Turbulent flame speed based on mass flow rate of reactants

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Abstract

Starting with an integral formulation of mass flow rate of reactants through an ensemble of isotherms within a statistically planar, turbulent premixed flame, a scaling for the corresponding turbulent flame speed is derived. Closure relations for the local flame displacement speed and scalar dissipation rate anomaly are invoked and a new length scale quantifying the fluctuation distance of the isotherms within the premixed flame structure is introduced. Damköhler’s hypotheses are not used at any stage. Eventually, the scaling is extended to expanding turbulent premixed flames.

1 Introduction

Turbulent flame speed has been a topic of active research since Damköhler’s 1940 paper [1]. Of the two hypotheses proposed in this paper, the first hypothesis suggests that for premixed flames in weak turbulence, the turbulent flame speed is proportional to the flame surface area. The second hypothesis suggests that for premixed flames in intense turbulence, the turbulent diffusivity instead of thermal diffusivity determines the turbulent flame speed, which results in a corresponding $Re_T^{1/2}$ scaling. Here $Re_T = u'_\text{rms} l_I/(S_L l_F)$ and $S_L$ is the flame speed of an unstretched, planar, laminar premixed flame [2]. $u'_\text{rms}$ is the root mean

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square of the fluctuating velocity. $l_I$ is the integral length scale, $l_F$ is the diffusion thickness of the flame. Note $S_L l_F = \alpha$ the thermal diffusivity, and with unity Schmidt number $Sc = 1$ assumption $\nu = S_L l_F$. The reader is recommended to refer to Driscoll et al. [3] for a state of the art interpretation of the Damköhler’s hypotheses based on recent measurements. As such, since 1940s several expressions of the form $S_T = f(S_L, u'_{rms}, l_I, l_F)$ have been sought. Clavin suggested a quadratic relation between $S_T$ and $u'_{rms}$ [4]. Yakhot used renormalization theory to derive an expression for $S_T$ [5]. Lipatnikov and Chomiak [6] introduced a turbulent Markstein number to obtain a turbulent flame speed expression for expanding turbulent flames. Kolla et al. [7] used the transport equation of the averaged scalar dissipation rate, their associated closures, and the KPP theorem [8] to derive an expression for turbulent flame speed for large Damköhler number ($Da$) flames. Kerstein et al. [9] used the $G-$equation to derive an expression for $S_T / S_L$ as a volume integral of the absolute gradient of the level set function $G$ [9]. The $G-$equation approach was also utilized by Peters [10] to obtain turbulent flame speeds in both the corrugated and thickened flamelet regimes. Chaudhuri et al. [11] extended Peters’s spectral formulation of the $G-$equation to derive an expression for turbulent flame speed. Some of the issues with $G-$equation approach are restrictive initial condition as in [9], averaging issues [12, 13], and their interpretation towards obtaining scaling relations for dissipation rate of the level-set function itself. The difficulty in utilizing averaged transport equations of progress variables to determine turbulent flame speed involves closures of the several terms and their applicability over large ranges of $Re_T$ and $Ka$. Here $Ka$ is the Karlovitz number. The reader could refer to the following review papers and books for a much more detailed exposition on this topic [14, 8, 15, 16, 3, 17, 18].

In many cases, the derivations of turbulent flame speed begin with Damköhler’s hypotheses and often the turbulent flame speed itself is not rigorously defined. Perhaps there is a need to revisit turbulent flame speed theoretically, from first principles, without invoking any hypothesis or ambiguous definitions. In this paper, we initiate the derivation of turbulent flame speed of statistically planar premixed flames, from first principles, by rigorously estimating the averaged mass flow rate through an ensemble of propagating surfaces. Such a mass flow rate constitutes the basis of the turbulent flame speed defined in this paper. However, in later stages, we do introduce closures of local flame displacement speed and mean
scalar dissipation rate. A new length scale based on the statistics of fluctuation distance of individual iso-scalar surfaces is also introduced.

2 Derivation

Consider a statistically planar premixed flame in a rectangular cuboid domain with a square cross-section - a configuration widely adopted in fundamental turbulent premixed flame studies. Turbulent, premixed reactants enter from one of the square-faces with a mean velocity in the $x-$direction to interact with the statistically stationary premixed flame downstream. We are only interested in conditions with turbulence Reynolds number $Re_T > 100$ and Karlovitz number $Ka > 1$.

The standard temperature based progress variable $c$ is defined as

$$c = \frac{T - T_u}{T_b - T_u}$$  \hspace{1cm} (1)

Here, $T_u$ is the temperature of the unburnt reactants and $T_b$ is the temperature of the fully burnt products. Consider an iso-$c$ surface given by $c = c^*$, within the flame structure of finite thickness. It is necessary to recognize that this surface could be wrinkled, multiply folded, disconnected and/or distributed over large part of the domain. The only necessary condition to define the iso-$c$ surface, locally, is $\nabla c \neq 0$. The mass flow rate through such a surface is given by

$$\dot{m}_{c^*} = - \int_{A_{T_{c^*}}} \rho \vec{v}_r \cdot \hat{n} dA$$ \hspace{1cm} (2)

Here $\rho$ is the local density, $\vec{v}_r$ is the flow velocity relative to the local surface, $\hat{n}$ is the local surface normal pointing towards lower temperature flow and $A_{T_{c^*}}$ is the total area of the surface defined by $c = c^*$. Now, the local flow velocity relative to the velocity of the local surface is given by $\vec{v}_r$, where

$$\vec{v}_r = \vec{u} - \vec{v}_f$$ \hspace{1cm} (3)

Here $\vec{u}$ is the local flow velocity and $\vec{v}_f$ is the local surface velocity. The following identity for local flame surface velocity is well known
\[ \vec{v}_f = \vec{u} + S_d \cdot \hat{n} \]  

(4)

where \( S_d \) is the local flame displacement speed. Using Eqs. [3] and [4] in Eq. [2] we rewrite the mass flow rate through the surface as:

\[ \dot{m}_{c^*} = - \int_{A_{T_{c^*}}} \rho (-S_d \hat{n}) \cdot \hat{n} dA \]  

(5)

Based on the \( \dot{m}_{c^*} \) we can define a surface specific turbulent flame speed \( S_{T_{c^*}} \) as

\[ \rho_u S_{T_{c^*}} A_0 = \dot{m}_{c^*} \]  

(6)

\( A_0 \) is the area projected by \( A_{T_{c^*}} \) onto the inlet plane of the cuboid. This is of course equal to the cross sectional area of the cuboid. Equating Eq. [5] and Eq. [6] we get

\[ \rho_u S_{T_{c^*}} A_0 = - \int_{A_{T_{c^*}}} \rho (-S_d) dA \]  

(7)

which yields

\[ S_{T_{c^*}} = \frac{1}{A_0} \int_{A_{T_{c^*}}} \tilde{S}_d dA \]  

(8)

Here \( \tilde{S}_d = \rho S_d / \rho_u \) is the density weighted flame displacement speed. However, as noted before, LHS represents the surface specific turbulent flame speed. We can transform it to a generalized turbulent flame speed by averaging over all \( c = c^* \), by integrating from \( c_{\text{min}} \) to \( c_{\text{max}} \). These are 0 and 1, respectively. Therefore,

\[ S_T = \frac{1}{(c_{\text{max}} - c_{\text{min}})} \int_{c_{\text{min}}}^{c_{\text{max}}} S_{T_{c^*}} dc^* \]  

(9)

Substituting Eq. [8] into Eq. [9] we obtain:

\[ S_T = \frac{1}{A_0} \int_0^1 \int_{A_{T_{c^*}}} \tilde{S}_d dA dc^* \]  

(10)

Now, the area integral could be transformed to a volume integral using the delta function \( \delta(c - c^*) \),

\[ S_T = \frac{1}{A_0} \int_0^1 \int_V \tilde{S}_d \delta(c - c^*) |\nabla c^*| dV dc^* \]  

(11)
Using the well-known relation
\[
\int_{c^*} f(c^*) \delta(c - c^*) \, dc^* = f(c)
\] (12)
we arrive at
\[
S_T = \frac{1}{A_0} \int_V \tilde{S}_d \lvert \nabla c \rvert dV
\] (13)
which could also be written using volume average denoted by \( \langle \rangle \). Note that using the level
set formulation given by \( G \)–equation and starting with the initial condition \( G(x,0) = x \),
Kerstein et al. [9] obtained an expression similar to Eq. 13 albeit in terms of gradient of \( G \).

Now our volume of interrogation is the portion of the cuboid with lateral dimensions \( L \) and axial dimension equal to the flame brush thickness \( \delta_T \). Also note \( L^2 = A_0 \). Therefore
Eq. 13 yields:
\[
S_T = \frac{L^2 \delta_T}{A_0} \langle \tilde{S}_d \lvert \nabla c \rvert \rangle
\] (14)
The RHS of this equation can be simplified with the assumption \( \langle \tilde{S}_d \lvert \nabla c \rvert \rangle \approx S_L \langle \lvert \nabla c \rvert \rangle \) for unity Lewis number (\( Le \)) flames. Alternatively, in the paragraphs below (till the end of the paragraph associated with Eq. 17) we show how a similar relation could be obtained using closure models for \( \tilde{S}_d \).

There is a vast literature establishing linear and non-linear relations between flame speed and stretch rate for steady, laminar premixed flames [20, 21, 22, 23, 2]. However, in the \( Ka > 1 \) limit we are considering, local flame structure could be significantly different from steady, stretched, laminar flames. As such, it has been recently shown that in intense turbulent premixed flames, the largest deviations of local \( \tilde{S}_d \) from \( S_L \) originate from flame-flame interactions [24] which ultimately leads to self-annihilation of the local flame surface. \( \kappa \) is defined as the local curvature i.e. \( \kappa = (\kappa_1 + \kappa_2) \) where \( \kappa_1 \) and \( \kappa_2 \) are the principal curvatures, with the convention that a surface convex towards reactants implies positive \( \kappa \). Also, the thermal thickness of a standard laminar premixed flame is defined as \( \delta_L = (T_b - T_u)/\lvert \nabla T \rvert_{max} \).

In moderate to intense turbulence, large portions of any iso-scalar surface within a flame are characterized by \( \kappa \delta_L \leq -1 \). Since their local radius of curvature is smaller than the flame thickness and the surface is propagating inwards, flame-flame interaction at some level is inevitable, in those portions. Since these portions of the flame are undergoing flame-flame
interaction – an inherently transient phenomena, the weak-stretch theories developed for stretched, steady, laminar premixed flames are not expected to be applicable. This was explicitly showed by Dave and Chaudhuri [24] who also analyzed a cylindrical, imploding, interacting and hence unsteady laminar premixed flame and showed that for the interacting stage $S_d \approx -2\alpha_0\kappa$ while $\kappa\delta_L \ll 0$. Now, for the non-interacting portions that are weakly stretched, the local flame displacement speed could be explained by the two-Markstein length weak stretch theories [25, 26, 24]. However, in those portions, to a leading order $\tilde{S}_d \approx S_L$. Indeed, the stretch rate deviates $\tilde{S}_d$ from $S_L$ but that deviation is much smaller than $S_L$ itself. In such a scenario, a model equation applicable for both non-interacting and interacting portions could be written as $\tilde{S}_d = S_L - 2\tilde{\alpha}_0\kappa$ for $\kappa \leq 0$. This was shown using a DNS database of lean $H_2 - air$ premixed flames for a fixed equivalence ratio [27]. For $\kappa > 0$ it appears from DNS data, that while a linear relation between $\tilde{S}_d - \kappa$ holds, the slope is different from $2\tilde{\alpha}_0$. As such Peters [10] proposed a similar linear relation between $S_d$ and $\kappa$ across corrugated flamelet and thin reaction zone regimes, albeit with different numerical coefficients. In any case, a very specific form of the $\tilde{S}_d - \kappa$ relation is not necessary to arrive at a leading order scaling of $S_T$. Hence, the following generic linear relationship between $\tilde{S}_d$ and $\kappa$ is considered:

$$\tilde{S}_d = S_L - A_1\kappa \quad \forall \kappa \leq 0$$

$$\tilde{S}_d = S_L - A_2\kappa \quad \forall \kappa > 0$$

(15)

$S_L$ is the unstretched planar laminar flame speed. Note that $A_1, A_2$ are functions of $\tilde{\alpha}_0$, heat release rate and $Le$ for non-unity $Le$ flames. Substituting Eq. 15 into Eq. 14 we get

$$S_T = \delta_T \langle S_L | \nabla c | \rangle - \delta_T \langle A_1\kappa | \nabla c | \rangle_{\kappa \leq 0} - \delta_T \langle A_2\kappa | \nabla c | \rangle_{\kappa > 0}$$

(16)

Now, from DNS data it appears that for $|\kappa|\delta_L > 1, \kappa|\nabla c| \approx k_0$ holds, statistically. Here $k_0$ is an $O(1)$ constant whose sign and magnitude could depend on the sign of $\kappa$. This can be explained from the limiting condition of flame-flame interaction which leads to very large negative $\kappa$, small $|\nabla c|$, and large $\tilde{S}_d$. During the end stages of flame-flame interaction, as $\kappa \to \infty, |\nabla c| \to 0$. Furthermore, large positive $\kappa$ is typically generated by positive normal straining [28]. Orthogonal to the positive normal strain rate, compressive strain rate aligns with the direction of the local scalar gradient in small $Da$ (and hence typically larger than
unity $Ka$) turbulent premixed flames [29] as in passive scalar turbulence [30], statistically. Clearly, extensive normal strain would lead to reduction of the magnitude of the scalar gradient while increasing positive curvature. Simultaneously, compressive normal strain would result in amplification of the scalar gradient magnitude while reducing the positive curvature. Thus increase (decrease) of $\kappa$ is often associated with decrease (increase) of $|\nabla c|$; hence their product could be assumed to be a constant. As such, from DNS data [31, 27] it can be ascertained that for either sign of $\kappa$, the product $\kappa|\nabla c|$ tends to respective constants, statistically. We can write that for $\kappa \leq 0$, $\kappa|\nabla c| \approx -k_1$ while for $\kappa > 0$, $\kappa|\nabla c| \approx k_2$. where both $k_1, k_2$ are positive constants. Substituting these into Eq. 16 we get:

$$\frac{S_T}{S_L} = \delta_T \langle |\nabla c| \rangle + \frac{\delta_T}{S_L} (\mathcal{A}_1 k_1 - \mathcal{A}_2 k_2)$$ (17)

For close to unity $Le$ flames, the second term is essentially a difference of two constants of similar magnitudes, should be much smaller than the first term, and hence could be neglected. For $Le < 1$ we expect $\mathcal{A}_2 < \mathcal{A}_1$ and hence for non-unity $Le$, $S_T/S_L$ will be amplified w.r.t. unity or greater than unity $Le$ conditions, all other parameters held fixed. Such amplification of $S_T$, for $Le < 1$ flames is discussed extensively in [15]. In any case, it is apparent that while the first term on the RHS of Eq. 17 is the leading order term, in certain conditions, the second term on the RHS could lead to non-negligible corrections. A complete quantitative understanding of the entire second term needs further work. In the rest of the paper, we will focus on the leading order first term on the RHS of Eqn. 17 where $\langle |\nabla c| \rangle$ is the important factor.

For intensely turbulent flames $\langle |\nabla \tilde{c}| \rangle \ll \langle |\nabla c'| \rangle$, where $c(x, y, z, t) = \bar{c}(x, t) + c'(x, y, z, t)$. Hence, it is reasonable to assume:

$$\langle \nabla c \cdot \nabla c \rangle^{1/2} \approx \langle \nabla c' \cdot \nabla c' \rangle^{1/2}$$ (18)

Given that local scalar dissipation rate $\chi$ is nearly log-normally distributed, in intense turbulent premixed flames [32, 33], it is also reasonable to assume $\langle \chi^n \rangle / \langle \chi \rangle^n \approx 1$ where $\chi = 2\alpha(\nabla c' \cdot \nabla c')$. Therefore,

$$\langle |\nabla c'| \rangle = \langle (\nabla c' \cdot \nabla c')^{1/2} \rangle \approx \langle \nabla c' \cdot \nabla c' \rangle^{1/2}$$ (19)
Given that quasi-lognormal distribution of local scalar dissipation rate holds in intensely turbulent premixed flames, one can invoke the scaling originating from scalar dissipation rate anomaly (since the RHS in Eq. 20 is independent of diffusivity, it is ostensibly an “anomaly”) well established for passive scalars in isotropic turbulence \[34\]. The implicit assumption is that for \(Ka \geq O(1)\), the scalar dissipation rate statistics is independent of dilatation originating from local heat release rate, to the leading order. Hence, we write:

\[
\langle \chi \rangle = 2\alpha \langle \nabla c' \cdot \nabla c' \rangle \sim \frac{u'_r \langle c'^2 \rangle}{l_I} = \frac{u'_r \langle c'^2 \rangle_r}{r} \tag{20}
\]
yielding

\[
\langle |\nabla c'| \rangle \approx \langle |\nabla c'| \rangle \sim \left[ \frac{u'_r \langle c'^2 \rangle}{2\alpha l_I} \right]^{1/2} \tag{21}
\]
The length scale \(r\) could be any length scale within the inertial range. Note that there exist sophisticated models for mean scalar dissipation rate \[35, 7\] for turbulent combustion especially for lower \(Da\) flames. However, in \(Ka > 1\) turbulence, the scalar dissipation rate anomaly scaling is expected to hold to the leading order, as evident from the scaling by Kolla et al. \[7\]. Substituting Eq. 21 into Eq. 17, we get to the leading order:

\[
\frac{S_T}{S_L} \sim \delta_T \left[ \frac{u'_r \langle c'^2 \rangle}{2\alpha l_I} \right]^{1/2} \tag{22}
\]

Next, we need to find a scaling relation for \(\langle c'^2 \rangle\). To that end, we linearize the monotonically increasing function \(\bar{c}(x,t)\) within the flame brush. The mean flow is along \(x\)–coordinate. \(x\) represents the axial direction; \(y, z\) representing the transverse directions of the cuboid. Note that the \(\bar{c}(x,t)\) is not necessary a linear function with distance, but is assumed here to retain mathematical tractability of the analysis. A more elaborate function like error function could be used as well. Outside the flame brush \(\bar{c}(x,t)\) becomes 0 and 1 on the unburnt and burnt sides, respectively. Assuming:

\[
\bar{c}(x,t) = \frac{x}{\delta_T}
\]
\[
c(x,y,z,t) = \bar{c}(x,t) + c'(x,y,z,t) \tag{23}
\]
\[
\Rightarrow c = \frac{x}{\delta_T} + c'
\]
\( \bar{c}(x,t) \) represents averaged \( c(x,y,z,t) \) over y-z direction at any instant \( t = t \). Next, we set:

\[
c = c^*
\]

Therefore

\[
c^* = \frac{x_{c^*}}{\delta_T} + c'
\]

\[
\Rightarrow x_{c^*} = \delta_T (c^* - c')
\]

Here, \( x_{c^*} \) denotes the \( x \)-coordinates of the surface \( c = c^* \). Utilizing \( x_{c^*} \), we can obtain the statistic of the distance over which the surface \( c = c^* \) fluctuates given by the variance of \( x_{c^*} \), denoted by \( \ell_{T_c^*}^2 \).

\[
\ell_{T_c^*}^2 = \frac{1}{L^2} \int_y \int_z (x_{c^*} - \bar{x}_{c^*})^2 dydz
\]

Substituting Eq. 23 into Eq. 25 we get:

\[
\ell_{T_c^*}^2 = \frac{\delta_T^2}{L^2} \int_y \int_z (c^* - c' - c^* + \bar{c}')^2 dydz
\]

Since, \( \bar{c}' = 0 \), the above equation leads to

\[
\ell_{T_c^*}^2 = \frac{\delta_T^2}{L^2} \int_y \int_z (-c')^2 dydz
\]

Next we average the above equation over the flame brush thickness \( \delta_T \) in the \( x \) direction to obtain a generalized flame surface fluctuation distance \( \ell_{T} \) given by

\[
\ell_T^2 = \frac{\delta_T^2}{L^2} \int_y \int_z (-c')^2 dxdydz
\]

This yields a closure for \( \langle c'^2 \rangle \) in terms of \( \delta_T \) and \( \ell_T \).

\[
\ell_T^2 = \delta_T^2 \langle c'^2 \rangle
\]

Substituting Eq. 29 into Eq. 22 we get

\[
\frac{S_T}{S_L} \sim \left[ \frac{u'_{rms} \ell_T^2}{S_L l_F l_I} \right]^{1/2}
\]

\( l_F \) is the diffusion thickness of a standard laminar premixed flame. The largest flame surface fluctuations determining its variance should be induced by the largest length scales of turbulence. Hence, it is reasonable to assume \( \ell_T \sim l_I \), yielding

\[
\frac{S_T}{S_L} \sim \left[ \frac{u'_{rms} l_I}{S_L l_F} \right]^{1/2}
\]
Assuming $S_L l_F = \alpha \approx \nu$, we get
\[ \frac{S_T}{S_L} \sim Re_T^{1/2} \] (32)
to the leading order. This is also the expression that was obtained by Damköhler [1] in the intense turbulence limit, by replacing thermal diffusivity with turbulent diffusivity and retaining identical chemical time scales between laminar and turbulent flame configurations. Despite years of research turbulent diffusivity remains incompletely understood, especially for reactive scalars. In any case we have not used turbulent diffusivity neither any assumption on the chemical time scales. Equation 32 is also consistent, in part, with the results from [10, 7, 11, 36], often derived for global consumption speed, using different techniques and associated assumptions.

The form of the scaling provided by Eq. 32 is consistent with the “bending behavior” of turbulent flame speed observed in DNS. However, a very large database focusing on turbulent flame speed scaling over a wide range of $Ka$ is rare. Aspden et al. [37] using DNS with detailed chemistry showed that the consumption speed $S_{T,GC} \sim Re_T^{1/2}$ holds over three decades of $Ka$ out of the four decades of $Ka$ investigated for both $H_2$– and $CH_4$–air turbulent premixed flames. However, the number of data-points are limited. When reactants are fully consumed the $S_T$ defined in this paper should be equal to $S_{T,GC}$. The large DNS database of Yu and Lipatnikov [38] obtained using single step chemistry clearly showed that $S_{T,GC}/S_L \sim Re^{1/2}$, for small $Da$. Experimentally obtained statistically planar turbulent flame speeds are not common. The configuration that is closest to the statistically planar turbulent premixed flame is the turbulent expanding flame configuration. However, the results derived for statistically planar flame configuration cannot be directly applied in the expanding flame configuration. For an expanding premixed flame with average radius $\langle R \rangle \gg l_F$, we can consider a sector of the turbulent expanding flame to be a statistically quasi-planar, quasi-steady flame enclosed in a cuboid box with lateral dimensions equal to the $\langle R \rangle$. Indeed the characteristic dimensions of the expanding flame $\langle R \rangle$, flame-brush thickness $\delta_T$ are monotonically increasing with time $t$. Furthermore, $\delta_T$ monotonically increases with $\langle R \rangle$. In view of this the averaged scalar dissipation rate, measured within the cuboid of lateral dimension $\langle R \rangle$ is obtained from Eq. 20 as:
\[ \langle \chi \rangle_{\langle R \rangle} = 2\alpha \langle \nabla c' \cdot \nabla c' \rangle_{\langle R \rangle} \sim \frac{u'_{\langle R \rangle} \langle c'^2 \rangle_{\langle R \rangle}}{\langle R \rangle} \] (33)

The rest of the derivations proceeds similar to that of the statistically planar flames with the difference that in the expanding flame configuration the flame surface fluctuation length scale \( \ell_T \sim \langle R \rangle \). Substituting these yields:

\[ \frac{S_T}{S_L} \sim \left[ \frac{u'_{\langle R \rangle} \langle R \rangle}{S_L l_F} \right]^{1/2} \] (34)

Similar scaling has been experimentally demonstrated by at least five groups in the last decade [39, 40, 41, 42, 43, 44, 45]. Indeed, given the constitutive relations, scalings introduced, the match between the experimental and theoretical results should not be considered evidence of a “proof” that \( S_T/S_L \sim Re_T^{1/2} \) is universal. Different scalings resulting from physics or configuration not considered in the present derivation is certainly possible and merit further exploration.

3 Conclusions

Starting with the mass flow rate of reactants passing through an ensemble of isotherms constituting a statistically planar turbulent premixed flame, a leading order scaling of the turbulent flame speed: \( S_T \sim Re_T^{1/2} \) is obtained. To this end, the local flame displacement speed closure originating from flame-flame interaction, validated over a range of \( Ka \) for \( H_2 \)-air turbulent premixed flames is used. The scalar dissipation rate anomaly is also used alongside a linearized mean progress variable profile which yields a simplified scaling of the isotherm fluctuation distance - a new length scale. Finally, the scaling obtained is extended to sufficiently large expanding flames experiencing negligible mean stretch.

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