Ignition of a Cloud of Droplets

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ABSTRACT

The sprays in gas turbines play a significant role in both the design and performance of the combustors. Most of the earlier spray combustion models are based on the premise that individual drop combustion occurs. Recent experiments on spray combustion reveal that a common flame exists around a large number of droplets (group combustion) in the vicinity of the injector while far down stream individual drop combustion occurs. Compared to the results predicted for individual drop combustion, the group combustion modeling results in a) lower ignition temperature, b) lesser burning rate and c) more soot formation. An unified approach is given here for modeling both the ignition and combustion of a cloud of droplets.

The quasi-steady ignition problem of a cloud of droplets is analyzed for spherically symmetric conditions. Chemical reaction is accounted for regions both within and outside the cloud. Quasi-steady conservation equations for a cloud of droplets are reduced to a simple form by using a modified version of Schwab-Zeldovich formulation. A general analysis is presented so that pure evaporation and diffusion controlled combustion can be considered in addition to the ignition of a cloud of droplets. For a few simple cases, an algebraic relation for the burning rate of a chemically reacting cloud of droplets is given in a form analogous to the result for a droplet. For complex cases, a numerical method is used for obtaining the results. A computer program has been developed to determine the pure evaporation rate, diffusion controlled burning rate and the rate of burning with chemical reaction for a cloud of droplets having non-uniform size and number density inside the cloud. Results are generated for the ignition temperatures. Parametric results showing the effects of oxygen mass fraction and cloud radius are also presented. Ignition is found to start in the region outside the cloud for a range of group combustion numbers studied. Under quiescent conditions, the ignition temperature of a cloud of droplets is deduced to be significantly lower than that for a single droplet.

NOMENCLATURE

\(A\) preexponential factor
\(a\) radius coordinate for a single droplet
\(b\) radius of liquid droplet
\(I\) transfer number for combustion of a single droplet
\(T\) transfer number
\(V\) specific heat
\(D\) diffusion coefficient
\(G\) activation energy
group combustion number, (eq. 16d)

\(h_T\) thermal enthalpy
\(h_c\) heating value per kg of fuel
\(L\) Latent heat
\(n\) nondimensional burning rate (eq. 16j)
\(\dot{m}_p\) mass flow rate
\(p\) vapor production rate per unit volume
\(\dot{m}_c\) vapor consumption rate per volume
\(\dot{m}_n\) mass flow rate at the cloud periphery
\(\dot{n}_d\) Nusselt number based on radius of droplet
\(\dot{n}_p\) order of reaction with respect to fuel and oxidizer
\(\dot{q}\) heat generation rate per unit area
\(\dot{q}_t\) heat loss rate per unit area
\(s_{15}\) universal gas constant
\(S_{21}\) cloud radius (Fig. 1)
\(\chi\) radius (Fig. 1)
\(S_{21}\) eqs. (23c), (23d) and (24c)
\(T\) temperature
\(\dot{V}_P\) mass fraction
\(\dot{V}_T\) eq. (12b)
\(\dot{V}_M\) Schwab-Zeldovich variable
\(Y\) eqs. (21b) and (22b)
eqs. 16
\(c\) stoichiometric mass of oxygen density
\(c_0\) fuel volume fraction, eq. (16c)
\(c_{ref}\) reference density evaluated at reference temperature
\(\phi\) nondimensional coupling function

\(c\) critical
\(c_{f,c}\) fuel chemically consumed
\(F\) fuel
\(a\) flame
\(G\) group of droplets
\(B\) generation
\(L_k\) liquid
\(O_2\) oxygen
\(P\) fuel vapor produced

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The design of the combustors for gas turbines and steam power plants must be optimized towards achieving high combustion efficiency and low pollutant emissions at widely varying loads. The sprays play a major role in both the design and performance of combustors. Therefore considerable research has been carried out in the past few decades on modelling the combustion of sprays. The spray combustion models are based on the premise that individual drop combustion occurs. However recent experimental research on spray combustion reveal that a sheath flame exists around the boundary of the spray core in the vicinity of the spray injector, while individual drop combustion occurs for downstream of the injector. Thus there exists a common flame around a group of droplets (group combustion) rather than a flame around each droplet (drop combustion). The group combustion model of a cloud of droplets yields a very low burning rate compared to the rate predicted with the single drop combustion model; further the group combustion leads to increased volume of fuel rich zone which promotes soot formation. On the other hand fuel rich conditions may reduce NO\(_x\) formation. The ignition temperature under group ignition model is expected to yield a lower value compared to the ignition temperature predicted with the single drop ignition model. Thus the ignition temperature, combustion rate and the pollutants depend upon whether group combustion or individual drop combustion occurs for the droplets in the sprays. The spray conditions in gas turbines as existing in the vicinity of the injector are conducive to the occurrence of group ignition and combustion. Hence group ignition and group combustion models are appropriate for modeling the spray in gas turbines and as well as to interpret the experimental data on combustion behavior in gas turbines. Group ignition and combustion are more likely for fuel sprays in diesel engines since, relative to the gas turbine combustors, the sprays are more dense. The reduced group ignition temperature is expected to reduce the required compression ratio for the self ignition of the spray. The present research carried out in two parts deals with the group ignition (part I) and group combustion (part II) of a cloud of droplets. Further discussions in the present paper pertain to group ignition (part I).

Extensive research has been carried out in the recent decades on the ignition and combustion of a single drop of fuel. An excellent review of the status of ignition and combustion of liquid droplets is available in ref. [1]. The results from the combustion of single drops could be readily applied to an industrial burner if the spray produced by the atomizer is dilute enough that only weak interaction occurs between the droplets [2]. If the interdroplet spacing is less than about 7000 times the diameter of the droplet, then the interaction between the droplets leads to a reduction in evaporation/burning rate [3, 4]. If the spacing between the droplets is further reduced, then oxygen is effectively blocked from reaching the individual droplets inside a cloud of droplets due to blowing effects. The diffusion controlled group combustion problem has been analyzed previously by Labowsky and Rosner [3] and Chiu and Liu [5]. Chiu and Liu defined group combustion number G as

\[
G = 3 \times (\text{Fuel Volume Fraction}) \left( \frac{\text{cloud radius}}{\text{droplet radius}} \right)^2
\]

[The G number of Chiu and Liu is same as the square of Thiele Modulus defined by Labowsky and Rosner in quiescent atmosphere. The G number represents a ratio of blowing velocity of fuel vapor to gas diffusion velocity of \(O_2\). If G number exceeds a critical value \(G_c\), then the flame stands outside the cloud and if \(G < G_c\), then there is burning of individual droplets inside the cloud. Chigier and McGrath [6] observed a sheath flame around the outer periphery of a spray essentially validating the group combustion theory. Further if the diameter of a droplet is very small, establishment of the gas phase flame around the droplet may not be possible [7], which again may lead to group combustion.

Corsi and Sichel [8] analyzed the problem of nonsteady vaporization of a cloud of droplets of monodisperse droplets and obtained results for vaporization wave velocity using asymptotic techniques. Using steady state conservation equations for the reacting region outside the cloud and frozen region inside the cloud and matching conditions to the inwardly propagating wave front of non-reacting cloud, they obtained ignition temperatures [9]. The present work, independently carried out, accounts for the chemical reaction in regions both
within and outside the cloud and presents a numerical
scheme to obtain exact steady state solution for the
ignition temperatures of a cloud of droplets having non-
uniform size and number density inside the cloud.
For a special simple case, implicit algebraic relation for the
burning rate of a chemically reacting cloud of droplets is
given in a form analogous to the relation of a burning
single droplet.
Consider a cloud of radius \( R_c \) containing densely
packed droplets (Fig. 1). The ignition process of a
group of droplets, is illustrated in Fig. 2A. For a plane
source (reaction occurring at a single surface)
at temperature \( T_R \), the curve ABC shows the heat gener-
ation rate per unit area (\( Q_G \)) vs the reaction surface
area at temperature \( T_G \). The line GIDH shows the heat loss rate
(\( Q_H \)) from the reaction surface just at the time of
ignition. According to the thermal theory of ignition, \( I_G \)
is the ignition point for a group of droplets. At \( G, T_R = 0 \).
The heat generation rate per unit area is a
strong function of temperature \( T_R \) and a weak function of
fuel and oxidizer mass fractions. Hence for a single
droplet the plot \( Q_G \) vs \( T_R \) is approximately the same as
that for a cloud. However the heat loss rate \( Q_H \) is
inversely proportional to the radius of the reaction zone
(\( \theta_R \)). The line SIGT shows the \( \theta_R \) vs \( T_R \) relationship for
a single droplet. Since \( \theta_R \) is very small for a single
droplet, the heat loss rate is quite high. The point
\( I_G \) denotes the ignition condition for a single droplet.
It is obvious that the free stream temperature required
for ignition of a single droplet \( T_R(\theta_R) \) is higher
than \( T_R(\theta_G) \) for a group of droplets. The ensuing
analysis and results essentially confirm this hypoth-
esis. It should be noted that even a large droplet can
exhibit a similar qualitative behavior. However the
cloud takes considerable space to distribute the mass
into very finely dispersed droplets inside the cloud and the
blowing rate of such a cloud is expected to be
higher compared to the rate for a single droplet of
same mass both of which will lead to a reduction in
ignition temperature.

2. CONSERVATION EQUATIONS

For the purpose of analysis, the system of interest
will be divided into three zones I, II and III as shown in
Fig. 1. The zones I, II and III will be
called as the film region, the bulk gas region and the
single phase gas region respectively.

2.1 Assumptions

i. Spherical symmetry exists and \( \zeta = \text{constant} \)

ii. The three zone model is valid. For zone I,
\( \dot{\alpha}(\text{property})/\dot{\alpha} = \text{constant} \) and no significant chemical reaction
occurs. For zone II, \( \dot{\alpha}(\text{property}) = \text{constant} \) and
chemical reaction is significant. The assumption of pure evap-
oration in zone I is justified in view of the fact that
the characteristic thickness of the film zone is of
the order of \( \alpha_I \) while the interdroplet distance is of
the order \( (1/2 \alpha_I)^3 \) which is much larger than \( \alpha_I \) for dilute
clouds. Further the zone II is hotter compared to zone
I and hence significant chemical reaction is expected to be
taken place in zone II compared to zone I.

iii. For the sake of simplicity, a quasi-steady be-
behaviour is assumed for all the three zones. For zone I,
the assumption is valid since \( \tau / \tau_{\text{rev}} \gg 1 \). For the
zones II and III, the quasi-steady assumption is ques-
tionable. The thermal diffusion time scale to the cen-
tre of a cloud of radius \( R_c \) cm is of the order of \( R_c ^2 \)
while the sum of heating and evaporation time for a
droplet of radius 50 \( \text{cm} \) is of the order of about 15 ms.
Hence only an outer layer of droplets with a thickness of
about 0.1 \( \text{cm} \) may evaporate. A quasi-steady assump-
tion will lead to larger burning rate and hence the re-
action zone will be located at a larger radius for the
steady analysis than the location obtained with non-
steady analysis. The quasi-steady analysis provides a
lower bound on the temperature required to ignite the
cloud.

A few more assumptions are stated in the later
sections of the text.

The quasi-steady conservation equations both for
the two phase cloud regime and the single phase gas re-
gime are given below:

2.2 Conventional Form

Mass

\[
\frac{d\dot{\alpha}_I}{d\tau} = \dot{\alpha}_I^* + 4\pi^2 \]

(1)

where

\[
\dot{\alpha}_I^* = n_2 \dot{\alpha}_I a_1 \ln (1+\delta), \quad \tau < R_c
\]

(2a)

\[
= 0, \quad \tau > R_c
\]

(2b)

In view of assumption (ii)

\[
\dot{\alpha}_I = \dot{\alpha}_I, \quad \tau < R_c
\]

(3a)

\[
\dot{\alpha}_I = \dot{\alpha}_I, \quad \tau > R_c
\]

(3b)

Species

Fuel:

\[
\frac{d}{d\tau} (\dot{\alpha}_I - \dot{\alpha}_I^*) = \dot{\alpha}_I - \dot{\alpha}_I^* \frac{4\pi^2}{4\pi^2}
\]

(4)

where

\[
\dot{\alpha}_I^* = A \dot{\alpha}_I \dot{\alpha}_I Y_0 \exp (-E/RT)
\]

(5)

Oxidizer:

\[
\frac{d}{d\tau} (\dot{\alpha}_I - \dot{\alpha}_I^*) = \dot{\alpha}_I - \dot{\alpha}_I^* \frac{4\pi^2}{4\pi^2}
\]

(6)

Energy

\[
\frac{d}{d\tau} (\dot{\alpha}_I^* - \dot{\alpha}_I^*) = \dot{\alpha}_I - \dot{\alpha}_I^* \frac{4\pi^2}{4\pi^2}
\]

(7)

iv. It is implicitly and justifiably assumed that the
volume of chemically reacting zone II is almost same
as the sum of volumes of zones I and II and the volume
occupied by fuel droplets. (i.e. point masses)

The thermal enthalpy uses reference condition as the
temperature of surface of the droplet. Surface
temperature is related to the partial pressure of fuel
vapor through the Clapeyron equation. The partial
pressure of vapor can be estimated from the following equa-
tion for pure evaporation in zone I:

\[
Y_0 \frac{Y_I \dot{\alpha}_I + B}{Y_{I,\text{w}} \left( 1 + B \right)} \quad \tau < R_c
\]

(9a)

Another useful relation is given as

\[
Y_{0,\text{w}} = \frac{Y_I \dot{\alpha}_I}{1 + B}, \quad \tau > R_c
\]

(9b)

It should be noted that \( Y_{I,\text{w}} \) and \( Y_{0,\text{w}} \) are generally a
function of the radius \( r \) within the cloud.

2.3 Schwab-Zeldovich Form

The fuel vapor source term \( \dot{\alpha}_I \) and the chemical
reaction term \( \dot{\alpha}_I^* \) can be eliminated in equations (4),
(6) and (7) through suitable coupling of equations (1),
(4), (6) and (7).
The coupled equations are given below:

\[
\frac{d}{d\tau} (\dot{\alpha}_I - \dot{\alpha}_I^*) = \frac{d}{d\tau} \left( (4\pi^2) \frac{d(\dot{\alpha}_I^*)}{d\tau} \right) = 0
\]

(10a)

\[\text{Relative velocity effects can be included by replacing ln(1+\delta) by B and } \dot{\alpha} \text{ by } \dot{\alpha}_{\text{N}}\]
where
\[
\beta_{TF} = \left\{ \frac{h_F}{h_C} + Y_F / (1 - L_c) \right\} - 1
\]  
(10b)
\[
\frac{d}{dr} \left( \frac{\delta_{O_2}}{\delta_{O_2} F} \right) - \frac{d}{dr} \left( \frac{\rho D_4 \delta_{O_2}^2}{dr} \right) = 0
\]  
(11a)
where
\[
\delta_{O_2} F = Y_F \delta_{O_2} - 1
\]  
(11b)
\[
\frac{d}{dr} (\delta F) - \frac{d}{dr} (\rho D_4 \delta^2 \frac{dr}{dr}) = \delta_{O_2} F \cdot 4 \pi r^2
\]  
(12a)
where
\[
\delta_{TF} = 1 - Y_F
\]  
(12b)
Equations (10), (11) and (12) appear to be similar to the governing equations for a single droplet except that \( \delta \) is not constant for \( r < R_c \). Further equations (12) are unnecessary in obtaining results for diffusion controlled combustion and pure evaporation problems. The boundary conditions are given as
\[
Y_F = 1, 0 < \beta_{TF} \leq \beta_{TF,w}, \delta_{O_2} F \leq \delta_{O_2} F, w \text{ as } r \rightarrow \infty
\]  
(13a)
and
\[
\delta = \frac{d\delta}{dr} - \frac{d}{dr} \left( \frac{\rho D_4 \delta^2}{dr} \right) = 0 \text{ at } r = 0
\]  
(13b)
Equations (1), (10), (11) and (12) which are subject to the boundary conditions given as Eqs. (13), and relations given in eqs. (9) yield the solution for a chemically reacting cloud of droplets.

2.4 Non-dimensional Conservation Equations

The normalized coupling function \( \phi \) can be defined as
\[
\phi = \frac{\delta_{TF}}{\delta_{TF,w}} \text{ for } \delta_{TF}, \delta_{O_2} F
\]  
(14)
\[
\phi = \frac{\delta}{\delta_{TF,w}} \text{ for } Y_F
\]  
(15)
The conservation equations are reduced to the non-dimensional form by introduction of the following non-dimensional variables.

a) \( \xi = R_c / r \)

b) \( e = \delta / \delta_{TF,w} \)

c) \( T = \alpha = \alpha_{TF} \)

d) \( G = 3 \ln \left( \frac{R_c \delta_{TF,w} / \delta_{TF,w} \left( \frac{R_c}{\delta_{TF,w}} \right)}{1 - \xi} \right) \)

e) \( D_{II} = A \left( \frac{R_c \ln \left( \frac{R_c \delta_{TF,w} / \delta_{TF,w} \left( \frac{R_c}{\delta_{TF,w}} \right)}{1 - \xi} \right)}{\ln \left( \frac{R_c \delta_{TF,w} / \delta_{TF,w} \left( \frac{R_c}{\delta_{TF,w}} \right)}{1 - \xi} \right)} \right) \)

Using eqs. (16) in (1), (10), (11) and (12), the following equations are obtained in non-dimensional form mass
\[
\frac{d\alpha}{d\xi} + \left( G \frac{\ln (1 + B)}{A^2} \frac{\delta_{TF,w}^2}{\delta_{TF,w}^2} \right) = 0, \xi > 1
\]  
(17)
\[
\phi = (1 + B) \gamma
\]  
(20a)
\[
\phi = (1 + B) \gamma
\]  
(21a)

Similarly using eq. (9 a), eq. (15) can be written as
\[
\phi = (1 + B) \gamma
\]  
(22a)
where
\[
\gamma = \frac{Y_F - 1 + \frac{L_c}{h_c}}{A \left( \frac{R_c \ln \left( \frac{R_c \delta_{TF,w} / \delta_{TF,w} \left( \frac{R_c}{\delta_{TF,w}} \right)}{1 - \xi} \right)}{\ln \left( \frac{R_c \delta_{TF,w} / \delta_{TF,w} \left( \frac{R_c}{\delta_{TF,w}} \right)}{1 - \xi} \right)} \right)}
\]  
(21b)

Eqs. (17), (18), (19), the boundary conditions of eq. (20) and the relations (9) are sufficient for the solution of chemically reacting cloud of droplets.

3. ANALYSIS, RESULTS AND DISCUSSION

3.1 Integral Solutions

Integrating eqs. (18) and (19) twice and using the boundary conditions one can obtain
\[
\phi = \exp \left( -M \xi \right), \xi \leq 1
\]  
(23a)
\[
\phi = \exp \left( -S_1 \left( \frac{\xi}{S_2} \right) - S_2 \left( \frac{\xi}{S_1} \right) \right), \xi \geq 1
\]  
(23b)
where
\[
S_1 = \frac{\ln (1 + B) \delta_{TF,w}^2}{\delta_{TF,w}^2}
\]  
(23c)
\[
S_2(\xi) = \int_{1.0}^{\xi} \frac{\kappa}{\gamma_0} \frac{G \ln (1 + B)}{n_0^3} \, dn,
\]

(23d)

and

\[
\phi_F = \exp \left( -\zeta C + S_3(\xi) \right), \quad \zeta = 1.0,
\]

(24a)

\[
\phi_F = \exp \left( -S_1(\xi) - S_2(\xi) + S_3(\xi) \right), \quad \zeta \geq 1
\]

(24b)

\[
S_3(\xi) = \int_{0}^{\xi} \frac{[Y_F(t)]^{n_2} Y_{O_2}(t)^{n_2} Y_{O_2}(t)}{(1 - Y_F(t))^3 [0(t)]^{n_2} \gamma_0^{n_2} \gamma_0^{n_2} \gamma_0^{n_2}} \, d\xi.
\]

(24c)

Solution for the nondimensional burning rate \( M \) as a function of free stream temperature \( T_{\infty} \) is sought. Prior to presenting the numerical method and the results, a few simple solutions will be given below.

3.2 Explicit and Implicit Solutions

Explicit solutions for \( \alpha \) and \( \phi \) and implicit solution for \( M \) will be given for a few simple cases. As \( r > R_d \), the thermal enthalpy decreases but fuel mass fraction \( Y_F \) increases. As \( r < R_d \), the thermal enthalpy increases but the fuel mass fraction decreases. Because of the compensating effects of the fuel mass fraction \( Y_F \), as given by relation (9a) and hence the droplet temperature will be approximately constant inside the cloud. Further if

\[
G \equiv \frac{G_1}{\xi^q}
\]

then the following relations can be obtained for \( \alpha, \phi \) and \( M \) for a chemically reacting cloud. The details of derivation are shown in Appendix A.

\[
\alpha = \frac{(q-3)}{2} \frac{\Gamma(q-1)}{\Gamma(q-3/2)} \frac{\sqrt{G_1}}{\Gamma(q-2)} \frac{G(q-2)}{G(q-3/2)} \frac{(q-3)}{q-2}, \quad q \geq 2
\]

(26a)

\[
\phi = (1 + R_e) \exp \left(-\zeta C + S_3(\xi) \right), \quad \zeta \geq 1
\]

(26b)

\[
(1 + R_e) \gamma = \exp (-M)
\]

(27a)

\[
(1 + R_e) \gamma = \exp (-M)
\]

(27b)

The solution of \( \phi \) for \( \zeta \geq 1 \) is same as eq. (23a).

\[
M = \frac{1}{1 + \frac{2q-1}{q_1} \left( \frac{2-G(q-2)}{2-G(q-3/2)} \right) \left( \frac{1-G(q-3)}{2-G(q-3/2)} \right) \left( \frac{1}{G(q-2)} \right)}
\]

(28a)

where \( M_0 \) is the nondimensional mass burning rate of a chemically reacting single drop having a radius of \( R_e \). The expression for \( M_0 \) is the same as given in Ref. 2.

\[
M_0 = \ln \left[ 1 + \frac{h_T \omega_0}{h_c} \left( \frac{Y_{O_2} \omega_0}{Y_{O_2} \omega_0 + \gamma_0^2} \right) \right]
\]

(28b)

It should be noted that the relation for \( M/(M_0) \) given in eq. (28a) is true whether the problem of interest is pure evaporation, chemical reaction or diffusion controlled combustion. However \( M \) (equation (28b)) contains the unknown term \( Y_{O_2} \), which is assumed, (2) then, \( M \) is estimated using eq. (18b) for the given fuel volume fraction distribution and droplet size distribution; (3) eqs. (23) are utilized to obtain \( \phi \) for \( \zeta \geq 1 \) and (4) the profile for \( Y_F \) can be obtained from the knowledge of \( \phi \) and the assumed \( B \) profile using eqs. (14) and (10b). Similarly, the \( Y_{O_2} \) profile can also be obtained; (5) the calculated profiles \( Y_F \) and \( Y_{O_2} \) are used in the term \( S_3 \) (eq. 24c). In order to evaluate the temperature \( T \) and hence \( \theta \), the droplet surface temperature must be determined. From the known \( Y_F \) and \( \phi \) profiles inside the cloud and eq (9a), the surface temperature can be determined using Clapeyron equation. Many times the error in solution for the burning rate due to assumption of surface temperature same as boiling temperature is negligibly small. A profile for \( T \) and hence new \( Y_F \) profile are then calculated using \( \phi \) and eqs. (15) and (12b); (6) with the calculated "\( T \)" from step (4) and "\( Y_F \)" from step (5), a new "B" profile is obtained; (7) then steps (1) to (6) are repeated until successive profiles converge within a root mean square error of about 1%.

Convergence is rapid for diffusion controlled combustion and pure evaporation problems but difficulties were encountered for the ignition problem particularly for the solutions in the middle branch of Fig. 28. An under-relaxation technique was used in obtaining the new "B" profile.

\[
B_{\text{new}} = R_B \times B_{\text{new}} + (1 - R_B) B_{\text{old}}
\]

where \( RF \) is the under-relaxation factor, which has a value of 0.7.

The computer program using the above sequence is capable of dealing with spray clouds having arbitrary size and fuel volume fraction distributions. Further, evaporation, diffusion controlled combustion and ignition problems can be solved. The interaction effects can be readily incorporated.
Table 1. Data used in the calculations

Fuel:
Fuel: Dodecane C_{12}H_{26}, Stoichiometric oxygen: 3.48 kg/kj of fuel, Boiling point temperature: 490 K, Latent heat: 256 kJ/kg, Heating value: 44360 kJ/kg of gaseous dodecane [10].

Surrounding:

O_2: 0.23

T_{amb} = 298 K

Spray data:

r_0: 5 \times 10^{-5} m, R_c: 1 \times 10^{-2} m, R_l: 5 \times 10^{-5} m,

q: 0, Fuel volume fraction, \beta: 2 \times 10^{-6} \text{ (calculated)}

Overall mass density of cloud, \rho_c: 1 kg/m^3 (calculated)

Kinetics data [11]

Preexponential factor: 3.00 \times 10^8 1/s, Activation energy: 1.5 \times 10^6 kJ/k mole, Damköhler number: 1 \times 10^7 (calculated), Order with fuel, n_F = 1.0, Order with oxygen, n_O_2 = 1.0, Overall order, n = 1.0

Gas mixture:

\rho_{p,mix} = \rho_F \cdot 0.3648 + \rho_{O_2} \cdot \frac{8071}{T} + 1.5 \times 10^6 \frac{1}{T^2}, kJ/K mole

Numerical method data:

\Delta T = 0.01, \Delta r = 0.00667 (step size in integration), relaxation factor = 0.7

3.5 Fuel Data

The fuel and other data selected for the quantitative results are shown in Table 1. The overall global kinetic data for oxidation is taken from Williams [11] for decane: air mixture, since the global kinetics data for dodecane are not available. Further for the numerical results it is assumed that the cloud consists of uniformly sized droplets and droplet density is uniform inside the cloud. This approach is taken in order that the numerical results can be compared with simple solutions.

3.6 Quantitative Results and Discussion

Fig. 3 shows the total nondimensional mass burn rate M vs T_{amb} for the base data given in Table 1. According to the schematic shown in Fig. 2, there should be three branches of the solution to the problem: a lower branch (stable) AB, a middle branch BCD, and an upper branch EF. However, with the numerical scheme, so far only the lower branch leading to ignition and the upper branch solutions (which are almost the same as the results for diffusion controlled combustion) were obtained.

The point B represents the minimum temperature required to ignite the cloud of droplets. The required temperature T_B is around 750 K. The lower curve below AB (dotted line) represents the pure evaporation of spray. The ignition condition is clearly revealed in the plot of temperature profiles in Fig. 4. For the curve AB, there is no ignition and only simple evaporation takes place. Heat transfer occurs from the free stream to the cloud of droplets. For the curve CDE, a temperature peak starts developing around T_{amb} = 740 K. Then heat transfer takes place from the surface of maximum temperature (point B) to the ambient atmosphere. Thus the direction of heat transfer reverses. Beyond T_{amb} = 740 K, the temperature sharply rises to a value given by diffusion controlled combustion. One observes that within about 3% error, one may use an adiabatic ignition criterion as described in reference [12].

Fig. 4 exhibits the location of peak temperature (curve ABC) for an increasing ambient temperature. Because of the step size used in the calculation, the flame can be anywhere within the dashed area at a given ambient temperature. The flame appears to move away from the cloud. The curve BE plots the location of the flame for diffusion controlled combustion. For diffusion controlled combustion, \xi can be fixed exactly using eq. B-2 in Appendix B. The numerical scheme has been found to agree with the exact results for the location of flame.

Fig. 5 shows the effect of oxygen mass fraction on the dimensionless mass burning rate. The required ambient temperature for ignition increases as Y_{O_2,m} is reduced but not significantly. The diffusion controlled regime the flame moves away from the cloud as Y_{O_2,m} is reduced while the reverse happens for the ignition regime.

Fig. 6 shows the effect of reducing the cloud radius by a factor of 10, on the temperature profile. Due to lesser reaction zone volume the required ambient temperature jumps to 950 K from 740 K as cloud radius
is decreased from 1 cm to 0.1 cm. Further, the ignition location is within the vicinity of the cloud radius i.e. at smaller cloud radius with same fuel volume fraction, ignition may occur in zone II. It should be noted that results for the reduction of cloud radius are analogous to results for a single droplet in that the reaction zone volume is decreased which is responsible for higher ignition temperature.

The effect of atomization of spray on the ignition temperature could be studied by comparing the ignition temperatures of finer and coarser clouds of same mass. Fig. 8 shows the results. It is observed that qualitative trends appear to change slightly depending upon the criterion used to define the ignition condition. If $\Delta T (= T_{peak} - T_{ambient})$ is selected as $1\degree C$, the effect of drop size is negligible. If $\Delta T$ is set at $5\degree C$, then the decreasing drop size decreases the ignition temperature. This is explained as follows. From the $G$-number definition (eq. 14d), it is apparent that the $G$-number increases with the decreasing drop size. The blowing rate (or mass evaporation rate) increases with increased $G$-number (Fig. 2a). The increased blowing rate moves the reaction zone closer to the ambiance which decreases the heat loss from the reaction zone and hence decreases the ignition temperature. However, the experimental and theoretical studies on single droplet/sphere particle yield the reverse [14, 15]. The operational experience in the field indicates the ease of ignition with finer atomization. The group theory explains such a behavior. Since ignition is essentially a non-steady phenomenon, these results await confirmation from the non-steady analysis.

4. SUMMARY

A three zone theory for the ignition of a group of droplets is presented and results for ignition of a cloud of dodecane droplets are presented. Implicit algebraic relation for the nondimensional burning rate of a chemically reacting cloud of droplets is presented in a form analogous to the burning of a chemically reacting single droplet of radius same as the radius of the cloud. The ignition temperature for a cloud with larger cloud radius is less than a cloud with smaller cloud radius because of lower heat loss in the former. At smaller cloud radius ignition location moves towards the cloud indicating the possibility of drop ignition. A cloud could be ignited as low as at $700\degree K$. At reduced oxygen concentration which exists in the recirculation zone of boilers and gas turbines group combustion is possible even for very dilute clouds.

APPENDIX A

EXPLICIT . . . RESULTS FOR SPECIAL CASES OF CHEMICALLY REACTING CLOUDS

Rewrite eq. (17) as

$$
\left( \frac{d\theta}{dT} \right) \frac{M \theta^4}{G \theta^4} \xi = \ln (1 + B)
$$

(A-1)

Differentiating (A-1) with respect to $\xi$

$$
\frac{d}{d\xi} \frac{d\theta}{dT} \frac{M \theta^4}{G \theta^4} = -\frac{1}{1 + B} \frac{d(1+B)/d\xi}{\xi}
$$

(A-2)

From eqs. (21)

$$
\alpha = (1 + B) \gamma
$$

(A-4)

Using eq. (21) in eq. (18a) and then integrating

$$
M \alpha = -[1/(1+B) \gamma] \frac{d(1+B)/d\xi}{\xi}
$$

(A-3)

Since $\gamma$ is approximately constant inside the cloud (section 4.3, text), eq. (A-3) can be written as

$$
M \alpha = -\frac{1}{(1+B)} \frac{d}{d\xi} (B + 1)
$$

(A-4)

Using (A-4) in the right hand side of eq. (A-2),

$$
\frac{d}{d\xi} \left( \frac{\theta^4}{M \theta^4} \right) - M \alpha = 0 \quad \xi \geq 1
$$

(A-5)

Equation (A-5) is amenable to simple integration, if

$$
G \theta^4 = G_0 \theta_0^4
$$

(A-6)

where $G_0$ is a constant.

Using (A-6) in (A-5) and integrating [Ref. 16, p. 137-138], one can obtain an expression for $\alpha$ as given in eq. (26a)

Integrating eq. (A-4)

$$
(B + 1) = (1 + B) \exp(-M \xi \omega \eta + 1)
$$

(A-7)
Using eq. (A-7) in eq. (21), the nondimensional coupling function profile can be obtained as shown in eq. (27).
Using eqns. (18b) and (26b) in eq. (A-7) and then using integral tables [17], the following expression for $M$ is obtained

$$M = \left[ \ln \left( 1 + \frac{2}{2 - q} \right) \right] \left[ \frac{3 - q}{1 - q} \right]$$

$$+ \left[ \frac{1 - q}{1 - q} \left( \frac{1}{2 - q} \right) \right]$$

$$\sqrt{\frac{1}{2 - q} \left( \frac{1}{2 - q} \right) \left( \frac{1}{2 - q} \right)} \right]$$

$$\forall \ q \leq 2.$$  \hspace{1cm} (A-8)

Using eqns. (23a), (21a) and (27b) in (A-8), an implicit expression for $M$ is obtained as shown in eq. (28).

**APPENDIX B**

**DIFFUSION CONTROLLED COMBUSTION**

The flame is located at $\phi_f = \gamma_{O_2} = 0$ and hence $\phi_{O_2} = 1/[1 + \Phi_{O_2}]$. Thus

$$\phi_f = 1/[1 + \Phi_{O_2}]$$  \hspace{1cm} (B-1)

Since for group combustion, the flame is outside the cloud ($\xi < 1.0$), eq. (23a) yields the flame location as

$$\xi_f = \frac{1}{M} \ln \left( 1 + \gamma_{O_2} \omega_{O_2} \right)$$  \hspace{1cm} (B-2)

where $M$ is known from eqs. (28) with $\gamma_{O_2} = 0$. In order that $\xi_f \leq 1.0$, then eq. (B-2) yields the condition that

$$M \geq \ln \left( 1 + \Phi_{O_2} \omega_{O_2} \right)$$  \hspace{1cm} (B-3)

Using eq. (16j) in (B-3)

$$M \geq \frac{4\pi cD \Theta_c}{\ln \left( 1 + \Phi_{O_2} \omega_{O_2} \right)}$$  \hspace{1cm} (B-4)

From eqs. (B-3) and eqs. (28) with $\gamma_{O_2} = 0$ the critical $\Theta_c$ numbers above which there exists a group combustion can be quantitatively evaluated.

The flame temperature is obtained from eqs. (B-1), (10b) and (14). The result is found to be same as the adiabatic flame temperature

$$h_{f, f} = h_{T, \omega} = \left( \frac{\Phi_{O_2} \omega_{O_2}}{\gamma_{O_2}} \right) h_{c} - 1 - h_{T, \omega} / \left( 1 + \Phi_{O_2} \omega_{O_2} \right)$$  \hspace{1cm} (B-5)

5. **REFERENCES**

Table 1

PHYSICO-CHEMICAL CONSTANTS FOR LIQUID n-DODECANNE

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>\rho (gm/cm^3)</td>
<td>0.749</td>
</tr>
<tr>
<td>\text{C}_{pl} (cal/gm\degree K)</td>
<td>0.5</td>
</tr>
<tr>
<td>L_{298} (cal/gm)</td>
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</tr>
<tr>
<td>Q (cal/gm-fuel)</td>
<td>10630.</td>
</tr>
<tr>
<td>\eta</td>
<td>3.52</td>
</tr>
<tr>
<td>(\rho D)_\infty (gm/cm·sec)</td>
<td>$3.0 \times 10^{-4}$</td>
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<tr>
<td>T_c (\degree K)</td>
<td>659.</td>
</tr>
<tr>
<td>\alpha (cm²/sec)</td>
<td>$8.83 \times 10^{-4}$</td>
</tr>
<tr>
<td>\text{C}_p (cal/gm\degree K)</td>
<td>0.25</td>
</tr>
<tr>
<td>\text{P}_c (atm)</td>
<td>17.9</td>
</tr>
<tr>
<td>a</td>
<td>4.12</td>
</tr>
<tr>
<td>b (\degree K)</td>
<td>1626.</td>
</tr>
<tr>
<td>c (\degree K)</td>
<td>93.</td>
</tr>
</tbody>
</table>

Octane:
\[ A = 9.9 \times 10^6 \]

\[ n = \frac{241}{10} \]

\[ T_c = 568.5 \]

\[ \text{PC} = 399.5 \]

\[ \text{B} = 300.0 \]

\[ \rho = 707.0 \]