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Transport equation for premixed flame curvature conditioned to reaction zone in turbulent flow

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ABSTRACT

A compact transport equation is obtained for modeling evolution of flame curvature field in a turbulent flow. While known curvature transport equations are reduced to the newly derived one, the latter contains significantly fewer terms. The newly derived equation is also conditioned to flame reaction zone of a finite thickness and various terms in the conditioned transport equation are analyzed by processing two Direct Numerical Simulation (DNS) databases by Dave and Chaudhuri (Evolution of local flame displacement speeds in turbulence, *J. Fluid Mech.* 884 (2020) A46) and by Yuvraj et al. (How “mixing” affects propagation and structure of intensely turbulent, lean, hydrogen-air premixed flames, *Combust. Flame* 273 (2025) 113,903). Both DNS sets deal with complex-chemistry hydrogen-air flames. In one case, the equivalence ratio ϕ is equal to 0.81, diffusional-thermal effects are weakly pronounced, and turbulence is moderately intense (Karlovitz number $Ka = 13$). In another case, $\phi = 0.4$, diffusional-thermal effects play an important role, and turbulence is more intense ($Ka = 115$). Nevertheless, major qualitative trends found by analyzing the DNS data are similar in both cases. First, the data show that evolution of conditioned curvature is primarily controlled by two terms, which describe (i) curvature production by non-uniform velocity field and (ii) curvature reduction due to flame propagation. Second, application of Helmholtz-Hodge decomposition to the DNS velocity fields shows that the former term is controlled by rotational motions, contrary to the local flame strain rate, which is generated by irrotational motions in both flames. This fundamental difference between the effects of turbulent velocity field on flame strain rate and curvature should be considered when modeling such effects.

Novelty and significance statement: Transport equation for premixed flame curvature field is obtained in a compact form. A new transport equation for curvature conditioned to flame reaction zone is derived. DNS data obtained from two lean hydrogen-air turbulent flames show that the r.h.s. of the latter equation involves two predominant terms which describe (i) curvature production by velocity field and (ii) curvature reduction due to flame propagation. Application of Helmholtz-Hodge decomposition to the DNS velocity fields shows that the former term is controlled by rotational motions, contrary to the local flame strain rate, which is generated by irrotational motions. The derived equations open new perspectives for modeling the influence of turbulence on local premixed flame structure and burning rate. Performed analyses of the newly derived conditioned equation have generated new knowledge. Specifically, finding that evolutions of curvature and flame strain rate are controlled by rotational and irrotational motions, respectively, is significant from fundamental perspective.

1. Introduction

Rapidly growing interest [1] in combustion of lean mixtures of hydrogen or H₂-containing fuel blends calls for research into diffusional-thermal effects, which trigger laminar flame instability [2]

and greatly increase turbulent burning velocity U_T [3–7]. This increase in U_T is associated [8] with appearance of highly curved inherently laminar reaction zones in turbulent flows. Significant influence of such zones on U_T was clearly shown in many Direct Numerical Simulation (DNS) studies reviewed recently [9,10].

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While statistics of local flame curvature in turbulent media were explored both in experiments, e.g. [11–16], and in DNS studies, e.g. [17–19] with more references can be found in recent review articles [20–22], models capable for predicting these statistics have not yet been elaborated. Since the issue is of crucial importance for modeling lean H_2 -air flames, there is urgent need for advancing new approaches to bridge this fundamental knowledge gap. This work responds to such a call by introducing and analyzing a new transport equation for local flame curvature.

Relevant equations were earlier derived for a single surface [23] and for curvature field [24–26]. In the latter papers, equivalent transport equations are written in different forms, see Eqs. (9)–(10) and the Supplementary Material. However, they involve many terms and are difficult to analyze. Published results [26–31] of DNS analyses of various terms in those transport equations (i) show that several terms have large magnitudes and opposite signs but (ii) do not emphasize few predominant terms that should be the focus of attention when developing models. If a transport equation involves two terms that have large magnitudes, but opposite signs, separately modeling each term does not seem to be the best task. Indeed, even a small error in evaluating one term can yield a large error when computing the sum of the two terms. A solution could consist in combining such terms and modeling them jointly.

The present work aims to seek such a solution by considering a compact form of transport equation for flame curvature field. Moreover, the work aims at introducing a new transport equation for curvature conditioned to flame reaction zone. Furthermore, the behavior of few predominant terms in the newly derived conditioned transport equation is studied by analyzing two recent DNS databases [32,33].

Transport equations for curvature are derived in the next section. The DNS attributes are summarized in Section 3. Results of analyses of the DNS databases are discussed in Section 4, followed by Conclusions.

2. Derivation

2.1. Instantaneous local equations

Let us begin with a transport equation for combustion progress variable c , written in the following well-known kinematic form [23–26, 34]

$$\frac{D^*c}{D^*t} = \frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} - S_d |\nabla c| = \frac{\partial c}{\partial t} + v_i^c \frac{\partial c}{\partial x_i} = 0, \quad (1)$$

where

$$S_d = \frac{1}{\rho |\nabla c|} \left[\frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right) + \dot{\omega}_c \right] \quad (2)$$

is displacement speed relative to the flow; $\mathbf{v}^c = \mathbf{u} + S_d \mathbf{n}$ is flame velocity vector in the laboratory framework; $\mathbf{n} = -\nabla c / |\nabla c|$ is the unit vector normal to isoc surface; ρ is the density; D is molecular diffusivity; $\dot{\omega}_c$ is mass rate of product creation; and the Einstein summation convention applies to repeated indexes.

Application of vector-operator ∇ to Eq. (1) yields

$$0 = \frac{\partial}{\partial x_i} \left(\frac{D^*c}{D^*t} \right) = \frac{D^*}{D^*t} \left(\frac{\partial c}{\partial x_i} \right) + \frac{\partial c}{\partial x_j} \frac{\partial v_j^c}{\partial x_i}. \quad (3)$$

Consequently,

$$\begin{aligned} \frac{D^*n_i}{D^*t} &= -\frac{1}{|\nabla c|} \frac{D^*}{D^*t} \left(\frac{\partial c}{\partial x_i} \right) + \frac{1}{|\nabla c|^2} \frac{\partial c}{\partial x_i} \frac{D^*}{D^*t} |\nabla c| \\ &= -\frac{1}{|\nabla c|} \frac{\partial c}{\partial x_j} \frac{\partial v_j^c}{\partial x_i} + \frac{1}{|\nabla c|^3} \frac{\partial c}{\partial x_i} \frac{\partial c}{\partial x_j} \frac{D^*}{D^*t} \left(\frac{\partial c}{\partial x_j} \right) \\ &= -n_j \frac{\partial v_j^c}{\partial x_i} - \frac{1}{|\nabla c|} n_i n_j \frac{\partial c}{\partial x_k} \frac{\partial v_k^c}{\partial x_j} \end{aligned} \quad (4)$$

and we arrive at the following transport equation

$$\frac{D^*n_i}{D^*t} = \frac{\partial n_i}{\partial t} + v_j^c \frac{\partial n_i}{\partial x_j} = (n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k, \quad (5)$$

derived by Candel and Poinot [24] using a different method. Here, δ_{ij} is Kronecker delta. Below, Eq. (5) is rewritten in the following form:

$$\frac{\partial n_i}{\partial t} + u_j \frac{\partial n_i}{\partial x_j} = (n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k - S_d n_j \frac{\partial n_i}{\partial x_j}. \quad (6)$$

Thus, terms that describe (i) advection of an iso- c surface by the flow and (ii) self-propagation of this surface are separated on the left-hand side (l.h.s.) and the latter term is moved to the right-hand side (r.h.s.).

This is done, because the influences of advection and molecular diffusion (which directly affects the self-propagation velocity S_d) on the evolution of the normal vector $\mathbf{n}$ differ fundamentally [35]. To show this difference, let us compare two limiting cases: (i) evolution of a material surface ($S_d = 0$) in a turbulent flow and (ii) self-propagation of a front in quiescent media ($\mathbf{u} = 0$) at a constant speed S . Here, a new symbol, S , is introduced to distinguish the constant speed of the front from S_d defined by Eq. (2).

In the former case, the smoothness of the surface is well known [36] to be preserved and critical or zero-gradient points [35], where $\nabla c = 0$, $0 < c < 1$, and the normal vector $\mathbf{n}$ is ill-defined, do not appear.

If $\mathbf{u} = 0$ and S_d is substituted with a constant S , Eq. (5) reduces to the inviscid vector Burgers equation

$$\frac{\partial n_i}{\partial t} + S n_j \frac{\partial n_i}{\partial x_j} = (n_i n_j - \delta_{ij}) S \frac{\partial n_k}{\partial x_j} n_k = 0, \quad (7)$$

because $n_k n_k = 1$ and $n_k (\partial n_k / \partial x_j) = 0$. For this equation, discontinuities of the normal field appear due to the front propagation for an initially smooth field $\mathbf{n}(\mathbf{x}, t)$ [37]. Such shock solutions correspond, e.g., to flame cusps [2] that appear on an initially smooth isoc surface due to its self-propagation. In the case of a flame of a finite thickness, molecular diffusion smooths out such cusps, results in variations in S_d defined by Eq. (2) and appearance of the critical points [35], where $\nabla c = 0$ and $0 < c < 1$.

For these reasons, the term $\mathbf{v}^c \cdot \nabla \mathbf{n}$ on the l.h.s. of Eq. (5) is split into advection and propagation terms.

By taking a scalar product of the vector-operator ∇ and Eq. (6), we arrive straightforwardly at

$$\begin{aligned} \frac{\partial \kappa_m}{\partial t} + u_j \frac{\partial \kappa_m}{\partial x_j} &= -\frac{1}{2} \frac{\partial u_j}{\partial x_i} \frac{\partial n_i}{\partial x_j} \\ &+ \frac{1}{2} \frac{\partial}{\partial x_i} \left[(n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k - S_d n_j \frac{\partial n_i}{\partial x_j} \right], \end{aligned} \quad (8)$$

where $\kappa_m = \nabla \cdot \mathbf{n} / 2$ is the mean curvature of an isoc surface and the first term on the r.h.s. is moved from the l.h.s. after splitting the scalar product of ∇ and the advection term $u_j \partial n_i / \partial x_j$ into two sub-terms.

It is worth stressing the two terms on the l.h.s. of Eq. (8) and the first term on the r.h.s. are linear with respect to n_i , whereas all non-linear terms are combined in the last term on the r.h.s. If a scalar product of the vector-operator ∇ and Eq. (5) is taken and the velocity $\mathbf{v}^c$ is retained, all terms on the r.h.s. of the equation for κ_m are non-linear with respect to n_i .

For comparison, Dopazo et al. [25] derived the following transport equation for curvature

$$\begin{aligned}
& \frac{\partial \kappa_m}{\partial t} + v_j^c \frac{\partial \kappa_m}{\partial x_j} = a_N \kappa_m + \frac{1}{2} n_j \frac{\partial a_N}{\partial x_j} \\
& - S_{ij} \frac{\partial n_j}{\partial x_i} - \frac{1}{2} \frac{\partial S_{ij}}{\partial x_i} n_j + \frac{1}{2} \frac{\partial W_{ij}}{\partial x_i} n_j + n_j \frac{\partial S_d}{\partial x_j} \kappa_m \\
& + \frac{1}{2} n_i \frac{\partial}{\partial x_i} \left(n_j \frac{\partial S_d}{\partial x_j} \right) - S_{ij}^a \frac{\partial n_j}{\partial x_i} - \frac{1}{2} \frac{\partial S_{ij}^a}{\partial x_i} n_j \\
& + \frac{1}{2} \frac{\partial W_{ij}^a}{\partial x_i} n_j
\end{aligned} \quad (9)$$

where $a_N = n_i S_{ij} n_j$ is normal strain rate, and the tensors S_{ij} , W_{ij} , S_{ij}^a , and W_{ij}^a are specified in the Supplementary Material.

Later, Yu et al. [26] arrived at another equation

$$\begin{aligned}
& \frac{\partial \kappa_m}{\partial t} + v_j^c \frac{\partial \kappa_m}{\partial x_j} = -\mathcal{K} \kappa_m + \kappa_m \nabla \cdot \mathbf{u} \\
& + n_j \frac{\partial S_d}{\partial x_j} \kappa_m + 2S_d \kappa_m^2 - \frac{1}{2} \frac{\partial^2 u_i}{\partial x_j^2} n_i - S_{ij} \frac{\partial n_j}{\partial x_i} \\
& + \frac{1}{2} n_j \frac{\partial a_N}{\partial x_j} + \frac{1}{2} n_i n_j \frac{\partial^2 S_d}{\partial x_i \partial x_j} - \frac{1}{2} \frac{\partial^2 S_d}{\partial x_i^2} \\
& - \frac{1}{2} S_d \frac{\partial n_j}{\partial x_i} \frac{\partial n_i}{\partial x_j}
\end{aligned} \quad (10)$$

where $\mathcal{K} = \nabla \cdot \mathbf{u} - a_N + 2S_d \kappa_m$ is flame stretch rate. Note that Eq. (2.22) in Ref. [26] is written for $\nabla \cdot \mathbf{n}^- = -2\kappa_m$ (the vector $\mathbf{n}^- = -\mathbf{n}$ points to burned gas).

Eqs. (9) and (10) have been derived by taking a scalar product of the vector-operator ∇ and Eq. (5), contrary to Eq. (6) adopted here to derive Eq. (8). As shown in Supplementary Material, the transport equations derived by Dopazo et al. [25] and by Yu et al. [26] are reduced to Eq. (8). In contrast, the structure of the r.h.s. of Eq. (8) is compact and simple, i. e., there is (i) a single source/sink term, which is associated with the influence of non-uniform velocity field on flame topology, and (ii) a transport-like term, which subsumes terms due to surface propagation.

2.2. Conditioned equations

To explore the behavior of curvature of a finite-volume zone in a flame, e.g., reaction zone, Eq. (8) can be conditioned to this zone. For this purpose, let's introduce the following indicator function:

$$I(\mathbf{x}, t) = H[c(\mathbf{x}, t) - c_1] - H[c(\mathbf{x}, t) - c_2], \quad (11)$$

where c_1 and c_2 designate boundaries of the studied zone with $c_1 < c_2$ and H is Heaviside function. The indicator function is equal to unity if $c_1 < c(\mathbf{x}, t) < c_2$ and vanishes otherwise. The evolution of $I(\mathbf{x}, t)$ is described by the following equation:

$$\begin{aligned}
& \frac{\partial I}{\partial t} + u_j \frac{\partial I}{\partial x_j} = \frac{dI}{dc} \left(\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} \right) \\
& = [\delta(c - c_1) - \delta(c - c_2)] S_d |\nabla c|.
\end{aligned} \quad (12)$$

Here, the derivatives dH/dc of the Heaviside functions $H(c - c_n)$ are substituted with Dirac delta functions $\delta(c - c_n)$, where $n = 1$ or 2 .

Using the continuity equation and Eq. (12), we arrive at the following identity:

$$\begin{aligned}
& \rho I \frac{\partial \kappa_m}{\partial t} + \rho I u_j \frac{\partial \kappa_m}{\partial x_j} = \frac{\partial}{\partial t} (\rho I \kappa_m) \\
& + \frac{\partial}{\partial x_j} (\rho u_j I \kappa_m) - \rho \kappa_m \left(\frac{\partial I}{\partial t} + u_j \frac{\partial I}{\partial x_j} \right) \\
& = \frac{\partial}{\partial t} (\rho I \kappa_m) + \frac{\partial}{\partial x_j} (\rho u_j I \kappa_m) \\
& - \rho \kappa_m [\delta(c - c_1) - \delta(c - c_2)] S_d |\nabla c|.
\end{aligned} \quad (13)$$

Subsequently, Eq. (8) multiplied with $\rho(\mathbf{x}, t)I(\mathbf{x}, t)$ and Eq. (13) yield

$$\begin{aligned}
& \frac{\partial}{\partial t} (\rho I \kappa_m) + \frac{\partial}{\partial x_j} (\rho u_j I \kappa_m) = -\frac{\rho I}{2} \frac{\partial u_j}{\partial x_i} \frac{\partial n_i}{\partial x_j} \\
& + \frac{\rho I}{2} \frac{\partial}{\partial x_i} \left[(n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k - S_d n_j \frac{\partial n_i}{\partial x_j} \right] \\
& + \kappa_m [\delta(c - c_1) - \delta(c - c_2)] \rho S_d |\nabla c|.
\end{aligned} \quad (14)$$

The first and second terms on the r.h.s. of Eq. (14) result directly from multiplication of the two terms on the r.h.s. of Eq. (8) with $\rho(\mathbf{x}, t)I(\mathbf{x}, t)$.

In a statistically stationary case analyzed in the rest of this paper, Reynolds-averaged continuity equation reduces to $\nabla \cdot (\bar{\rho} \mathbf{u}) = 0$ and Reynolds-averaged Eq. (12) multiplied with the density $\rho(\mathbf{x}, t)$ reads

$$\begin{aligned}
& \bar{\rho} \mathbf{u} \cdot \nabla \bar{I} = \nabla \cdot (\bar{\rho} \mathbf{u} \bar{I} - \bar{\rho} \mathbf{u} \bar{I}) \\
& = (\rho S_d |\nabla c|)_{c=c_1} - (\rho S_d |\nabla c|)_{c=c_2}.
\end{aligned} \quad (15)$$

Here, $\bar{q}$ and $\tilde{q} \equiv \overline{\rho q} / \bar{\rho}$ are Reynolds and Favre-averaged values, respectively, of the quantity q , whereas $q_{c=c_n}$ designates $\delta(c - c_n)q$.

The Reynolds-averaged Eq. (14) reads

$$\begin{aligned}
& \bar{\rho} \mathbf{u} \cdot \nabla (\bar{I} \langle \kappa_m \rangle_c) = \nabla \cdot (\bar{\rho} \mathbf{u} \bar{I} \langle \kappa_m \rangle_c - \bar{\rho} \mathbf{u} \bar{I} \kappa_m) \\
& + \frac{\rho I}{2} \frac{\partial}{\partial x_i} \left[(n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k - S_d n_j \frac{\partial n_i}{\partial x_j} \right] \\
& - \frac{\rho I}{2} \frac{\partial u_j}{\partial x_i} \frac{\partial n_i}{\partial x_j} + (\rho S_d \kappa_m |\nabla c|)_{c=c_1}^{c=c_2},
\end{aligned} \quad (16)$$

where $\langle \kappa_m \rangle_c \equiv \langle \kappa_m | c_1 < c < c_2 \rangle = \overline{\kappa_m I} / \bar{I}$ is the curvature conditioned to the zone studied and $q_{|c=c_2}^{c=c_1} \equiv q_{c=c_1} - q_{c=c_2}$. Finally, Eqs. (15)-(16) yield

$$\begin{aligned}
& \bar{\rho} \mathbf{u} \cdot \nabla \langle \kappa_m \rangle_c = \underbrace{\nabla \cdot (\bar{\rho} \mathbf{u} \bar{I} \langle \kappa_m \rangle_c - \bar{\rho} \mathbf{u} \bar{I} \kappa_m)}_{T_1} \\
& + \underbrace{\frac{\rho I}{2} \frac{\partial}{\partial x_i} \left[(n_i n_j - \delta_{ij}) \frac{\partial v_k^c}{\partial x_j} n_k - S_d n_j \frac{\partial n_i}{\partial x_j} \right]}_{T_2} \\
& - \underbrace{\frac{\rho I}{2} \frac{\partial u_j}{\partial x_i} \frac{\partial n_i}{\partial x_j}}_{T_3} + \underbrace{(\rho S_d (\kappa_m - \langle \kappa_m \rangle_c) |\nabla c|)_{c=c_1}^{c=c_2}}_{T_4}
\end{aligned} \quad (17)$$

Here, term T_1 is analogous to turbulent transport terms in a common Favre-averaged transport equation for combustion progress variable. It is linear with respect to the velocity vector $\mathbf{u}$ or the curvature κ_m . Term T_3 describes the influence of non-uniformities of the velocity field on the curvature of reaction zone. T_3 is linear with respect to components of the velocity vector $\mathbf{u}$ or the normal vector $\mathbf{n}$. Term T_4 stems from the influence of the self-propagation of that zone on its curvature. It is linear with respect to the curvature κ_m . Note that the product $\rho S_d |\nabla c|$ is nothing more than the sum of molecular diffusion and reaction terms in the transport equation for combustion progress variable, see Eqs. (1) and (2). Finally, term T_2 is a combination of several terms that are non-linear with respect to n_i . Physical meanings of various sub-terms in this combination are discussed elsewhere [25,26]. Here, they are not discussed, because many of these sub-terms require modeling, have large magnitudes and opposite signs [25,26], but cancel one another if considered jointly. Hence, a single term T_2 is adopted, because it may be neglected, as argued in Sect. 3.

In the following, various terms in Eq. (17) will be evaluated by processing the DNS data by Chaudhuri et al. [32,33], described in the next section.

3. DNS databases

Since (i) one of the two sets of DNS data adopted here was already

analyzed in our previous papers [38–47] and (ii) both sets were generated using basically the same numerical methods (while initial conditions were different), only a brief description of the DNS attributes and applied numerical diagnostic techniques follow. The reader interested in further details is encouraged to look into the cited papers.

Three-dimensional DNS data were obtained using PENCIL code [48] from statistically planar and one-dimensional, lean H_2 -air turbulent flames. Navier-Stokes equations were solved in compressible form. The mixture-averaged transport model and a chemical mechanism by Li et al. [49] were used in both cases.

Homogeneous isotropic turbulence was pre-generated using forcing at low wavenumbers in a separate cube with the fully periodic boundary conditions, was injected into the computational domains through their left boundaries and decayed along the mean flow direction. Major characteristics (rms velocity u' or Kolmogorov time scale τ_K) of the pre-generated turbulence are comparable in both cases. Longitudinal integral length scale $L_{11} = 3.0$ mm in both cases [32,33], whereas turbulent Reynolds numbers $Re_t = u'L_{11}/\nu = 950$ [32] and 800 [33] are slightly different and sufficiently high when compared to majority of recent three-dimensional complex-chemistry DNSs of premixed turbulent flames, reviewed elsewhere [22]. Here, ν is kinematic viscosity of unburned gas.

The major difference between the two simulated cases consists of equivalence ratios $\Phi = 0.81$ and 0.40. Accordingly, laminar flame speed $S_L = 1.85$ m/s, thickness $\delta_L = (T_b - T_u)/\max\{|\nabla T|\} = 0.36$ mm, time scale $\tau_f = \delta_L/S_L = 0.19$ ms, $u'/S_L = 3.6$, and Karlovitz number $Ka = \tau_f/\tau_K = 13$ in the richer case [32], whereas $S_L = 0.25$ m/s, $\delta_L = 0.6$ mm, $\tau_f = 2.4$ ms, $u'/S_L = 20$, and $Ka = 115$ in the leaner case [33]. Here, T is temperature, subscripts u and b refer to unburned and burned gases, respectively. In the following, the two cases are labeled F081_Ka13 and F04_Ka115, based on their equivalence ratios (letter F) and Karlovitz numbers. Diffusional-thermal effects [2,5,6,9,10] are well pronounced solely in case F04_Ka115, where, e.g., the peak fuel consumption rate is higher than the largest fuel consumption rate $\dot{\omega}_{F,m}^L$ in the unstretched laminar flame by an order of magnitude. Further details are discussed in [32,33].

In the following, variations of studied quantities within mean flame brushes are reported using mean (time- and transverse-averaged) combustion progress variable $\bar{c} = 1 - \bar{Y}_F/Y_{F,u}$, which is a monotonous function of the axial coordinate x . Here, Y_F is fuel mass fraction. Reaction-zone boundaries c_1 and c_2 are set as follows: $\dot{\omega}_F[c(\mathbf{x}, t) = c_n] = b\dot{\omega}_{F,m}^L$ with $b = 0.9$ (similar results were obtained by setting $b = 0.5$). Methods used to sample conditioned quantities are described elsewhere [44], where a single case F081_Ka13 is analyzed. When evaluating S_d in term T_2 in Eq. (17), all points where $\delta_L|\nabla c| < 10^{-9}$ were omitted to avoid singularities. When sampling T_4 , $\rho S_d|\nabla c|$ was computed using the r.h.s. of Eq. (2).

Moreover, Helmholtz-Hodge decomposition of the DNS velocity fields $\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_s(\mathbf{x}, t) + \mathbf{u}_d(\mathbf{x}, t)$ to rotational (solenoidal) and irrotational (dilatational, potential) subfields, $\mathbf{u}_s(\mathbf{x}, t)$ and $\mathbf{u}_d(\mathbf{x}, t)$, respectively, was performed. Accordingly,

$$\nabla \times \mathbf{u}_s = \nabla \times \mathbf{u}, \quad \nabla \cdot \mathbf{u}_d = \nabla \cdot \mathbf{u}. \quad (18)$$

Methods adopted for this purpose are described in detail elsewhere [44,50]. The basic difference between potential and solenoidal velocity subfields consists of the fact that the latter is dilatation-free. Thus, combustion-induced dilatation directly affects the potential velocity field only.

4. Results and discussion

Fig. 1 shows variations of normalized terms on the r.h.s. of Eq. (17) within mean flame brush. While the term magnitudes are larger in case F04_Ka115 characterized by a significantly higher Karlovitz number,

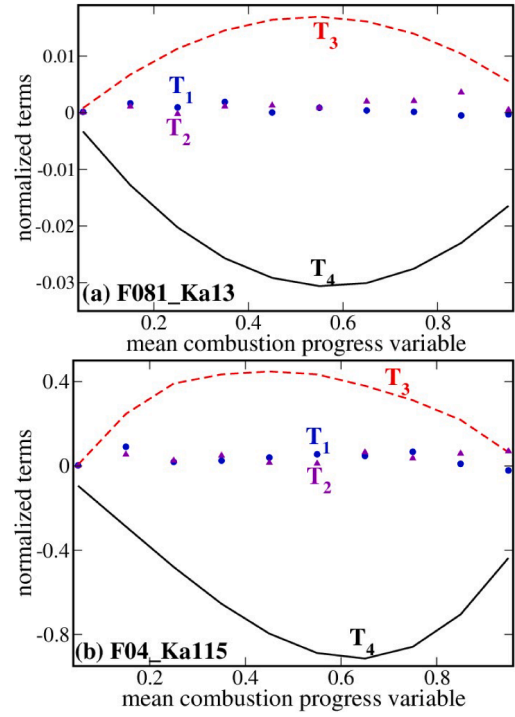


Fig. 1. Variation of normalized terms $(\delta_L^2 / \rho_u S_L) T_n$ ($n = 1, \dots, 4$) on the r.h.s. of Eq. (17) within mean flame brush.

major trends are similar in both cases. First, there are two predominant terms T_3 and T_4 , whose signs are opposite. The turbulent transport term T_1 and the combination T_2 of non-linear terms are very small and may be neglected. This feature of the newly derived Eq. (17) is very plausible for modeling.

Second, term T_3 is controlled by interaction between velocity gradient and the normal vector $\mathbf{n}$, is positive and acts to increase reaction-zone curvature.

Third, flame-propagation term T_4 reduces the curvature. The negative sign of T_4 can be explained by considering the simplest canonical model case of an expanding spherical laminar flame. In that case, $R_f(c_1) > R_f(c_{rz}) > R_f(c_2)$, where c_{rz} refers to the middle of the reaction zone. Hence, $0 < \kappa_m(c_1) < \kappa_m < \kappa_m(c_2)$, $\rho S_d(\kappa_m - \kappa_m < c) |\nabla c| < 0$ at $c = c_1$, and $\rho S_d(\kappa_m - \kappa_m > c) |\nabla c| > 0$ at $c = c_2$.

It is of interest to note that the ratios of the peak absolute values of terms T_n in cases F04_Ka115 and F081_Ka13 are about 26 both for $n = 3$ and $n = 4$. These ratios are also close to the ratio of $Ka^{3/2}$ in the two cases. Together with similar bell-like shapes of $T_3(\bar{c})$ - and $T_4(\bar{c})$ -curves in both cases, the proximity of these ratios imply the following empirical model of the two terms: $(\delta_L^2 / \rho_u S_L) T_n = \beta_n Ka^{3/2} \bar{c}(1 - \bar{c})$, where coefficients β_n are different for $n = 3$ and $n = 4$, with $\beta_3 > 0$, $\beta_4 < 0$, and $\beta_3 < |\beta_4|$. Such a model cannot be accepted by analyzing DNS data obtained from two flames only and more cases should be simulated to explore this observation. Nevertheless, it is worth noting that this model yields $T_n \propto (\tau_K \eta_K)^{-1}$ in line with the assumption that gradients of components of the normal and velocity vectors, e.g., in T_3 , scale as inverse Kolmogorov length scale η_K^{-1} and inverse Kolmogorov time scale τ_K^{-1} , respectively.

Finally, the magnitude of the negative flame propagation term T_4 is higher than the magnitude of the positive strain term T_3 . Consequently, $\langle \kappa_m \rangle$ decreases from positive values near the leading edge of flame brush (where $\langle \kappa_m \rangle > 0$ for simple topological reasons) to negative values near its trailing edge, where $\langle \kappa_m \rangle < 0$. This behavior of curvature conditioned to reaction zone is illustrated in Fig. 2a. Note that the normalized conditioned curvature is significantly larger in the leading

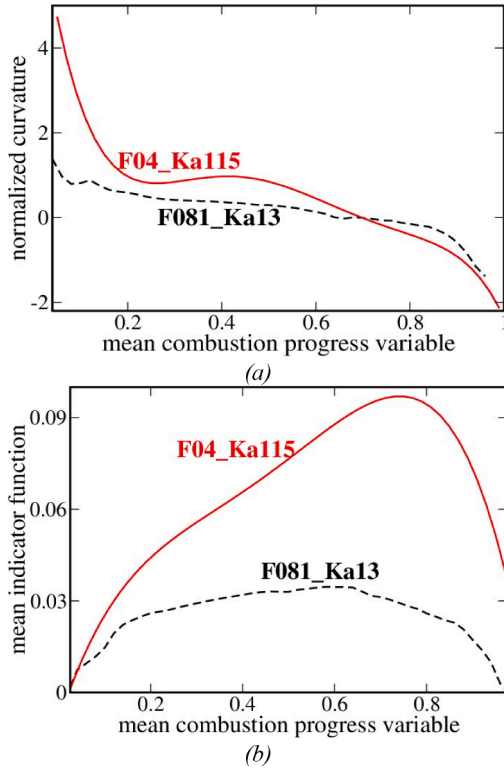


Fig. 2. Variations of (a) normalized conditioned curvature $\delta_L \bar{\kappa}_m \bar{I} / \bar{I}$ and (b) mean indicator function $\bar{I}$ along normal to mean flame brush.

zone (small $\bar{c}$) of flame brush in case F04_Ka115 when compared to case F081_Ka13. This difference is associated with diffusional-thermal phenomena that greatly affect the largest local curvature that a flame can sustain without extinction [2,6,8]. In lean H_2 -air mixtures, this critical curvature is known to be larger at lower ϕ .

For completeness, Fig. 2b reports variations of the mean indicator function $\bar{I}[\bar{c}(x)]$, i.e., probability of finding the reaction zone studied, along normal to mean flame brush. At higher Ka , this probability is significantly larger and peaks at larger $\bar{c}$ (red solid line). This difference between cases F081_Ka13 and F04_Ka115 implies more dense population of mean flame brush with reaction zones, with the effect being most pronounced at $\bar{c} = 0.75$, i.e., in the trailing half of mean flame brush. These trends are consistent with (i) significantly different normalized turbulent burning velocities $U_T/S_L = 5.4$ and $U_T/S_L = 19$ in cases F081_Ka13 and F04_Ka115, respectively, and (ii) DNS data [51] that show that large ratios of U_T/S_L in intense turbulence are mainly controlled by flame folding, i.e., multiple crossing of any normal to mean flame brush with highly wrinkled flame surface.

To illustrate some advantages of the compact Eq. (8) and its conditioned version, i.e. Eq. (17), let us decompose the non-linear term T_2 in Eq. (17) as follows:

$$\begin{aligned}
 T_2 = & \underbrace{-\frac{\rho I}{2} \frac{\partial}{\partial x_j} \left(n_1 \frac{\partial u_1}{\partial x_j} \right)}_{T_{21}} + \underbrace{\frac{\rho I}{2} \frac{\partial}{\partial x_j} \left(n_1 \frac{\partial u_1}{\partial x_k} n_k n_j \right)}_{T_{22}} \\
 & + \underbrace{\frac{\rho I}{2} \frac{\partial}{\partial x_j} \left(n_j n_i \frac{\partial S_d}{\partial x_i} \right)}_{T_{23}} - \underbrace{\frac{\rho I}{2} \frac{\partial}{\partial x_j} \left(\frac{\partial S_d}{\partial x_j} \right)}_{T_{24}} \\
 & - \underbrace{\frac{\rho I}{2} \frac{\partial}{\partial x_j} \left(S_d n_1 \frac{\partial n_j}{\partial x_1} \right)}_{T_{25}}.
 \end{aligned} \quad (19)$$

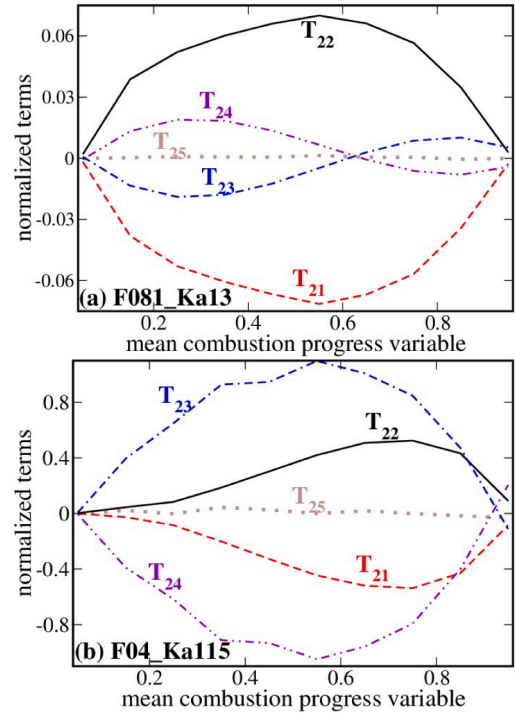


Fig. 3. Variation of normalized terms $(\delta_L^2 / \rho_u S_L) T_{2m}$ on the r.h.s. of Eq. (19) within mean flame brush.

Fig. 3 shows that while term T_{25} is small, other terms on the r.h.s. of Eq. (19) can be large. However, large (cf. ordinate axes in Figs. 1 and 3) terms T_{21} and T_{22} , which involve flow velocity, have opposite signs and almost cancel one another. Similarly, their counterparts that involve displacement speed, i.e., terms T_{24} and T_{23} , respectively, are significant, but have opposite signs and almost cancel one another. Thus, term T_2 has a small magnitude and may be neglected to the leading order despite its components are large. This situation is somewhat similar to the problem of modeling dissipation rate in turbulent flows, because the rate is well known to be a small difference between two large terms at high Reynolds numbers [52].

It is also of interest to note that signs of flame-propagation terms T_{23} and T_{24} can be opposite in the two cases studied. In the richer case, T_{23} (T_{24}) is negative (positive) at $\bar{c} < 0.6$, but positive (negative) at larger $\bar{c}$, see Fig. 3a. In the leaner case, T_{23} and T_{24} are positive and negative, respectively, in the largest part of the mean flame brush, see Fig. 3b. Moreover, magnitudes of T_{23} and T_{24} are significantly smaller than magnitudes of T_{21} and T_{22} in the richer case, see Fig. 3a, but the opposite relation between the term magnitudes is observed in the leaner case, see Fig. 3b. These differences (i) imply that the sub-terms discussed are sensitive to diffusional-thermal effects and (ii) make modeling each separate sub-term difficult.

Such difficulties can be further illustrated by comparing results conditioned to fuel consumption, see Fig. 1, and heat release, see Fig. 4, zones. The latter figure reports various terms on the r.h.s. of Eq. (17) or (19), conditioned to the heat release zone, whose boundaries θ_1 and θ_2 are set by applying a constraint of $\dot{\omega}_T[\theta(\mathbf{x}, t) = \theta_n] = 0.9 \dot{\omega}_{T,m}^L$ to unstretched laminar flame. Here, $\theta = (T - T_u)/(T_a - T_u)$ is temperature-based combustion progress variable invoked for symmetry reasons, i.e., for a pair of θ and $\dot{\omega}_T$ to correspond to a pair of c and $\dot{\omega}_F$; T_a is adiabatic combustion temperature; $\dot{\omega}_T = \sum_{k=1}^K h_k \dot{\omega}_k$ is heat release rate; $\dot{\omega}_{T,m}^L$ is its peak value in the unstretched laminar flame; h_k and $\dot{\omega}_k$ are the enthalpy and rate of formation, respectively, of species k ; K is the number of species. When exploring Eqs. (17) and (19) in the heat release zone, the displacement speeds $S_{d,T}$ of isotherm surfaces were used.

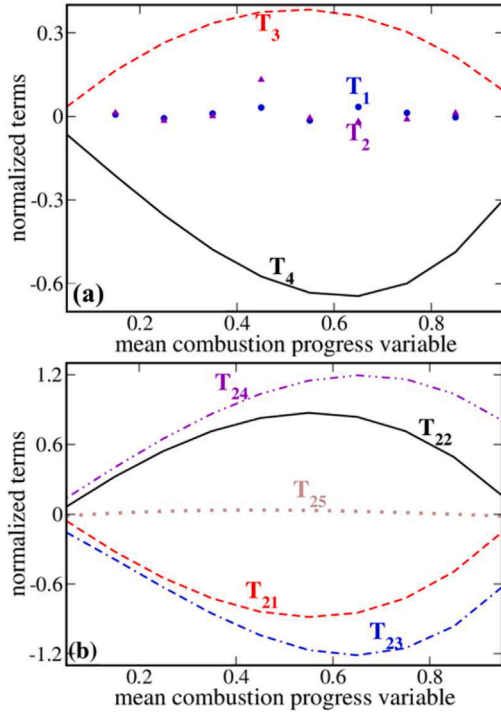


Fig. 4. Variation of normalized terms $(\delta_L^2 / \rho_u S_L) T_n$ on the r.h.s. of (a) Eq. (17) and (b) Eq. (19) within mean flame brush. Case F04_Ka115. The terms are conditioned to heat release zone.

The fields of $S_{d,T}(\mathbf{x}, t)$ were directly obtained from the DNS data and stored by Yuvraj et al. [33], see Eq. (2) in the cited paper.

Comparison of Figs. 3b and 4b shows that the sign of sub-term T_{23} or T_{24} conditioned to reaction (fuel consumption) zone is opposite to the sign of the same sub-term conditioned to heat release zone in the same turbulent flame. Accordingly, separately modeling T_{23} (or T_{24}) should allow for qualitative differences between the sub-terms conditioned to the two zones. This task appears to be challenging. The problem does not arise if compact Eqs. (8) and (17) are adopted. Indeed, comparison of Figs. 1b and 4a shows that the behavior of the major terms on the r.h.s. of Eq. (17) is similar regardless of whether the terms are conditioned to reaction or heat release zone.

It is also worth noting that variations in displacement speed significantly affect term T_4 that controls evolution of conditioned curvature. To show this, S_d evaluated using Eq. (2) was substituted with $S_d = \rho_u S_L / \rho$ in Eq. (17). The results obtained are plotted in Fig. 5. Comparison of black circles in Fig. 5 with black solid lines in Fig. 1 shows that magnitude of T_4 is significantly larger when S_d is evaluated using Eq. (2). If S_d was simply equal to $\rho_u S_L / \rho$, the positive T_3 would dominate on the r. h.s. of Eq. (17) and result in an increase in the conditioned curvature from the leading edge of flame brush to its trailing edge, but such a trend is obviously wrong for topological reasons. Note that the behavior of term T_3 is weakly affected by S_d , cf. curves plotted in red dashed lines in Figs. 1 and 5.

Eq. (17) also offers the opportunity to explore the influence of rotational and irrotational velocity fields on the evolution of conditioned curvature. Indeed, since only one of the two predominant terms on the r.h.s. of Eq. (17) involves flow velocity, one can easily compare magnitudes of term T_3 , evaluated by substituting velocity field $\mathbf{u}(\mathbf{x}, t)$ with its rotational or irrotational components, see Eq. (18). Fig. 6 shows that the flow-field term T_3 is controlled by rotational velocity in both cases, i.e., the influence of rotational velocity perturbations on the local reaction zone curvature and, hence, on the curvature contribution S_{d,κ_m} to the local stretch rate is much stronger when compared to irrotational velocity field. This trend is more pronounced in case F04_Ka115, see

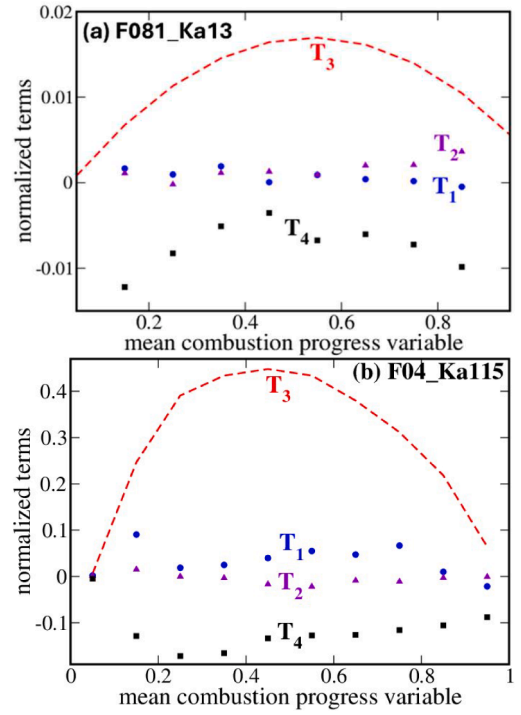


Fig. 5. Variation of normalized terms $(\delta_L^2 / \rho_u S_L) T_n$ on the r.h.s. of Eq. (17) where S_d is substituted with $S_d = \rho_u S_L / \rho$.

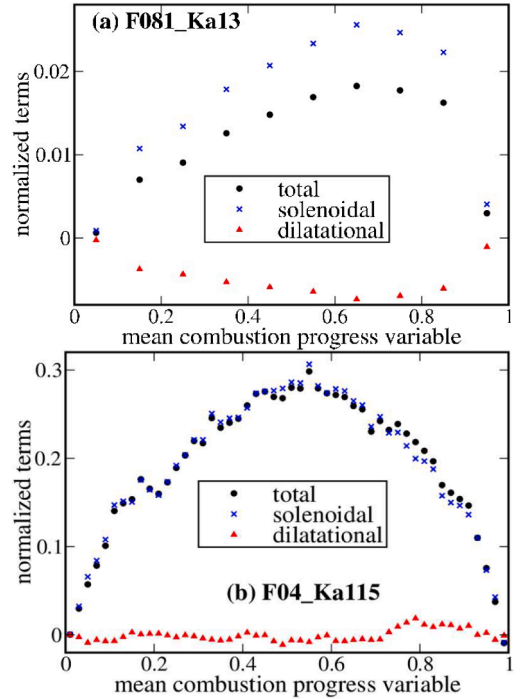


Fig. 6. Rotational (solenoidal) and irrotational (dilatational) contributions to normalized term $(\delta_L^2 / \rho_u S_L) T_3$ in Eq. (17).

Fig. 6b, characterized by a lower density ratio (4.29 when compared to 6.15) and a higher Karlovitz number. Since thermal expansion effects play a more important role at higher density ratios and lower Ka [21,53, 54], small contribution of irrotational (dilatational) velocity field to T_3 is more pronounced in case F081_Ka13, see Fig. 6a.

On the contrary, the tangential strain rate $a_t = \nabla \cdot \mathbf{u} - \mathbf{n} \cdot \nabla \mathbf{u} \cdot \mathbf{n}$ is

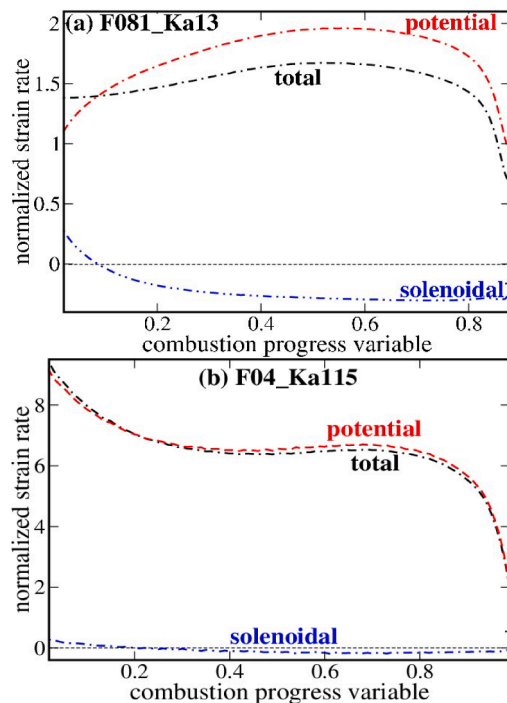


Fig. 7. Dependencies of normalized conditioned strain rate $(\delta_L/S_L) < a_t|c >$ and rotational (solenoidal) and irrotational (potential) velocity contributions to it, sampled from the entire flame brush, on the local value c of fuel-based combustion progress variable.

primarily controlled by irrotational velocity field, see Fig. 7, which shows dependencies of strain rates sampled from the entire flame brushes and conditioned to the local value $c(\mathbf{x}, t)$ of combustion progress variable on this local value. The emphasized trend is observed even at Ka as high as 115 and the density ratio as low as 4.29, see Fig. 7b.

Thus, inhomogeneous flow field affects flame stretch rate via two different channels; (i) rotational velocity fluctuations statistically act to bend reaction zones and (ii) irrotational velocity fluctuations (induced by thermal expansion) act to strain these zones. This fundamental difference between the influence of turbulent flow on the two components of flame stretch rate (curvature and strain rate) should be properly addressed to develop predictive models. This point calls for future target-directed studies.

5. Conclusions

A compact transport equation is derived for modeling evolution of flame curvature field in a turbulent flow. This equation is further conditioned to reaction zone. Analyses of two DNS databases [32,33] show, first, that spatial variations of the conditioned curvature are mainly controlled by two terms, which describe (i) curvature production by non-uniform velocity field and (ii) curvature reduction due to flame propagation. Second, application of Helmholtz-Hodge decomposition to the DNS velocity fields shows that the former term is controlled by rotational motions, contrary to the local flame strain rate, which is generated by irrotational motions in both flames. This fundamental difference between effects of turbulent velocity field on flame strain rate and curvature is worth consideration when modeling such effects.

CRedit authorship contribution statement

Andrei N. Lipatnikov: Writing – original draft, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization.
Vladimir A. Sabelnikov: Writing – review & editing, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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