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Contribution of small scale turbulence to burning velocity of flamelets in the thin reaction zone regime

Ömer L. Gülder *

Institute for Aerospace Studies, University of Toronto, 4925 Dufferin Street, Toronto, Ont., Canada M3H 5T6

Abstract

There is a growing body of experimental evidence that passive surface character of the premixed flamelets may not be preserved beyond medium turbulence intensities, and their thermal structure deviate from that of a laminar flamelet. Further, the experimental measurements of flame surface characteristics indicate that the flame surface area is not the dominant factor in increasing the turbulent burning velocity under the conditions corresponding to the thin reaction zones regime. Approaches to estimating the turbulent burning rates based on the area increase of the premixed flame front surfaces may not be the right models and may require additional mechanisms for proper representation of the burning rate. This paper proposes a simple scheme to estimate the contribution of the flame front alteration by small scale turbulence on flamelet burning velocity. An expression was derived to estimate the contribution of flame front alteration as a consequence of the small scale turbulent eddies that may penetrate into the preheat layer of the premixed flame front. The derivation was based on the experimental evidence of flame front alteration by active eddies penetrating into the preheat layer and enhancing the transport. As a first approximation it was assumed that these active eddies have a characteristic size about the Taylor microscale. Further, the formalism that demonstrates that within the turbulence cascade the volume occupied by a certain size eddy and its characteristic velocity obey power-law relationships (i.e. structure functions) that are dictated by the intermittency of the turbulent field, was used. The predictions of the proposed expression were compared to the available experimental data.

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Keywords: Premixed turbulent combustion; Premixed combustion regimes; Thin reaction zone regime; Flame surface density; Small scale turbulence

1. Introduction

A frequent assumption made in modelling and simulation of premixed turbulent combustion is that the reaction is confined to thin flame fronts. The propagation of these fronts and associated events are governed by the interaction of the heat

and mass transport and the chemistry within the flame front. This strong coupling between the chemistry and the heat and mass transport is handled in flamelet models by assuming that the flame front is a thin passive interface that locally propagates with a laminar burning velocity. Then at high Damköhler numbers, a premixed flame front can be taken as consisting of regions of reactants and products separated by thin laminar flamelets. Since the instantaneous behaviour of these thin layers is the same as those of laminar flames,

* Fax: +1 416 667 7799.

E-mail address: ogulder@utias.utoronto.ca

turbulent burning velocity can be approximated by the product of the flamelets surface area and laminar burning velocity corrected for the effect of stretch and flame curvature. However, there is a growing body of experimental evidence that the approaches based on the flamelet hypothesis may not be always valid over the range of conditions of practical interest, see for example [1–3].

The most recent regime diagram for the premixed turbulent combustion, shown in Fig. 1, extends the traditional flamelet regime further up to $Ka = 100$ from the previous upper limit of $Ka = 1$, where Karlovitz number, Ka , is defined as the ratio of chemical time scale to the Kolmogorov time scale. The region between $Ka = 1$ and $Ka = 100$ is called the “thin reaction zones”, and the flamelet assumptions are claimed to be still valid [4].

Two of the widely used sub-grid scale models in large eddy simulation of premixed turbulent combustion are the power-law and flame surface density approaches [5,6]. In these models, as stated above, the turbulent flame speed can be represented as the product of the laminar flame speed, S_L , corrected for the effects of stretch (strain and curvature) and the wrinkled flame surface area. As shown in [1–3], passive surface character of the flamelets may not be preserved beyond certain turbulence conditions, and flamelet formulations may require corrections due to effects other than surface area growth and flame stretch. This implies that the structure of the flame front deviates from the thermal structure of a laminar flame. This may not necessarily imply flame thickening, but may involve alterations in the thermal structure of the flame front.

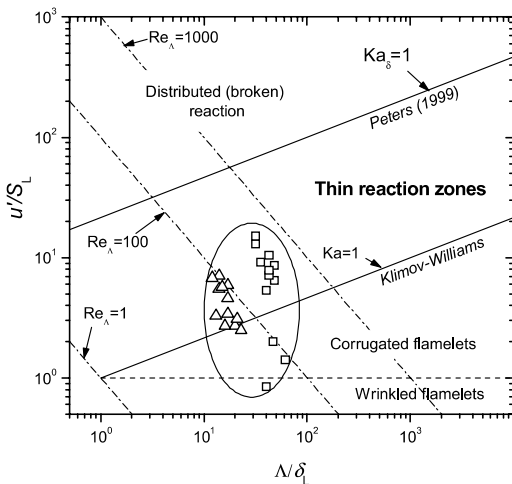


Fig. 1. Diagram of premixed turbulent combustion regimes (adapted from [3]). Note the range of the thin reaction zone regime, and $Ka_s = 100 Ka$. Circled area shows the two sets of data in Fig. 2.

The probability of the flame front alteration in the thin reaction zones regime by penetration of smaller size eddies into the flame front, and the enhancement of heat and mass transport should not be ignored, and there is some experimental evidence of this happening [7]. This paper proposes a simple scheme to estimate the contribution of the flame front alteration by small scale turbulence on flamelet burning velocity. The proposed formulation can be used in flamelet models and premixed turbulent combustion closures to include the contributions of flame front alteration by small scale turbulence. The alteration of the flame front by strain and curvature is not included in this formulation. Strain and curvature effects are understood relatively better than the alteration of flame front by penetrating small scale eddies, and several models exist to estimate the strain and curvature effects on flamelet velocity.

2. Background

Overall heat release Q within the turbulent flame brush of volume V can be written as $Q = \int \rho_u S_L \Delta H \Sigma dV$, where ρ_u is the unburned mixture density, S_L is the laminar burning velocity, Σ is the flame surface density, and ΔH is the enthalpy of reaction of the premixed mixture. For a well-defined geometry of a flame front, overall heat release can be also expressed in terms of a turbulent burning velocity S_T as $Q = \rho_u S_T \Delta H A_o$, where A_o is the area perpendicular to the direction of the flame propagation. These expressions for Q yield

$$\frac{S_T}{S_L} = \frac{\int \Sigma dV}{A_o} \quad (1)$$

Equation (1) is equivalent to the Damköhler's hypothesis that

$$\frac{S_T}{S_L} = \frac{A_T}{A_o} \quad (2)$$

where A_T is the surface area of the turbulent flame front. Another approach of estimating A_T , in addition to Eq. (1), is to use fractal geometry [8], i.e.

$$\frac{A_T}{A_o} = a (\varepsilon_o / \varepsilon_i)^{D_f - 1} \quad (3)$$

where D_f is the fractal dimension ε_o is the outer cutoff, ε_i is the inner cutoff, and a is a constant of order unity. Equation (3) assumes that the wrinkled flame sheet structure displays self-similarity.

Experimental data [1,3] fail to validate Eq. (1). Further, there is a growing body of experimental evidence that does not support Eq. (2) (see [2] for a critical assessment of the experimental fractal dimension data published). Figure 2 shows

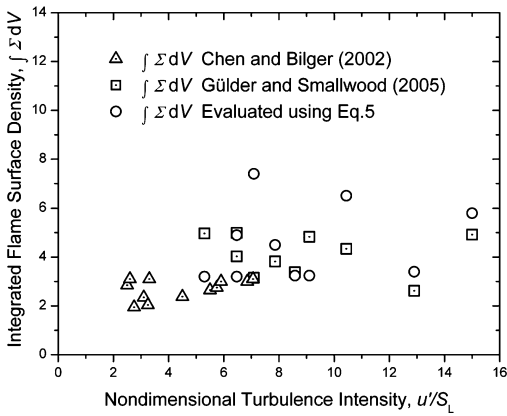


Fig. 2. Integrated flame surface density data from [1] and [3] plotted as a function of non-dimensional turbulence intensity. Also plotted are the integrated flame surface densities evaluated by using Eq. (5) from the same flame images as in [3].

the experimental data [1,3] that represent the right hand side of the Eq. (1) plotted against non-dimensional turbulence intensity, u'/S_L . The experimental setup used to obtain the data used in this study is described in detail in [2]. A brief outline will be given here. The turbulent premixed conical flames were produced by two axisymmetric Bunsen-type burners with inner nozzle diameters of 11.2 and 22.4 mm. Premixed turbulent propane–air flames with equivalence ratios of 0.8 and 1.0 were stabilized by using an annular propane pilot for low turbulence flames and a hydrogen pilot for high turbulence ones. Perforated plates positioned three nozzle diameters upstream of the burner rim controlled the turbulence levels. The turbulence parameters were measured by LDV under reacting conditions where the flow is seeded by fine silicone oil droplets. The length scales, A , and turbulence intensities, u' were measured on the burner centerline at the nozzle exit. The instantaneous flame fronts were visualized both by laser induced fluorescence of OH and by Mie scattering. A tunable excimer laser (Lambda Physik EMG 150T MSC) was used for both techniques. The dimensions of the laser sheet at the burner centerline were about $17\text{ cm} \times 100\ \mu\text{m}$ (FWHM) in the vertical and horizontal planes, respectively. The sheet thickness was less than $150\ \mu\text{m}$ over the full flame width. The optical detector was a large pixel format CCD detector (1242×1152 pixels) giving a flame image spatial resolution of $150\ \mu\text{m}$. At each condition, a minimum of one hundred flame images were captured. The flame front contours were obtained from the LIF of OH and Mie scattering images by the methods described in [2,3]. The flame surface density, based on the gradient of the progress variable across the flame front [9], is given as

$$\Sigma(x) \equiv \langle \Sigma'(x) \rangle = \langle |\nabla c| \delta(c - c_f) \rangle \quad (4)$$

where c is the mean progress variable, ∇c is the spatial flame front gradient, $\delta(c - c_f)$ is the instantaneous flame front position (δ is the Kronecker delta), and $\Sigma'(x)$ is the instantaneous local flame surface density. More recently Shepherd [10] proposed a new technique of obtaining flame surface density from two-dimensional flame front images (see also [11,12]). A two-dimensional estimate of Σ may be calculated from

$$\Sigma(c) = \frac{L(c)}{A(c)} \quad (5)$$

where $L(c)$ is the flame-front length and $A(c)$ is the flame-zone area. The data in Fig. 2 were evaluated by using Eq. (4) (square symbols), and by Eq. (5) (circle symbols).

The area increase in terms of flame surface density integrated over the flame brush displays a very weak, if any, sensitivity to u'/S_L , Fig. 2. Most recent fractal dimension data published in literature [2,13,14] are shown in Fig. 3. As discussed in [2], area increase calculated from experimentally measured fractal parameters, D_f , ε_o , ε_i , is not capable of predicting the observed turbulent burning rates. This implies that the other mechanism(s) may have a non-trivial contribution to the flame propagation in addition to the flame surface area increase by turbulence.

In Eqs. (1) and (2), the laminar burning velocity, S_L , is treated as $S_L = I_o S_L^o$, where I_o is defined as a factor accounting for the strain and curvature effects and usually expressed as a function of the Markstein number, and S_L^o is the unstretched

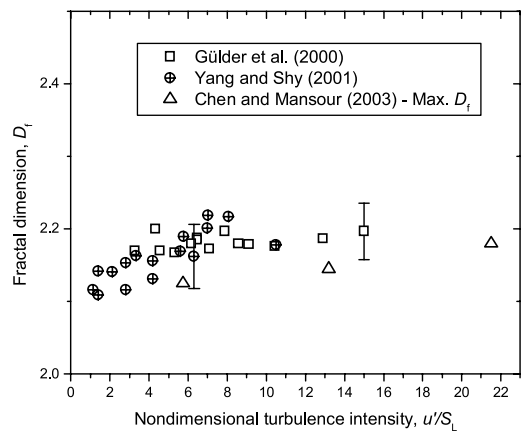


Fig. 3. Comparison of the experimental fractal dimension data from recent studies [2,13,14]. For clarity typical error bars are shown only. Note that the data of [14] represent the maximum values of fractal dimensions measured at the indicated turbulence intensity.

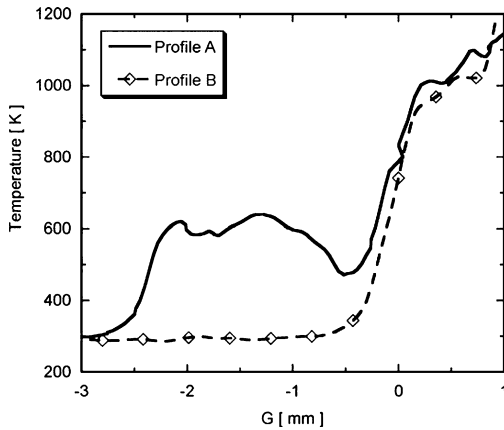


Fig. 4. Temperature profiles upstream of thin reaction zones in a turbulent premixed flame [7]. Solid line (profile A) is the temperature profile when a turbulent eddy was penetrated the preheat zone enhanced the heat transport from the reaction zone to the regions ahead of the preheat zone. Dashed line (profile B) is the profile in the absence of any eddies within the preheat zone.

laminar burning velocity of a planar flame front. In a recent experiment [7], it was shown that eddies of certain size may penetrate the preheat zone of the flame front and increase the temperature ahead of the preheat zone by enhanced transport of heat and species from the reaction zone, Fig. 4. However, the probability density function of temperature ahead of the preheat zone (obtained from numerous single temperature realizations) shows that probability of an eddy penetrating the preheat zone and transporting heat from the reaction zone to regions ahead of the preheat zone is small. The conditional averages of the temperatures ahead of the preheat zone for different turbulence intensities show trivial differences [7].

3. Formulation

Here, it will be argued that the penetration of active eddies of certain size into the preheat layer of the premixed turbulent flame front is not a rare event and may be expressed in terms of the probability of the occurrence of certain size eddies at a given time. This argument is based on the intermittency of the turbulence field and the associated structure functions [15]. With this concept, it may be possible to formulate an effective local burning velocity to replace the S_L in Eqs. (1) and (2), such that

$$S_e = J_o J_o S_L^o \quad (6)$$

where J_o can be defined as the factor of enhancement due to increased effective transport within the preheat layer by the active eddies that may penetrate into the preheat zone of the flame front.

A central assumption in Kolmogorov's theory is the self-similarity of the random velocity field at inertial-range scale [16,17]. Further, turbulence is intermittent meaning that it displays activity during only a fraction of the time, which decreases with the scale. Intermittency is commonly expressed as the structure functions that follow power-laws in the inertial range [15,18]. It is possible to define an intermittency factor [15], in terms of the Kolmogorov capacity dimension D_c and the integral length scale Λ

$$p_x = (x/\Lambda)^{3-D_c} \quad (7)$$

that approximates the fraction of the volume filled by active eddies of scale x . Velocity of the active eddies of size x can be expressed as [15]

$$u_x \sim u'(x/\Lambda)^{(D_c-2)/3} \quad (8)$$

Assuming that active eddies of size x can penetrate the preheat layer, we can define a "micro-turbulent" diffusivity within the preheat layer of the flame front as $\mathfrak{D}'_{mt} \sim xu_x$ in the presence of a penetrating eddy. Taking the intermittency into account gives the effective diffusivity as

$$\mathfrak{D}_{mt} \sim p_x \mathfrak{D}'_{mt} \sim xu'(x/\Lambda)^\alpha \quad (9)$$

where $\alpha = (7 - 2D_c)/3$. For $D_c = 2.8$ [17,18] we get $\alpha \approx 0.5$.

In the turbulence cascade, the next scale under the integral length scale (or the outer scale) is the Taylor microscale. The Taylor microscale can be viewed as the spatial scale across which local velocity values may be treated as approximately invariant [19]. The Taylor microscale can also be understood as the internal viscous shear-layer thickness associated with the large-scale motion spanning the full transverse extent, Λ , of the flow. Therefore it is the smallest scale generated by a Λ -size eddy and defines the range of scales directly connected to integral-scale dynamics by viscous action [20]. As a first approximation, we can take the Taylor microscale as the typical size of the active eddies of size x . A Taylor microscale size eddy may or may not be able to wrinkle the reaction zone sheet, but can stir the preheat zone (even if its characteristic size is larger than the preheat zone thickness) and enhance transport from the reaction zone to the preheat zone and to fresh gas ahead of the preheat zone, provided that it has sufficient strength.

The Taylor microscale, λ , can be used to define the Taylor Reynolds number, see e.g. [21],

$$Re_\lambda = (u'\lambda)/\nu \approx Re_\Lambda^{1/2} \quad (10)$$

where Re_Λ is the Reynolds number based on the integral length scale Λ , defined as $Re_\Lambda = (u'\Lambda)/\nu$.

Then, using Eq. (10), we can express Eq. (9) as follows:

$$\mathfrak{T}_{mt} \sim \nu Re_\lambda^{1/2} \tag{11}$$

For laminar flames we can write the premixed flame velocity as

$$S_L^o \sim \mathfrak{T} / \delta_L^o \tag{12}$$

where \mathfrak{T} is the molecular diffusivity and $\delta_L^o \equiv \mathfrak{T} / S_L^o$ is the Zeldovich thickness. In a similar manner, we can define an enhanced burning velocity as

$$S_e \sim (\mathfrak{T}_{mt} + \mathfrak{T}) / \delta_e \tag{13}$$

where δ_e is the corresponding diffusion thickness, and should be on the same order of magnitude as the Taylor microscale, λ . Since the Schmidt number is $Sc = \nu / \mathfrak{T}$, we have

$$J_o = S_e / S_L^o \approx \left[1 + Sc Re_\lambda^{1/2} \right] (\delta_L^o / \lambda) \tag{14}$$

Using the definition of the Karlovitz number, $Ka = (u' / S_L) (\delta_L^o / \lambda)$, Eq. (14) can be written as

$$J_o \approx \left[1 + Sc Re_\lambda^{1/2} \right] (u' / S_L)^{-1} Ka \tag{15}$$

which should be valid for large values of non-dimensional turbulence intensity. Equation (14) can be used, along with Eq. (6), to estimate the contribution of small scale turbulence to flamelet burning velocity. In the following section, this exercise has been carried out using the available experimental data [1,3].

4. Discussion

The integrated flame surface density data from [1] and [3] (same data as in Fig. 2) replotted in Fig. 5. These integrated flame surface densities, data representing the right hand side of Eq. (2), were corrected by the corresponding values of J_o evaluated from Eq. (14), and plotted in Fig. 5 as blank circle symbols. The difference between blank circle symbols and the integrated flame surface densities represent the contribution to the flamelet velocity by small scale turbulence that increases the transport within the preheat layer. Also shown are the experimentally determined turbulent burning velocities evaluated at $c = 0.5$ (full circle symbols) and $c = 0.05$ (full square symbols), where c is the mean progress variable. The discrepancy between the integrated flame surface densities and the experimental turbulent burning velocities is significant. When the influence of the flame front alteration taken into account using Eq. (14), then the predictions are more close to the measured turbulent burning velocities, Fig. 5.

Up to the non-dimensional turbulence intensities of about 5–7, it seems that the changes in the surface area of the flame play a role in turbulent flame propagation as can be seen in Figs. 2 and 3, and there is experimental and numerical evidence that increase in flame surface area is the dominant factor in increasing the turbulent burning velocity with turbulence intensity within the “corrugated flamelets” regime shown in Fig. 1, see, for example [22,23]. However, this effect

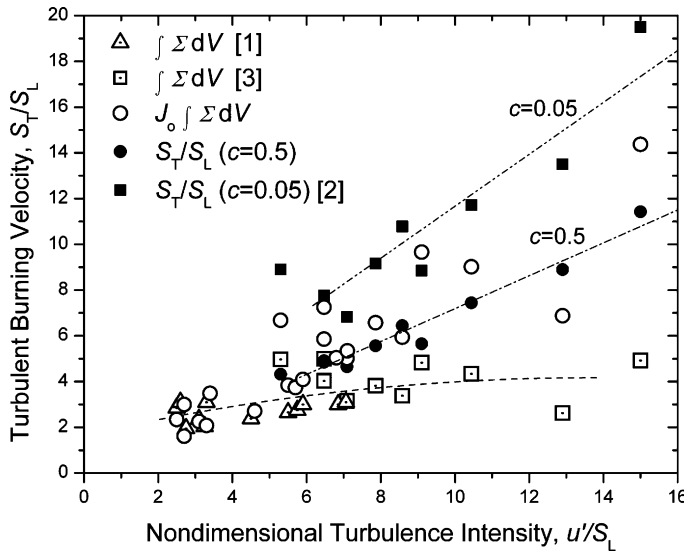


Fig. 5. Integrated flame surface density data of [1] and [3] are replotted from Fig. 2. Also shown are the experimentally determined turbulent burning velocities (for the data of [2,3]) evaluated at $c = 0.5$ (full circles) and $c = 0.05$ (full squares), using the same methodology as described in [22], where c is the mean progress variable. Two dot-dash straight lines are approximate linear fits to experimental turbulent burning velocity data. Blank circles represent the product of J_o [Eq. (14)] and integrated flame surface density [i.e., right hand side of the Eq. (3)].

seems to diminish as the turbulence intensities increase further. In the regime of thin reaction zones, the probability of alteration of the flame front (most probably the preheat zone) by the penetration of active eddies may not be negligible, and the flamelet models applied to the thin reaction zones regime may need correction to take into account flame front alteration. It should be emphasized that the thickness of the flame front is much larger than the Zeldovich thickness. Most recent measurements indicate that flame front thickness, defined as $\delta_{th} \equiv (T_b - T_u)/|\nabla T|_{max}$, may be estimated as $7.4(\mathfrak{Z}/S_L^0)$ [22], where T_b and T_u are the burned and unburned gas temperatures, respectively, and ∇T is the temperature gradient within the flame front. In [22], the reaction zone thickness, measured as the thickness of the CH layer, is larger than 0.5 mm which is comparable to or larger than the Taylor microscale measured under the same conditions.

Zimont [24] and Ronney and Yakhot [25] proposed formulations based on the *ad hoc* assumption that the flame front gets thicker with increasing turbulence intensity. It is postulated that [25] the laminar flame front will be thickened by the small scales of turbulence increasing the transport rates and wrinkled by the large scales. Both formulations [24,25] assumed that the small scales of turbulence would broaden the flame front and increase transport rates within the flame front causing faster burn rates. The distinction of the current formulation is that the intermittency arguments and structure functions were used to estimate the probability of existence of a certain size eddy at a given location.

The experimental turbulent burning velocity data in Fig. 5 do not explicitly show the bending effect, although the bending effect is shown to be physically present by several investigators, both experimentally and numerically (see, e.g. [25]).

5. Concluding Remarks

There is sufficient experimental evidence that the flame surface area increase is not the dominant mechanism in increasing the turbulent burning velocity under the conditions corresponding to the thin reaction zones regime. When the non-dimensional turbulence intensity, u/S_L , exceeds about 6–7, the flame surface area increase estimated by the fractal analysis or flame surface density approaches does not explain the observed increases in the turbulent burning velocity. One of the potential contributors is the enhancement of the transport within the flame front by small size eddies that could penetrate into the preheat layer. An expression has been derived to estimate the contribution of flame front alteration, as a consequence of the small scale turbulent eddies that may penetrate into the preheat layer of the premixed flame

front, to the flamelet burning velocity. The derivation was based on: (a) there is experimental evidence of flame front alteration by active eddies penetrating into the preheat layer and enhancing the transport, (b) these active eddies have a characteristic size approximating the Taylor microscale, and (c) within the turbulence cascade the volume occupied by a certain size eddy and its velocity obey power-law relationships (i.e. structure functions), dictated by the intermittency of the turbulent field. The predictions of the proposed expression agree with the limited experimental data on premixed turbulent burning velocities.

Acknowledgments

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Comments

Heinz Pitsch, Stanford University, USA. First, in your evaluation of the turbulent burning velocity in the thin reaction zones regime, you use the laminar burning velocity as the propagation speed of the instantaneous flame front and show then that the resulting turbulent flame speed is too low. However, in the theory for the thin reaction zones regime by Peters, [1] the propagation speed of the instantaneous flame is given by $s_{\kappa} = D\kappa$, where D is the diffusivity and κ is the local flame curvature. He argues that this value is much higher than the laminar burning velocity in this regime. Did you evaluate the turbulent flame speed based on this expression and if so, how does it compare to your data?

Second, in using the Taylor micro-scale as the thickness for the broadened flame thickness in the thin reaction zone regime; both in laminar flames and in the theories of Damköhler and Peters, this thickness depends on a chemical time scale, whereas in your model, the thickness is independent of the chemistry. What is the basis for this assumption?

Reference

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Reply. Our evaluation, based on the measured curvature averaged over the whole flame surface and the molecular diffusivity corresponding to the reaction zone temperature, yielded s_{κ} values very similar to unperturbed laminar burning velocities. The proposal that s_{κ} should be used instead of the laminar burning velocity in the thin reaction zone regime is based on the two-dimensional DNS data [1]. Figure 7a in [1] verifies our evaluation that the contribution of s_{κ} is trivial for lean (equivalence ratio 0.8) flames for the normalized curvature of about 0.4–0.8.

The physical model adapted in this work does not necessarily invoke broadening of the flame thickness. Use of

the Taylor micro-scale as the diffusion thickness is a first approximation, as stated in the paper.

Reference

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Jerzy Chomiak, Chalmers University of Technology, Sweden. Since 1976 [1] I have been arguing that in high Reynolds number flow the small scale intermittency and coherence may play an important role in flame propagation, which changes from a surface reaction mechanism to a leading point mechanism with much lower surface densities, as shown in your experiments.

Since 1976 [1] I have been arguing that in high Reynolds number flow the small scale intermittency and coherence may play an important role in flame propagation, which changes from a surface reaction mechanism to a leading point mechanism with much lower surface densities, as shown in your experiments.

Reference

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Reply. The idea that at high enough Karlovitz numbers the nature of flame propagation cannot be explained by laminar flamelet concepts is not new. Contributions of small scale turbulence is considered by Chomiak ([1] in above comment) and ([24,25] in paper), among others. The intermittency of small scale turbulence and how it would affect the turbulent flame structure are also discussed by many including [1]. The contribution of the current work is to formulate the effect of small scale turbulence using the intermittency structure functions and compare the predictions to experimental data.