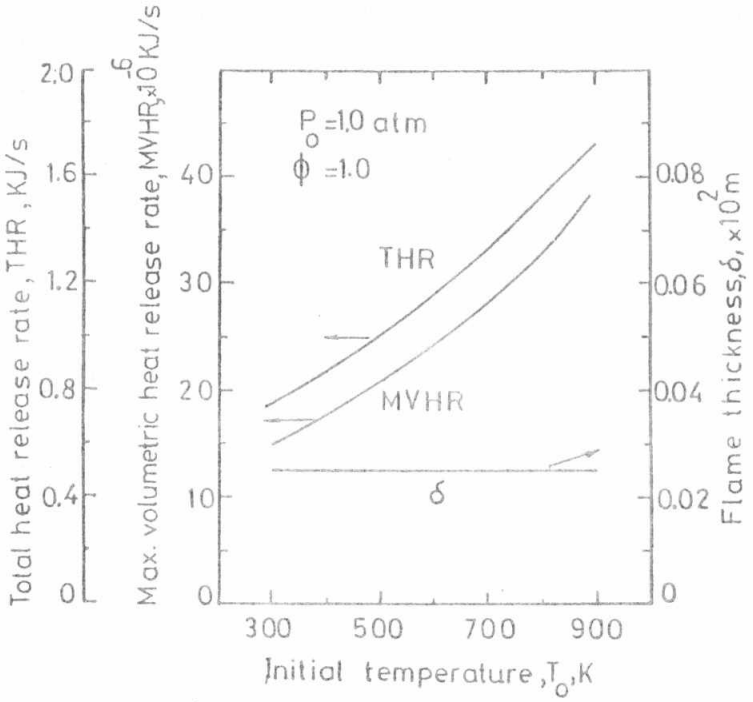

Fig.5. Variation of Maxium Volumetric Heat Release Rate, Total Heat Release Rate and Flame Thickness with Initial Temperature

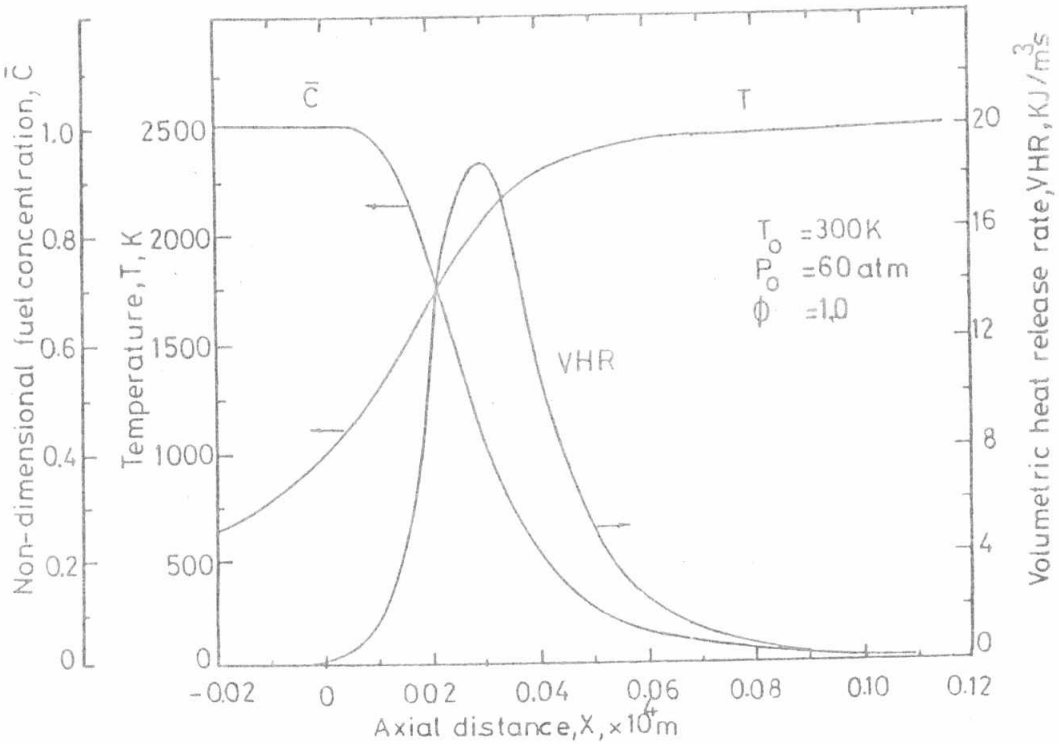

Fig.6. Axial Distribution of Temperature, Fuel Concentration and Volumetric Heat Release Rate at High Initial Pressure

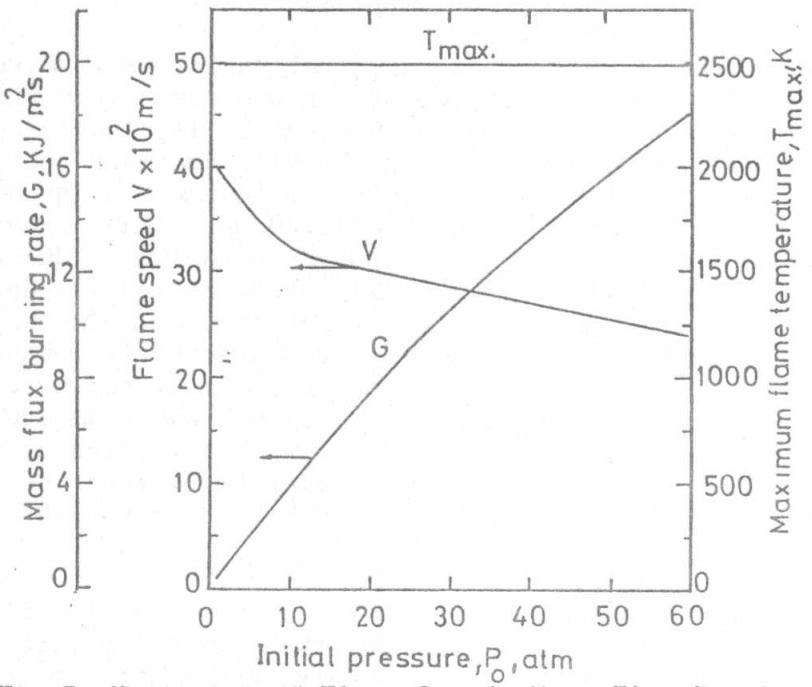

Fig.7. Variation of Flame Speed, Mass Flux Burning Rate and Maximum Temperature with Initial Pressure

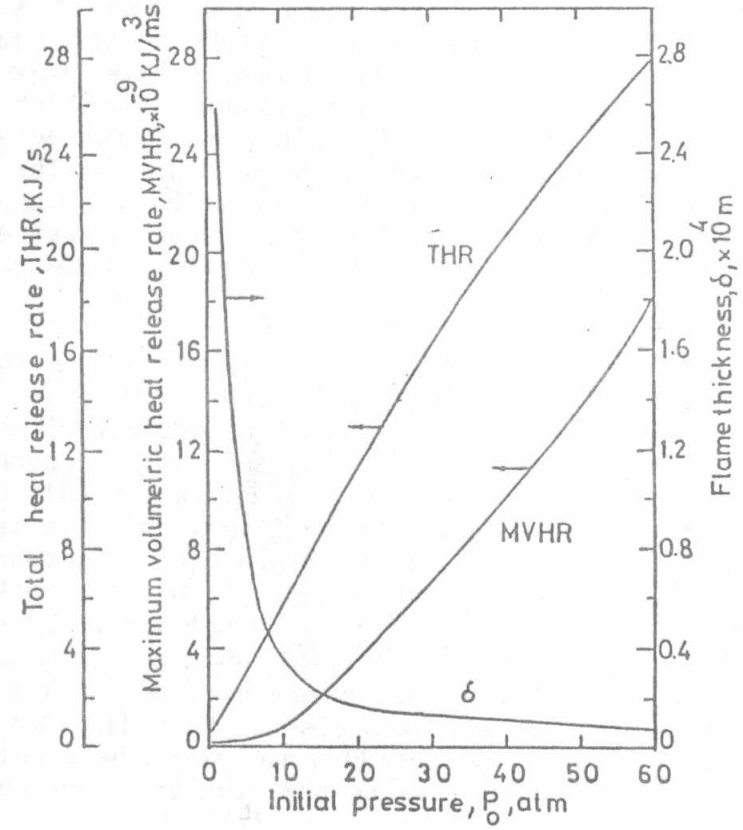

Fig.8. Variation of Maximum Volumetric and Total Heat Release Rates, and Flame Thickness with Initial Pressure

Figure (8) exhibits the variation of flame thickness, maximum volumetric and total heat release rates with pressure in the same range from 1 to 60 atm. The decrease in flame thickness with pressure is clearly seen, but the intriguing feature of such curve is the huge decrease that occurs in flame thickness when the pressure increases to 10 atm as compared to the decrease occuring in the interval from 10 to 60 atm, which means that the flame thickness is very sensitive to pressure up to 10 atm. Beyond this value the decrease in thickness takes place at a continually decreasing rate until the curve tends to flatten out beyond 50 atm. The variation of maximum volumetric heat release rate with pressure is also shown in Fig.(8). It shows a trend opposite to that of flame thickness since it increases with pressure at a rather small rate up to 10 atm, and a very high rate beyond that. The total heat release rate exhibits a tremendous increase with pressure, as shown in Fig.(8). The similarity between the mass flux burning rate in Fig.(7) and total heat release rate in Fig.(8) clearly indicates their direct proportionality.

An important operating parameter which has a great effect on flame behavior is the fuel air ratio. Figure (9) provides the flame structure and heat release pattern for the diesel flame at equivalence ratio, ϕ, equal to 0.9. Since the mixture in this case is a weak mixture, it can be expected that the produced flame would be a weak one, in the thermal sense. This is indicated in Fig.(9) where the maximum flame temperature is about 2150 K, which is considerably less than the stoichiometric maximum temperature. The volumetric heat release rate pattern has a peak value of about 6.1×10^6 Kj/m^3 s, which is once more much less than the peak exhibited by the stoichiometric flame, $14{,}6 \times 10^6$ Kj/m^3 s. The total heat release rate declines remarkably at $\phi=0.9$ to a value of 0.422 Kj/s compared to 0.766 Kj/s for the flame at $\phi=1$. The flame structure shown in Fig.(9) reflects a thicker flame compared to the stoichiometric one shown in Fig.(1). The flame thickness is calculated in this case to be 0.32 mm. Concerning the effect of ϕ on flame speed, the results of the solution show a great effect of ϕ on it, as this decreases to 0.24 m/s at $\phi=0.9$ compared to about 0.40 m/s at $\phi=1$.

Recalling the results presented so far, it is clear that the various initial and operating conditions affect the diesel flame in a conflicting manner. Thus, it is thought useful to assess the combined effects of these conditions on the flame, as diesel fuel may practically be burned under high initial temperature and pressure and lean mixture condition. The solution of the flame equations gives a flame speed for this case equal to 1.63 m/s. The axial profiles of flame temperature, fuel concentration, and volumetric heat release rate is shown in Fig.(10). The peak temperature reaches 3090 K, and the maximum volumetric heat release rate is about 47×10^9 Kj/m^3 s. Both figures are remarkably higher than their corresponding values at the atmospheric pressure and temperature, and stoichiometric mixture. The flame thickness experiences also a sharp diminution as its value is calculated to be 0.008 mm. Finally, the total heat release rate for this flame increases much relative to the stantard flame as its value reaches 62.7 Kj/s.

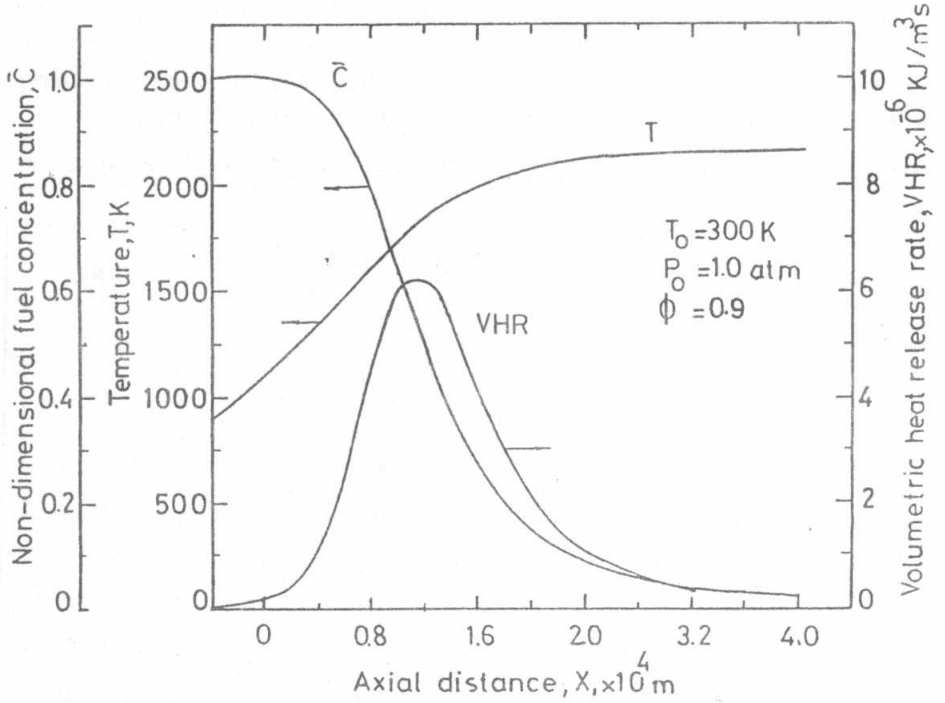

Fig.9. Axial Distribution of Temperature, Fuel Concentration and Volumetric Heat Release Rate at Equivalence Ratio Equal 0.9

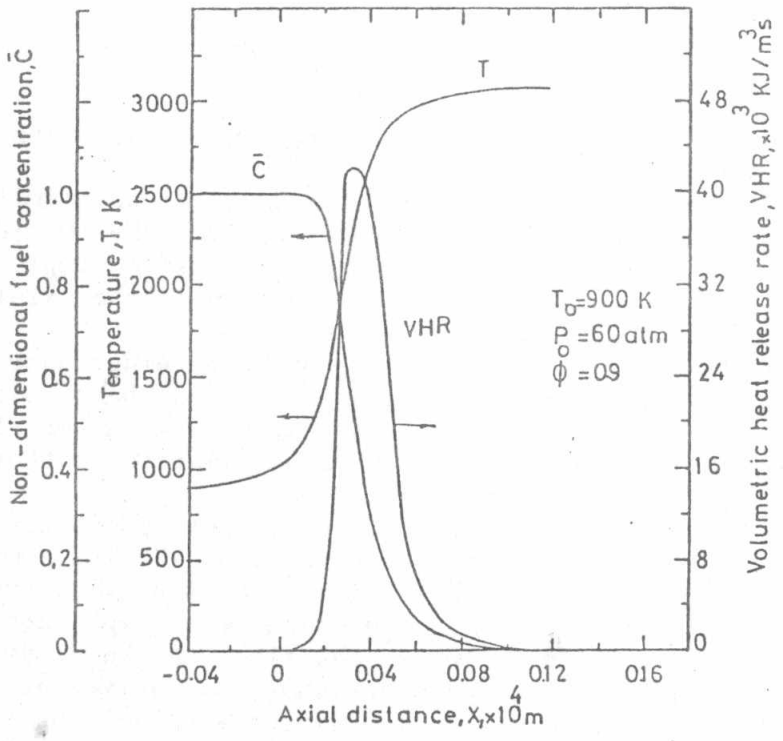

Fig.10. Axial Distribution of Temperature, Fuel Concentration and Volumetric Heat Release Rate for Lean Diesel Fuel-Air Flame at High Initial Temperature and Pressure

The following table summarizes the values of the various parameters characterizing the diesel flame at the various studied conditions.

Table 1 Diesel flame characteristics at different conditions

Condition T_o K, p_o atm, ϕ	300, 1, 1	900, 1, 1	300, 60, 1	300, 1, 0.9	900, 60, 0.9
V m/s	0.398	2.69	0.24	0.24	1.63
G Kg/m^2 s	0.497	1.12	18.15	0.303	40.7
T_{max} K	2490	3090	2490	2150	3090
δ mm	0.26	0.26	0.007	0.32	0.008
MVHR Kj/m^3 s	14.9×10^6	38.7×10^6	18.5×10^9	6.1×10^6	47×10^9
THR Kj/s	0.766	1.726	27.98	0.422	62.7

CONCLUSIONS

The following conclusions can be drawn in light of the results presented in the previous sections.

1. The numerical solution of the laminar flame equations modelling the burning of premixed diesel fuel-air mixture provides the burning velocity (flame speed) of the resulting propagating flame, and a complete picture of the internal structure and heat release pattern in the axial and transverse directions of the duct.
2. Preheating the diesel fuel-air mixture before burning causes an increase in burning velocity, peak flame temperature and total heat release rate. The flame thickness remains, however, unaffected. The volumetric heat release rate profile shows a higher peak value relative to that of a flame without preheating.
3. Burning diesel fuel in pressurized medium affects pronouncedly the resulting flame. The volumetric heat release rate exhibits a much higher peak value compared to the atmospheric flame. The mass flux burning rate and total heat release rate increase tremendously at high burning pressure. On the other hand, the burning velocity and flame thickness decrease at high pressure. The peak flame temperature shows no variation.
4. Decreasing the equivalence ratio to 0.9 decreases all the parameters characterizing the diesel laminar flame behavior except the flame thickness, which increases in response to the decrease in equivalence ratio.

5. Burning diesel fuel under the combined effects of initial and operating conditions, more or less, similar to practical ones, produced a much thinner flame relative to stoichiometric and atmospheric flame, but faster one with higher peak temperature and maximum volumetric and total heat release rates.

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NOMENCLATURE

C	mass of fuel per unit mass of mixture
C_o	mass of fuel in unburned mixture per unit mass of that mixture
$\bar{C}$	non-dimensional fuel concentration, C/C_c
c_p	average specific heat of mixture at constant pressure, Kj/Kg K
E	activation energy, Kj/Kmol
G	mass flux burning rate (eigenvalue of flame equations), $Kg/m^2 s$
H	heat of combustion of fuel, Kj/Kg fuel
k	pre-exponential frequency factor, $cm^{3/2}/mol^{\frac{1}{2}}\ atm^{0.3}\ K\ s$
L	distance separating the parallel plates, m
p	pressure, atm
R	universal gas constant, 8.313 Kj/Kmol K
T	temperature, K
t	time, s
u	x-component of mixture velocity, m/s
V	flame speed (burning velocity), m/s
w	rate of consumption of fuel per unit volume and time, $Kg/m^3 s$
x	axial coordinate system
y	transverse coordinate system

δ flame thickness, m
λ average thermal conductivity of mixture, Kj/m s K
ρ mixture density, Kg/m^3
ϕ equivalence ratio

Subscripts

o upstream boundary (environmental or initial condition)

Abbreviations

MVHR maximum volumetric heat release rate, Kj/m^3 s
THR total heat release rate, Kj/s