Drag Effects in Spherical Polydisperse Spray Flame Propagation

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Extended Abstract

Introduction

The propagation of a flame through an initial pre-mixture of an oxidizer and a mist of liquid fuel droplets is of particular relevance to the process of ignition in many practical aerospace and other engineering applications. Attempts at understanding the complex physical-chemical two-phase interaction at ignition under such circumstances, coupled to the subsequent flame evolution, have recently provided close-up details using a DNS simulation [1]. Previous work on the behavior of spherically propagating spray flames was performed by the author [2-4] using analytical means to arrive at an evolution equation for the flame front, and a comprehensive survey of previous research work on this topic can be found in these publications. Various aspects of the extinction and propagation such as the influence of initial liquid load [2], vaporization Damkohler number, droplet drag effects[3] and spray polydispersity [4] were examined in detail and shed important light on the way in which the continued life or death of the flame front can be impacted upon by these spray-related parameters.

In the current work previous analyses are extended to account for spray polydispersity coupled to droplet drag effects for the first time. The criticality of correctly accounting for the spray's actual size distribution rather than describing the spray as monodisperse using some average droplet diameter (such as the Sauter mean diameter) is demonstrated.

The Model

Consider an unconfined domain containing a mixture of fuel droplets, fuel vapor, oxygen and an inert gas. At time t = 0 the mixture is ignited and, under appropriate conditions, a flame front begins to propagate outwards with spherical symmetry through the mixture. The main assumptions of the model are as follows:

- (a) Velocities are small compared to the speed of sound.
- (b) Viscous dissipation and the work done by the pressure are negligible.
- (c) Constant transport properties determined primarily by those of the gas phase.
- (d) Dufour and Soret effects are negligible.
- (e) One step first order chemical reaction with Arrhenius kinetics and a large dimensionless activation energy θ .
- (f) Reactant composition fuel rich and far from stoichiometric.
- (g) A slowly varying flame with $O(\theta^{-1})$ heat losses.
- (h) Lewis number not too close to one, $|Le l| \approx O(1)$.
- (i) Variable gas density.

(j) The droplets are taken to have the same temperature as the host environment until reaching the fuel's boiling temperature.

(k) Downstream of the flame front vaporization is initiated when the temperature of the droplets is that of the liquid fuel's boiling temperature.

The situation under consideration is sketched in Fig. 1.



Figure 1: Spherical Spray Flame Configuration

Under the aforementioned assumptions the governing equations assume the following form

$$\frac{\partial\rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho u \right) = 0 \tag{1}$$

$$\rho \frac{\partial T}{\partial t} + \rho u \frac{\partial T}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) + (1 - \alpha) exp(\frac{1}{2}(T - 1))\hat{\delta}(r - F(t))$$

$$- K(T) - \eta S_v$$
(2)

$$\rho \frac{\partial m_O}{\partial t} + \rho u \frac{\partial m_O}{\partial r} = \frac{1}{Le} \frac{\partial}{\partial r} \left(r^2 \frac{\partial m_O}{\partial r} \right) - exp(\frac{1}{2}\theta(T-1))\hat{\delta}(r-F(t))$$
(3)

$$\rho \frac{\partial m_{d,j}}{\partial t} + \rho u \frac{\partial m_{d,j}}{\partial r} = -S_{v,j} , \quad j = 1, 2...N_s$$
(4)

$$\rho m_{d,j} \frac{\partial u_{d,j}}{\partial t} + \rho m_{d,j} u_{d,j} \frac{\partial u_{d,j}}{\partial r} = \frac{m_{d,j}}{\varepsilon_j} \left(u - u_{dj} \right) + \Psi_j m_{d,j+1} \left(u_{d,j+1} - u_{d,j} \right), \quad j = 1, 2...N_s$$
(5)

$$\rho = \frac{1}{T} \tag{6}$$

in which ρ is the mixture density, *u* is the velocity, *T* is the temperature, α is the ratio of the unburned gas temperature to the adiabatic burned gas temperature, F(t) is the location of the flame front, $\hat{\delta}$ is the delta function, $K(T) = h(T^4 - \alpha^4)$ represents radiant heat losses with *h* the heat loss coefficient, η is the latent heat of vaporization of the droplets in the spray, m_0 is the mass fraction of oxygen, *r* is the radial coordinate and *t* is time. Note that these quantities have been normalized in the usual fashion. The rate of vaporization, S_v , is based on the use of the sectional method for describing the spray and , $m_{d,j}$ is the mass fraction of liquid fuel in size section *j* of the spray. The reader is referred to reference [5] for the details of the method. The expression for $S_{v,j}$ is

$$S_{\nu,j} = \rho \Delta_j m_{d,j} - \rho \Psi_j m_{d,j+1}$$
(7)
with

$$\Psi_{Ns} = 0 \tag{8}$$

in which Δ_j and Ψ_j are the sectional vaporization Damkohler numbers, the former relating to the rate of loss of droplets from section j to the next section down and the latter to the rate at which droplets enter section j as they become ineligible for membership of section j+1 owing to a reduction in their size due to vaporization. The sectional vaporization numbers are computed using the relationships

$$(\Delta_{j}, \Psi_{j}) = 1.5E(\{3d_{u,j} - 2d_{l,j}\} / \{d_{u,j}^{3} - d_{l,j}^{3}\}, d_{l,j+1} / \{d_{u,j+1}^{3} - d_{l,j+1}^{3}\})$$
(9)

where E is an evaporation coefficient and d_{uj} and d_{lj} define the smallest and largest droplet radius, respectively, associated with size section j. In addition,

$$S_{\nu} = \sum_{j=1}^{N_s} S_{\nu,j}$$
(10)

with N_s being the number of size sections into which the initial droplet distribution has been subdivided.

The location of the onset of liquid fuel vaporization is uniquely determined by means of T_{ν} , which is a reference temperature (taken here as the boiling temperature). This value is a property of the given fuel.

Eqs(5) are the sectional momentum equations with $u_{d,j}$ being the sectional droplet velocity. The first term on the right hand side is the drag term whereas the second term describes the change of momentum resulting from the transfer of droplets from size section j+1 to size section j as a result of evaporation. ε_i are associated with sectional drag coefficients. The drag coefficient parameters, \mathcal{E}_i , are based on using an approximate expression [6] for the droplet drag coefficient $C_D = 24 / Re_d$, with Re_d the droplet's Reynolds number, and the sectional drag force per unit mass . For droplets of about 50 μm in diameter typical values of ε are found to be of the order of 10^{-2} which indicates a situation in which there will be fairly rapid dynamic adjustment of the droplets to the velocity of their host carrier gas. Since ε_i is proportionate to the average droplet in section *j* these drag radius parameters can be according ordered to $\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \dots < \varepsilon_{N_{\epsilon}} (=\varepsilon) << 1$. ε will be referred to as the Stokes number.

The aforedescribed equations can be brought to an analytically tractable form by exploiting two small parameters viz. the inverse of the activation energy θ^{-1} and ε both of which are much less than unity. After much mathematical development the final form of the evolution equation for the flame front is found:

$$\frac{dS}{dR} + S^2 \ln S^2 = \frac{2S}{R} - l - \Gamma S^2 \Im$$
⁽¹¹⁾

in which S relates to the flame velocity, R to the instantaneous flame radius, l to radiative heat loss, Γ is the non-dimensional latent heat of vaporization and the parameter \Im contains within it spray-related terms, viz. $\Omega_{j,i}$ which is expressed in terms of the initial sectional mass fractions and evaporation numbers, and the sectional drag parameters, ε_i :

$$\mathfrak{T} = \left[\delta - \sum_{j=l}^{N_S} \sum_{i=j}^{N_S} \Omega_{ji} \left\{ \frac{T_{\nu}(1-\alpha)}{(T_{\nu}-\alpha)} \right\}^{-\frac{A_i}{\alpha S^2}} \left\{ 1 - \varepsilon_j \Delta_i \left[\frac{1}{T_{\nu}} - 1 \right] \right\} - f(S) \right]$$
(12)

where f(S) is a complicated polydisperse spray-related function.

Results and Discussion

The flame front evolution equation is solved numerically and some typical results are presented for three different initial size distributions. Relevant data is listed in Tables 1 and 2.

Table 1: The droplet size sections (in μm)

Section Number	1	2	3	4	5	6	7	8	9
Lower Diameter $d_{l,j}$	1	5	10	20	30	40	50	70	90
Upper Diameter $d_{u,j}$	5	10	20	30	40	50	70	90	110

In Table 1 the way in which the range of droplet sizes is divided into size sections is defined. In Table 2 three droplet size distributions in the fresh unburned mixture are described. Distribution 1 is initially mono-sectional with all droplets located in the 40-50 μm size slot. Distribution 2 is initially bi-disperse with about 80% of the liquid fuel in droplets in the 70-90 μm range and the remaining 20% comprised of 10-20 μm droplets. Finally, the third distribution has droplets spread out throughout the entire range of droplet sizes. The three distributions have in common a Sauter mean diameter (SMD) of 44.8 μm .

Table 2: Droplet distributions and mean droplet sizes.

Section	1	2	3	4	5	6	7	8	9	SMD
Distribution 1	0	0	0	0	0	1	0	0	0	44.8
Distribution 2	0	0	.207	0	0	0	0	0	.793	44.8
Distribution 3	.0006	.0006	.0229	.0793	.1662	.2464	.2349	.1547	.1034	44.8

Unless stated otherwise representative data used for the calculations was: $\alpha = 0.16$, $T_v = 0.2$, l = 0.3, E = 20 and $\Gamma = 0.8$.



Figure 2: Spray flame evolution for distribution 1 and different values of the Stokes number.

In Fig.2 the flame velocity is plotted as a function of the radius for initial droplet distribution 1 and different values of the Stokes number. For this distribution, irrespective of the drag parameter, the flame extinguishes (i.e. $S \rightarrow 0$ for a finite value of R) although the flame's demise is delayed as $\varepsilon \rightarrow 0$. As ε grows the droplets remain in a given vicinity for a longer period of time thereby focusing the heat loss due to evaporation, leading to earlier extinction.



Figure 3: Spray flame evolution for distribution 2 and different values of the Stokes number.

The same figure is redrawn in Figure 3 for initial droplet distribution 2. In contrast to that shown in Figure 2 for this case it is seen that all flames survive irrespective of the drag parameter. This is presumably due to the fact that most liquid fuel is concentrated in larger droplets (section 9) which evaporate more gradually than the droplets initially in section 3, the latter evaporating rapidly.



Figure 4: Spray flame evolution for distribution 3 and different values of the Stokes number.

In Fig.4 the evolution of the flame fronts propagating through spray distribution 3 is drawn for different values of the Stokes number, ε . In this case, either the flame is sustained or extinguishes, depending on the Stokes parameter. For $\varepsilon > 0.1$ flame propagation occurs. For some critical value of ε between 0.1 and 0.5 extinction happens.

Two immediate conclusions may be drawn from these figures; both the actual distribution and the Stokes number together are critical in determining whether the developing spray flame will extinguish or not, *despite the fact that the sprays all have the same SMD*.

This can be viewed differently by considering Fig. 5 in which the evolution of the point of onset of evaporation is shown for all three distributions. It is clear that for distributions 1 and 3 the flames eventually extinguish whereas for distribution 2 a steady flame propagation rate is established.

Finally, it is noted that the velocity profiles for the liquid phase (not shown here) agree well with a full numerical calculation of the governing equations. Thus, the current theory demonstrates quite clearly that care must be exercised when characterizing a polydisperse spray via its SMD.



Figure 5: Evolution of evaporation onset location for all initial spray distributions.

References

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