Modelling of Droplet Combustion and Formation of Nitric Oxide

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Abstract

In the present work, an unsteady, spherically symmetric, diffusion controlled droplet combustion model is developed and analyzed by solving partial differential equations of heat and mass transfer, numerically, to get temperature, oxidizer mass fraction and fuel mass fraction profiles. The model is subjected to variation in initial droplet diameters, type of fuels, ambient pressures and temperatures and ambient oxidizer concentrations. It is observed that the above parameters significantly affect the combustion characteristics like flame temperature, flame radius and instantaneous flame to droplet radius ratio. For nitric oxide concentration estimation, the Olikara and Borman procedure (modified for single droplet combustion) is followed. Results indicate that No concentration increases with an increase in temperature, pressure and ambient oxidizer concentration.

Nomenclature

D_o, r_{1O}	Original or initial droplet diameter and radius respectively.
D, F	Instantaneous droplet and flame diameters respectively.
R_f, r_f, r_F	Instantaneous flame radius.
T	Temperature at instantaneous time (t) at a radial distance (r) from the droplet centre.
t/t_1	Non-dimensional time.
r/r_f, R/R_f	Non-dimensional radius.
λ_1	A variable defined as mesh ratio = k/h^2 where h and k are mesh sizes in radial and time directions respectively.

Subscripts:

B	Boiling
F, f	Flame
L	Liquid
∞	Ambient atmosphere.

Introduction

The varied applications of spray combustion in Diesel engines, industrial furnaces, gas turbines, rocket engines etc. have lead to numerous studies on both spray combustion and associated processes such as droplet evaporation and combustion. Objectives have been to establish design criteria for efficient and stable combustorsand to examine the formation and destruction of pollutants such as soot, unburned hydrocarbons, NO. However, combustion of spray is a complex process which involves simultaneous heat, mass and momentum transfer together with chemical reaction. The chief factors affecting the combustion of spray droplets are (i) dropsize (ii) composition of fuel, (iii) ambient gas composition, its pressure and temperature etc., and hence it is difficult to obtain detailed and accurate information by direct studies on spray combustion. Therefore, it is felt that the most essential prerequisite is to have a thorough knowledge

of the mechanism of single droplet evaporation and combustion at elevated pressures and temperatures since it serves as a fundamental step for understanding the nature of supercritical combustion in actual combustors of Diesel engines, rocket engines etc. [1].

The mathematical model

The transient droplet combustion model as shown in Fig. 1, developed for the present study is based on the following major assumptions: [1] the fuel is a pure liquid having a definite boiling point and droplet surface temperature is equal to its boiling point temperature, [2] the system is spherically symmetric, [3] the fuel and oxidizer diffuse from droplet surface and ambient atmosphere in opposite directions to react instantaneously at the flame front in stoichiometric proportions at the adiabatic flame temperature, [4] lewis number is unity, (5) the thermophysical properties are calculated at an average temperature of $(T_F + T_n)$, and [6] radiation effects are neglected. With these assumptions, the heat and mass transfer outside the flame is expressed by the following linear, second order partial differential equations with variable coefficients [2]

$$\alpha \frac{\partial^2 T}{\partial r^2} + \frac{2\alpha}{r} \frac{\partial T}{\partial r} = \frac{\partial T}{\partial t} \quad \cdots \quad (1)$$

$$K_d \frac{\partial^2 Y}{\partial r^2} + \frac{2K_d}{r} \frac{\partial Y}{\partial r} = \frac{\partial Y}{\partial t} \quad \cdots \quad (2)$$

where T and Y are the temperature and oxidizer concentrations respectively at a distance 'r' from the droplet center at time 't', α is the thermal diffusivity and k_d is the binary diffusion coefficient. The boundary conditions based on this combustion model are as follows:

at $r = r_f$; $T = T_F$, $Y_o = 0$

at $r = r_\infty$; $T = T_\infty$, $Y_o = Y_{o,\infty} = 0.232$

at $t = 0$; $r = r_{LO}$, $T = T_B$, $Y_F = 1.0$

where $r_L = r_{Lo} (1 - t/t_1)^{1/2}$ for $(0 \le t \le t_1)$

here Y_F and Y_o are fuel and oxidizer mass fractions respectively, $Y_{o/\infty}$ is the oxidizer concentration in ambience, t is the instantaneous time (sec), t_1 is the droplet combustion lifetime (sec), r_{LO} is the original or the initial droplet radius, r_L is the instantaneous droplet radius at time 't'. The above equations were solved by using finite difference technique utilizing two level explicit schemes which are stable for $\lambda_1 < \frac{1}{2}$. The temperature profile and fuel and oxidizer concentration profiles around a spherically symmetric burning droplet are shown in Fig. 1. The location were the maximum temperature $T = T_F$ or the corresponding oxidizer concentration $Y_o = 0$ and $Y_F = 0$ occurs, was taken as the flame radius. Instantaneous time 't' was obtained from the computer results whereas 't_1' was got by the relationship coming out from the d^2 - law. Other parameters like instantaneous flame to droplet diameter ratio F/D were then calculated as a function of time. NO concentrations were estimated with the help of a computer programme based on the lines of Olikara and Borman [3] to solve for the mole fraction x_i of NO under specified conditions of temperature T, pressure P and equivalence ratio ϕ.
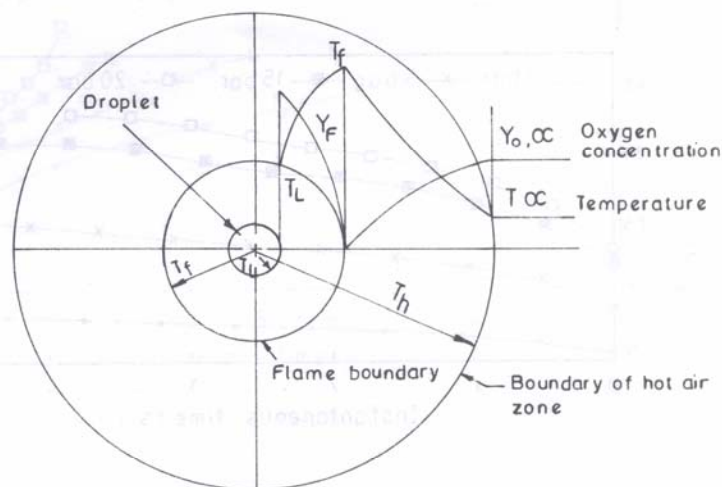
Fig. 1. Droplet combustion model

Results and discussion

Our results indicate that the fuel vapour and oxidizer concentration minima coincides with the temperature maxima due to the combustion reaction, the temperature increases with radius from the droplet surface where it is assumed equal to the boiling temperature of the fuel, becomes maximum at the flame and then decreases gradually to the ambient value of T_∞. The results indicate that the flame first moves away from the droplet surface and then towards it which suggests that the instantaneous flame to droplet diameter ratio F/D is continuously increasing with time. This behaviour is in good agreement with Waldman [4], under similar conditions, but is in contradiction with the quasisteady theory which predicts a large constant value of F/D ratio during droplet burning. Other conditions remaining same (T_∞ = 298 K, $Y_{o, \infty}$ = 0.232), as the ambient pressure p_∞ is increased to a value little less than the fuel's critical pressure, (for reduced pressure p_r = 0.91), for a 2000 micron n-heptane droplet, the adiabatic flame temperature is not affected much showing only a slight increase, but on the other hand the ratio (r_F/r_L) increases with time 't', Fig. 2. The present result is not in agreement with that of Kotake and Okazaki (5) who have numerically investigated the spherically symmetric combustion of a methanol droplet (D_o = 2000 microns), treating it as an unsteady diffusion controlled phenomenon. Their results suggest that (r_F/r_L) ratio decreases with an increase in p_∞, but a meaningful comparison cannot be made since these authors have not included the real gas effects at high ambient pressures in their model [4] and also the fuel used in both the studies are different (which may lead to difference in thermophysical properties and their subsequent effect on burning parameters like K_b, t_1, r_F etc). On the other hand in the present work once the boiling point temperature, adiabatic flame temperature [6], binary diffusion coefficient, combustion lifetime, burning constant etc. were evaluated at high pressure conditions using appropriate equations [7], they were used as input data in a computer programme to obtain the values of flame radius r_F at different times of droplet burning. The ratio r_F/r_L or F/D was then plotted against dimensionless time at increasing pressures.
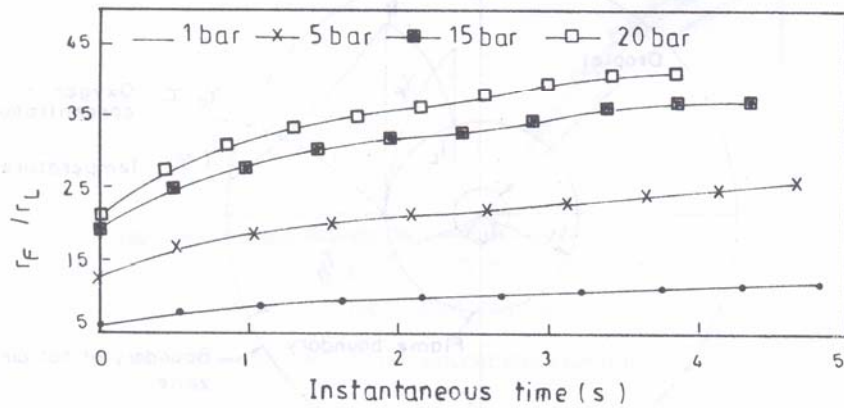
Fig. 2. Effect of ambient pressure on the variation of flame to droplet radius ratio with instantaneous
     Time

As the ambient temperature (T_∞) is varied from 100^0C to 700^0C, for $p_\infty = 1$ bar, and other conditions remaining same, it is observed that an increase in the ambient temperature leads to an increase in the corresponding adiabatic flame temperature values; the ratio (r_F /r_L) increases with instantaneous time 't'. Fig. 3, for an increase in the ambient temperature values. Our results show the same trend as reported by Kotake and Okazaki. An increase in the ambient oxygen concentration $Y_{o,\infty}$ from 11.6% to 46.4%, for $p_\infty = 1$ bar, $T_\infty = 298$K and for the same fuel and droplet size (2000) microns, results in the corresponding increase, in adiabatic flame temperatures; the ratio (r_F/r_L) increases with ambient oxidizer concentration increment. Fig. 4; our results are in fairly good agreement with those of Kotake and Okazake.
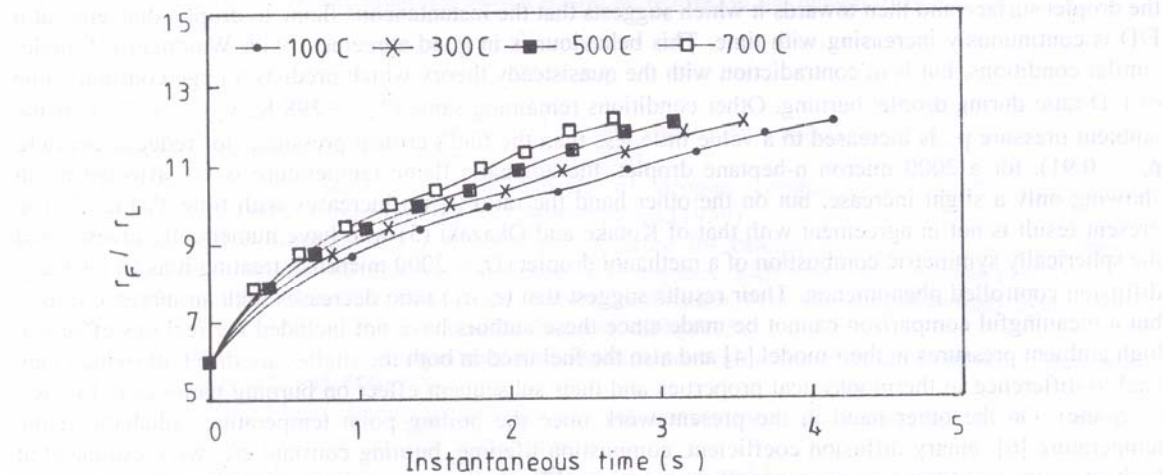

Fig. 3. Effect of ambient temperature on the variation of flame to droplet radius ratio with
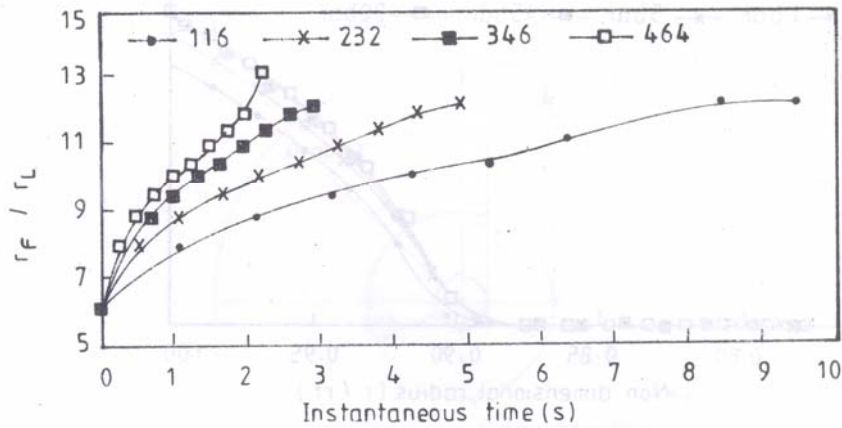   instantaneous time

Fig. 4. Effect of ambient oxidizer concentration on the variation of flame to droplet radius ratio with time

The temperature profile and the fuel concentration profile obtained earlier is then used to obtain the concentrations of NO using Olikara and Borman programme. As far as NO formation is concerned, it is generally by the extended Zeldovich mechanism,

$$O + N_2 \leftrightarrows NO + N$$
$$N + O_2 \leftrightarrows NO + O$$
$$N + OH \leftrightarrows NO + H$$
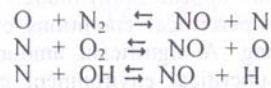
The rate of NO formation is strongly dependent on temperature. It is observed that NO formation peaks rapidly near the maximum temperature. Increasing the ambient temperature, Fig. 5, increases the flame temperature which increases the rate of formation of NO. Pressure also has a direct effect on reaction rates as well as an indirect one associated with the slight increase in flame temperature, Fig. 6. Similar behaviour for NO concentration variation has been reported by Bracco [8] considering ethanol drops burning in air.
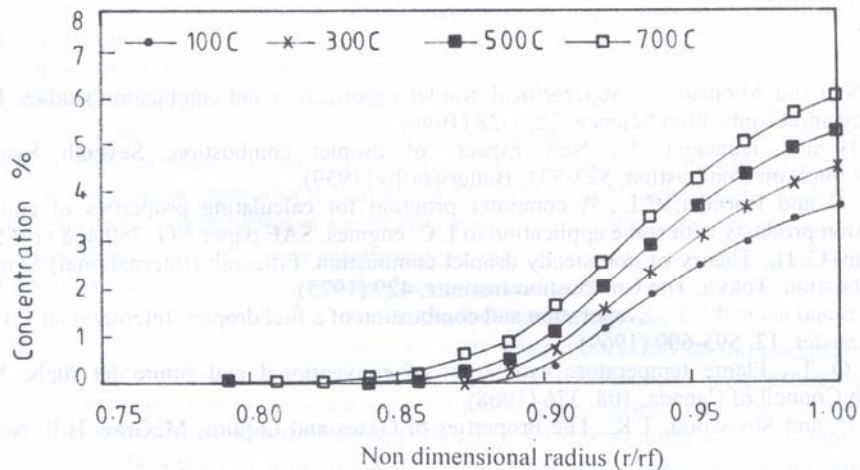

Fig. 5. Effect of ambient temperature on no concentration for n-heptane (t/T1 = 0.66)
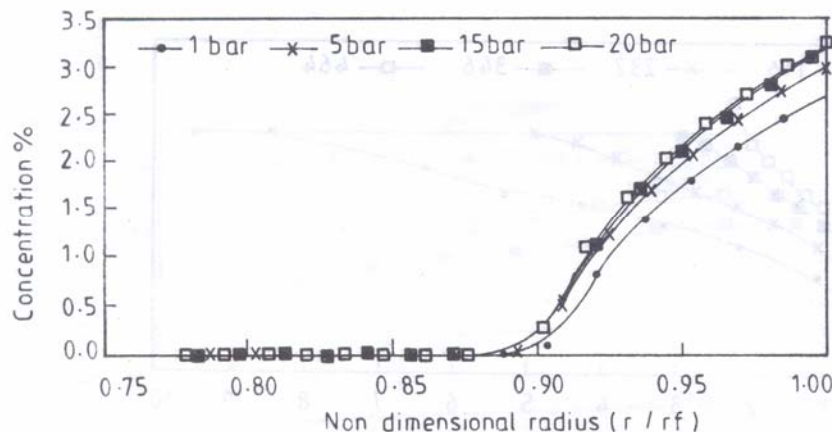
Fig. 6. Effect of ambient pressure on no concentration for n-heptane (t/T1 = 0.66)

Conclusion

Theoretical investigations by various authors have pointed that at sufficiently high ambient pressures, a fuel droplet can exceed its critical point during combustion. Under these conditions, the quasisteady combustion theories, employed with reasonable success at moderate pressures, can no longer accurately represent the droplet combustion process and a new burning regime must appear. Spray models currently in use normally do not include any special treatment of critical or supercritical conditions even though supercritical vaporization and combustion are likely to be occuring. A significant amount of research has been performed in understanding these processes under subcritical environment conditions; however, the common assumptions of gas phase quasisteadyness and ideal gas behavour that are employed in subcritical models become less valid as the ambient pressure increases, keeping this in mind the present model incorporates the real gas effect, making it more realistic. The results of the present study are compared with the existing numerical/experimental results under nearly identical conditions and appear to be in fairly good agreement. The present work can be further extended to the case of critical and subsequently supercritical droplet combustion and emission situations which would be helpful in the design of combustion chambers for optimum performance.

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