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Flamelet characteristics at the leading edge and through the flame brush of statistically steady incompressible turbulent premixed flames

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ABSTRACT

Conditional analysis is performed on statistical behavior of the flamelet characteristics at the leading edge and through the flame brush of incompressible turbulent premixed flames. The effective Lewis number is equal to unity with no stretch effect associated with differential diffusion. It is shown that the flamelet thickness, δ_f, is a crucial parameter to determine the local displacement speed, S_d, as well as the global turbulent burning velocity, S_T. There hold asymptotic relationships for S_T and conditional velocities at the leading edge in the statistically steady state. S_d is correlated with finite δ_f not in terms of stretch, but through independent effects of tangential strain rate and curvature. S_d and δ_f show strong correlations with curvature due to significant influence of tangential flux, while they show weak correlations dependent on the location in a flamelet with tangential strain rate. Flamelets tend to thicken according to the gradient of S_d due to focusing or defocusing of c transport for both positive and negative curvatures. The range of S_d is scaled by the tangential component, S_{dt}, with additional contribution of the normal S_{dn} component due to δ_f varying with curvature. Variation of S_{dt} is given in terms of the product of curvature and molecular diffusivity in the reaction–diffusion layer retaining a relatively invariant structure under turbulence. The stretched laminar flamelet model needs to be complemented by the additional effects of tangential flux and variation of finite δ_f in fully turbulent premixed flames.

1. Introduction

Many energy conversion devices including a spark ignition engine involve turbulent premixed combustion for homogeneous mixture of fuel and oxidant through which a wrinkled flame brush propagates. Reaction typically occurs in the localized thin reaction region called ‘flamelets’ which may be laminar or partially modified by turbulence with chemistry occurring faster than turbulent transport. Unlike mixing controlled nonpremixed combustion there remain significant uncertainties about their internal structure and how fast they burn through the turbulent burning velocity, S_T, of crucial engineering importance. A popular approach has been the stretched laminar flamelet model (LFM) [1] based on a collection of flamelets of negligible thicknesses moving at the displacement speed, S_d, added to stochastic turbulence. In the stretched LFM S_d has been expressed as

$$S_d/S_{Lu}^0 = 1 - KaMa \quad (1)$$

through the matched asymptotic solution for convection–diffusion and reaction–diffusion layers in a flamelet [2,3]. S_{Lu}^0 is the unstretched laminar flame speed. The Karlovitz number, Ka, is the nondimensional stretch given as a sum of the contributions of tangential strain rate and curvature. The Markstein number, Ma, is a property of the given premixture which becomes zero for a Lewis number equal to unity.

The stretched LFM is theoretically not valid, unless $\delta_f \ll R$ and $\delta_f \ll L$ for the minimum radius of curvature, R, and the flow scale, L, estimated as S_{Lu}^0 divided by the tangential strain rate [4]. The flamelet thickness, δ_f, given as the inverse of the maximum c gradient is about five to ten times L_m defined as D_{mu}/S_{Lu}^0 for molecular diffusivity, D_{mu}, in cold mixture. It has been shown that the minimum wrinkling scale is of a comparable order of magnitude with δ_f in typical premixed flame conditions [5–7]. The linear relationship in Eq. (1) was shown valid for a wide range of stretch in the laminar flame tip of a Bunsen burner [8] and for turbulent premixed flames in direct numerical simulation (DNS) [9]. It seems due to dominant influence of the curvature term over that by tangential strain rate and does not necessarily represent validity of the stretched LFM for the given flames [10,11]. There were reports on failure to reproduce the linear relationship for an unsteady flamelet wrinkled by a laminar toroidal vortex [12] and for a turbulent flame kernel of different kernel radii in the presence of mean curvature [13].

Finite δ_f was taken into account in the S_d expression through integral analysis [14,15], although with no consideration of the tangential

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flux due to curvature. Law & Sung [16] considered the effects of curvature for finite flamelet thickness in addition to those by stretch associated with differential diffusion. They described the smoothing mechanism by S_d varying with curvature to prevent sharp corners by Huygens propagation. Mikolaitis [17–18] performed analysis of highly curved flamelets for radii of curvature comparable with δ_f to show that the stretch alone is insufficient to explain large variation of S_d. He suggested existence of the minimum radius of wrinkling dependent on the mixture composition, for which S_d will vanish. Peters [19] extended the stretched LFM to consider the effect of tangential flux due to strong curvature by turbulence. S_d was decomposed into the contributions of the normal component, S_{dn}, and the tangential component, S_{dt}. Flame surface was defined at the interface between preheat zone and reaction zone with the latter retaining an invariant internal structure in the thin reaction zone regime. Flamelet thickening was attributed to small eddies penetrating into the preheat zone, although the influence of the smallest eddies was much smaller than expected in some experimental observations [10]. It was argued through scaling analysis that S_{dn} is dominant over S_{dt} for δ_f less than the Kolmogorov scale, η, in the corrugated flamelet regime. On the other hand S_{dt} due to curvature is dominant for δ_f larger than η in the thin reaction zone regime. Variation of S_d was explained primarily by the S_{dt} component given as a product of diffusivity and curvature [19]. It was shown later that curvature has strong influence on the S_{dn} component in both corrugated flamelet and thin reaction zone regimes [13]. Flamelets thicken with increasing absolute curvature, with the mean flamelet thickness greater than the unstretched δ_f in both regimes [20]. Behavior of δ_f and its dependence on curvature and tangential strain rate play a key role to determine the response of flamelets including S_d to turbulence [21]. In this work incompressible DNS is performed to investigate asymptotic behavior at the leading edge (LE) and conditional statistics through the flame brush of freely propagating 1-D flames in the statistically steady state. Some of the essential characteristics of real flames are retained in incompressible DNS, although with simplifications of the Lewis number equal to unity and no volume expansion with no feedback to turbulence. Previous observations in the references will be confirmed with description of the independent mechanisms of tangential strain rate and curvature affecting the flamelet structure and properties in turbulent premixed combustion.

2. Mathematical formulations

In this section we derive the equations for the orientation vector, $\mathbf{n}$, and the surface density function, Σ'_f, from the c equation in the surface propagation form involving S_d. They are averaged to describe transport of mean reaction progress variable, $\bar{c}$, mean orientation vector, $\langle\mathbf{n}\rangle_f$, and flame surface density, Σ_f, with corresponding conditionally averaged coefficient terms. c is defined in terms of temperature or deficient reactant species as

$$c = (T - T_u)/(T_b - T_u) \tag{2}$$

where the subscripts, u and b, represent unburned and fully burned gas. The continuous differentiable c varies between zero in unburned gas and unity in burned gas and satisfies everywhere in the domain

$$\frac{\partial c}{\partial t} + \mathbf{v}\cdot\nabla c = D_m \nabla^2 c + \dot{w}_c \tag{3}$$

$$\text{or } \frac{\partial c}{\partial t} - (v_n + S_d)\Sigma'_f = 0. \tag{4}$$

Eq. (4) is in the surface propagation form of an iso-c contour representing a flame surface. The unit normal vector on a flame is $\mathbf{n} = -\nabla c/|\nabla c|$. $\Sigma'_f (= |\nabla c|)$ is the surface density function or local flame surface density (FSD). It follows from the definitions that

$$\nabla c = -\mathbf{n}\Sigma'_f. \tag{5}$$

We take the divergence of Eq. (5) to obtain a higher order relationship for c as,

$$\nabla^2 c = \frac{\partial^2 c}{\partial n^2} - \Sigma'_f \nabla\cdot\mathbf{n}. \tag{6}$$

δ_f represents the flamelet thickness given as the inverse of $|\nabla c|$ or Σ'_f. $v_n = \mathbf{v}\cdot\mathbf{n}$ is the normal velocity component. S_d is given as a sum of the normal and tangential components as [22]

$$S_d = S_{dn} + S_{dt} \tag{7}$$

with

$$S_{dn} = \frac{1}{\Sigma'_f}\left(D_m \frac{\partial^2 c}{\partial n^2} + \dot{w}_c\right) \tag{8}$$

$$S_{dt} = -D_m \nabla\cdot\mathbf{n}\,. \tag{9}$$

n is the coordinate in the direction of $\mathbf{n}$ and $\nabla\cdot\mathbf{n}$ is twice the curvature on a flame surface at constant c. We obtain an equation for $\mathbf{n}$ by applying the gradient operator to Eq. (4) as

$$\frac{\partial}{\partial t}\left(\mathbf{n}\Sigma'_f\right) + \nabla\left[(v_n + S_d)\Sigma'_f\right] = 0. \tag{10}$$

The transport equation for Σ'_f may be derived by taking a scalar product of Eq. (10) with $\mathbf{n}$ as

$$\frac{\partial \Sigma'_f}{\partial t} + (v_n + S_d)\frac{\partial \Sigma'_f}{\partial n} = -\Sigma'_f \frac{\partial (v_n + S_d)}{\partial n}, \tag{11}$$

since it holds that

$$\mathbf{n}\cdot\frac{\partial \mathbf{n}}{\partial t} = \frac{1}{2}\frac{\partial}{\partial t}(\mathbf{n}\cdot\mathbf{n}) = 0. \tag{12}$$

The tangential gradient operator is defined as

$$\nabla_T \phi = \nabla\phi - \mathbf{n}\frac{\partial \phi}{\partial n}. \tag{13}$$

The tangential strain rate, $\nabla_T\cdot\mathbf{v}$, is defined as

$$\nabla_T\cdot\mathbf{v} = \nabla\cdot\mathbf{v} - \mathbf{nn}:\nabla\mathbf{v} \tag{14}$$

which may be approximated as $\nabla\cdot\mathbf{v} - \frac{\partial v_n}{\partial n}$ for sufficiently thin flamelets. The derivatives of S_{dn} and S_{dt} with respect to n may be given from Eqs. (8) and (9) as

$$\frac{\partial S_{dn}}{\partial n} = -\frac{\partial}{\partial n}\left(D_m \frac{\partial^2 c/\partial n^2}{\partial c/\partial n} + \frac{\dot{w}_c}{\partial c/\partial n}\right) \tag{15}$$

$$\frac{\partial S_{dt}}{\partial n} = -D_m \frac{\partial}{\partial n}(\nabla\cdot\mathbf{n}). \tag{16}$$

We define the temporal derivative tracking a flame element of fixed identity as

$$\left(\frac{D}{Dt}\right)_F \phi = \left[\frac{\partial}{\partial t} + (\mathbf{v} + S_d\mathbf{n})\cdot\nabla\right]\phi \tag{17}$$

for any scalar or vector quantity, ϕ, at a fixed c. Eqs. (4) and (11) may be rewritten as

$$\left(\frac{D}{Dt}\right)_F c = 0 \tag{18}$$

$$\left(\frac{D}{Dt}\right)_F \Sigma'_f = -\Sigma'_f \frac{\partial (v_n + S_d)}{\partial n} + \mathbf{v}\cdot\nabla_T \Sigma'_f. \tag{19}$$

Now we perform averaging of Eqs. (4), (10) and (11) to obtain the mean equations for $\bar{c}$, $\langle\mathbf{n}\rangle_f$ and Σ_f as

$$\frac{\partial \bar{c}}{\partial t} - \langle v_n + S_d\rangle_f \Sigma_f = 0 \tag{20}$$

$$\frac{\partial}{\partial t}\left(\langle\mathbf{n}\rangle_f \Sigma_f\right) + \nabla\left[\langle v_n + S_d\rangle_f \Sigma_f\right] = 0 \tag{21}$$