Flow topologies in different regimes of premixed turbulent combustion: A direct numerical simulation analysis

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The distributions of flow topologies within the flames representing the corrugated flamelets, thin reaction zones, and broken reaction zone regimes of premixed turbulent combustion are investigated using direct numerical simulation data of statistically planar turbulent H_2 -air flames with an equivalence ratio $\phi = 0.7$. It was found that the diminishing influence of dilatation rate with increasing Karlovitz number has significant influences on the statistical behaviors of the first, second, and third invariants (i.e., P , Q , and R) of the velocity gradient tensor. These differences are reflected in the distributions of the flow topologies within the flames considered in this analysis. This has important consequences for those topologies that make dominant contributions to the scalar-turbulence interaction and vortex-stretching terms in the scalar dissipation rate and enstrophy transport equations, respectively. Detailed physical explanations are provided for the observed regime dependences of the flow topologies and their implications on the scalar dissipation rate and enstrophy transport.

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I. INTRODUCTION

Turbulent flow fields often exhibit organized flow topologies in spite of their apparent chaotic nature. Perry and Chong [1] and Chong *et al.* [2] assigned all possible local small-scale three-dimensional flow topologies to eight categories based on the invariants P , Q , and R of the velocity-gradient tensor $A_{ij} = \partial u_i / \partial x_j$, where u_i is the i th component of velocity vector. The topologies, denoted by $S1$ – $S8$, distinguish eight regions in the three-dimensional P – Q – R phase space, as described in Fig. 1. Several previous studies [3–8] analyzed the flow properties in the Q – R plane for incompressible fluids (i.e., $P = -\nabla \cdot \vec{u} = 0$). For compressible flows ($P \neq 0$), however, one needs to account for P – Q – R space [9–12]. The analyses of topologies in nonreacting compressible flow turbulence have indicated that the unstable node-saddle-saddle and stable focal-stretching topologies in the Q – R plane dominate over other topologies.

In comparison to the large body of literature on local flow topologies in nonreacting turbulent flows, relatively little attention has been paid to their analysis in turbulent reacting flows [13–16].

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FIG. 1. Shown on top is the classification of S1–S8 topologies in the Q – R plane for (left to right) $P > 0$, $P = 0$, and $P < 0$. The lines r_{1a} (red), r_{1b} (blue), and r_2 (green) dividing the topologies are shown. Black dashed lines correspond to $Q = R = 0$. The bottom shows the classification of S1–S8 topologies: UF, unstable focus; UN, unstable node; SF, stable focus; SN, stable node; S, saddle; C, compressing; and ST, stretching.

Tanahashi *et al.* [13] used Q to distinguish strain-dominated and vorticity-dominated regions in a premixed flame and concluded that the vorticity vector remains perpendicular to the flame normal vector and that small-scale turbulence can survive even beyond the flame front. Grout *et al.* [14] analyzed the local flow topology of a nonpremixed jet in crossflow and reported that the highest heat release rates of the flame are associated with the regions with S8 topology. Recently, Cifuentes *et al.* [15,16] analyzed the topology distribution in a premixed turbulent flame based on a simple chemistry direct numerical simulation (DNS) database representing the flamelet combustion and demonstrated that the probability of finding focal (i.e., vortical) topologies decreases from the unburned gas side to the burned gas side. However, the differences in flow topology distribution within the flame for different regimes of premixed turbulent combustion are yet to be analyzed in the existing literature. These differences have important consequences on the scalar-turbulence interaction and vortex-stretching terms in the scalar dissipation rate and enstrophy transport equations, respectively [17,18]. Thus, the main objectives of this paper are (a) to identify the differences in the distribution of flow topologies in turbulent premixed flames representing different regimes of combustion and (b) to indicate the implications of the differences in topology distributions on the scalar-turbulence interaction and vortex-stretching terms.

A three-dimensional DNS database of statistically planar turbulent premixed H_2 -air flames with equivalence ratio $\phi = 0.7$ [19] has been considered spanning different regimes of premixed combustion. The rest of the paper will be organized as follows. The mathematical background and numerical implementation pertaining to the current analysis will be presented in the next section. This will be followed by presentation of results and their subsequent discussion. Finally, the main findings will be summarized and conclusions will be drawn in the final section of this paper.

II. MATHEMATICAL BACKGROUND AND NUMERICAL IMPLEMENTATION

Premixed combustion is often characterized using the nondimensional temperature $c_T = (T - T_0)/(T_{ad} - T_0)$, which increases from zero to unity from unburned to burned gases, where T , T_0 , and T_{ad} are the dimensional, unburned gas, and adiabatic flame temperature, respectively. The local flow topologies can be characterized by the invariants of the velocity-gradient tensor [1,2] $A_{ij} = \partial u_i / \partial x_j = S_{ij} + W_{ij}$, where $S_{ij} = 0.5(A_{ij} + A_{ji})$ and $W_{ij} = 0.5(A_{ij} - A_{ji})$ are the symmetric and antisymmetric components, respectively. Three eigenvalues λ_1 , λ_2 , and λ_3 of A_{ij} are the solutions of the characteristic equation $\lambda^3 + P\lambda^2 + Q\lambda + R = 0$, where P , Q , and R are the invariants of A_{ij} [1,2]:

$$\begin{aligned} P &= -(\lambda_1 + \lambda_2 + \lambda_3), \quad Q = 0.5(P^2 - S_{ij}S_{ij} + W_{ij}W_{ij}), \\ R &= (-P^3 + 3PQ - S_{ij}S_{jk}S_{ki} - 3W_{ij}W_{jk}S_{ki})/3. \end{aligned} \quad (1)$$

The discriminant $D = [27R^2 + (4P^3 - 18PQ)R + 4Q^3 - P^2Q^2]/108$ of $\lambda^3 + P\lambda^2 + Q\lambda + R = 0$ divides the P - Q - R phase-space into two regions: For $D > 0$ ($D < 0$), A_{ij} displays a focal (nodal) topology [1,2]. The velocity gradient tensor shows one real eigenvalue and two complex conjugate eigenvalues for focal topologies. By contrast, the velocity gradient tensor exhibits three real eigenvalues for nodal topologies. The surface $D = 0$ gives rise to two subsets r_{1a} and r_{1b} in P - Q - R phase space, which are given by [1,2] $r_{1a} = P(Q - 2P^2/9)/3 - 2(-3Q + P^2)^{3/2}/27$ and $r_{1b} = P(Q - 2P^2/9)/3 + 2(-3Q + P^2)^{3/2}/27$. In the region $D > 0$, A_{ij} has purely imaginary eigenvalues on the surface r_2 , which are given by $R = PQ$. The surfaces r_{1a} , r_{1b} , and r_2 , where r_2 is described by $PQ - R = 0$, divide the P - Q - R phase space into eight flow topologies, as shown in Fig. 1.

A three-dimensional DNS [19] database of freely propagating statistically planar turbulent H_2 -air premixed flames with $\phi = 0.7$, employing a detailed chemical mechanism [20] with nine species and 19 chemical reactions, is considered here. An equivalence ratio of 0.7 is chosen because the H_2 -air mixture for this equivalence ratio is known to be thermodiffusively neutral [21] such that the additional effects of preferential diffusion are eliminated. The unburned gas temperature T_0 is taken to be 300 K, which yields an unstrained laminar burning velocity $S_L = 135.6$ cm/s under atmospheric pressure. The DNS code solves fully compressible Navier-Stokes equations where spatial discretization is carried out by an eighth-order central difference scheme for internal grid points and the order of differentiation gradually decreases to a one-sided fourth-order scheme [19]. A fourth-order Runge-Kutta scheme is used for explicit time marching [19]. The flame is initialized by a one-dimensional steady initially planar laminar flame profile [22]. A precomputed auxiliary divergence-free, homogeneous, isotropic turbulence field is generated using a pseudospectral method [23] following the Passot-Pouquet spectrum [24] and is injected through the inlet. The mean inlet velocity has been changed gradually to match turbulent flame speed as the simulation progresses. In order to assess the extent to which the flames in this study can be qualified as statistically stationary, the temporal evolution of flame area has been monitored and the flame is considered to be statistically stationary when the flame area no longer varies with time. Turbulent inflow and outflow boundaries are taken in the direction of mean flame propagation and transverse boundaries are taken to be periodic. The nonperiodic boundaries are specified using an improved Navier-Stokes characteristic boundary condition technique [25].

The inflow values of normalized root-mean-square turbulent velocity fluctuation u'/S_L , turbulent length scale to flame thickness ratio l_T/δ_{th} , Damköhler number $Da = l_T S_L / u' \delta_{th}$, Karlovitz number $Ka = (\rho_0 S_L \delta_{th} / \mu_0)^{0.5} (u'/S_L)^{1.5} (l_T/\delta_{th})^{-0.5}$, and turbulent Reynolds number $Re_t = \rho_0 u' l_T / \mu_0$ for all cases are presented in Table I, where μ_0 is the unburned gas viscosity, $\delta_{th} = (T_{ad} - T_0) / \max |\nabla T|_L$ is the thermal flame thickness, and the subscript L is used to refer to unstrained laminar flame quantities. The turbulent length scale l_T is the most energetic scale of the Passot-Pouquet spectrum. The cases investigated in this study are nominally representative of three regimes of combustion: case A, corrugated flamelets ($Ka < 1$); case B, thin reaction zones ($1 < Ka < 100$); and case C,

TABLE I. List of inflow turbulence parameters.

Case	u'/S_L	l_T/δ_{th}	Re_t	Da	Ka
A	0.7	14.0	227	20.0	0.75
B	5	14.0	1623	2.8	14.4
C	14	4.0	1298	0.29	126

broken reaction zone regime ($Ka > 100$) [26]. It is worth noting from Table I that Ka in cases A–C is not modified independently of Da and Re_t and thus the differences in behavior among cases A–C should not be equated solely to the influences of Karlovitz number Ka . Instead, cases A–C, for the purpose of this paper, should be considered as three typical representative scenarios of the corrugated flamelet, thin reaction zone, and broken reaction zone regimes of premixed turbulent combustion, respectively.

The domain size is $20 \times 10 \times 10 \text{ mm}^3$ ($8 \times 2 \times 2 \text{ mm}^3$) in cases A and B (case C) and the domain has been discretized by a uniform Cartesian grid of $512 \times 256 \times 256$ ($1280 \times 320 \times 320$) cells. The smaller domain for case C is justified by the fact that the integral scale l_T is smaller in case C than in cases A and B (see Table I). The grid spacing was determined by the flame resolution, ensuring about ten grid points across δ_{th} , and in all cases the Kolmogorov length scale remains bigger than the grid spacing (i.e., $\eta \geq 1.5\Delta x$, where η and Δx are the Kolmogorov length scale and DNS grid spacing, respectively). For this resolution about seven to nine grid points reside across the thinnest species gradient. Case C has the highest value of turbulent Reynolds number and thus this case requires the smallest grid spacing to resolve the Kolmogorov length and flame thickness among all the cases considered here. For the purpose of computational economy a smaller computational domain than cases A and B has been chosen here for case C. Simulations have been carried out for $1.0t_e$, $6.8t_e$, and $6.7t_e$ (i.e., $t_e = l_T/u'$) for cases A–C, respectively, and this simulation time remains comparable to several previous analyses [15,16,27–29].

III. RESULTS AND DISCUSSION

Selected regions of instantaneous nondimensional temperature c_T , normalized first invariant $P^* = P \times (\delta_{th}/S_L)$, second invariant $Q^* = Q \times (\delta_{th}/S_L)^2$, and third invariant $R^* = R \times (\delta_{th}/S_L)^3$ fields when the statistics were extracted are shown in Fig. 2. Figure 2 also shows the flame location by the contour lines of $c_T = 0.1, 0.5, 0.7$ overlaid on the nondimensional temperature field. The c_T contours clearly show the increasing level of flame wrinkling as the turbulence intensity increases from cases A to C. In cases A and B the c_T isosurfaces lie close together, whereas in case C they are both much farther apart and the distance between neighboring isosurfaces varies greatly. This distinction is indicative of the different combustion regimes, which is often characterized in terms of the Karlovitz number. The Karlovitz number can be scaled as $Ka \sim \delta_{th}^2/\eta^2$, where η is the Kolmogorov length scale.

Since δ_{th} remains smaller than η in case A ($\delta_{th} \approx 0.9\eta$ and $\delta_r \approx 0.1\eta$), the flame undergoes no significant velocity fluctuations, which are dissipated at scales of the flame thickness. Eddies with sizes above the Kolmogorov scale wrinkle the flame. Since the reaction zone remains much thinner ($\delta_r \sim 0.1\delta_{th}$) it retains its quasilaminar structure. In case B, on the other hand ($\delta_{th} \approx 3.8\eta$ and $\delta_r \approx 0.4\eta$), eddies with sizes smaller than 4 times the Kolmogorov scale modify the internal structure of the flame thermal thickness, while the rest of the larger eddies only wrinkle the flame. Case C represents the broken reaction zone regime ($\delta_{th} \approx 11.2\eta$ and $\delta_r \approx 1.1\eta$), in which eddies with sizes smaller than 11 times the Kolmogorov scale modify the internal structure of the flame thermal thickness and the eddies at the Kolmogorov scale might modify the internal structure of the reaction thickness. Eddies with sizes greater than 11 times the Kolmogorov scale wrinkle the flame strongly, resulting in a considerable distortion of flame structure. This is evident from significant

FIG. 2. Selected regions of instantaneous nondimensional temperature c_T (row 1) (green contours show $c_T = 0.1, 0.5, 0.7$ isolines from left to right, shown close up in row 2), normalized first invariant $P^* = P \times (\delta_{th}/S_L)$ (row 3), second invariant $Q^* = Q \times (\delta_{th}/S_L)^2$ (row 4), and third invariant $R^* = R \times (\delta_{th}/S_L)^3$ (row 5) fields at the x – y midplane for (from left to right) cases A–C.

thickening of the flame and the large variations in the local flame thickness depending on the local turbulent flow conditions.

Note that there are no signs of localized flame extinction in case C in spite of large values of the Karlovitz number (i.e., $Ka > 100$). This is consistent with several previous DNS findings [30–33]. The above discussion suggests that distinctly different physical mechanisms are likely to govern the behavior of invariants in the three cases considered. It is also important to note from Table I that the values of Da , Ka , and Re_τ change from one case to another here and Ka is not modified in isolation. Thus, the alternations of Da and Re_τ in addition to the modification of Ka play a significant role in the differences in behavior of the invariants and their components among cases A–C.

Figure 2 shows that the qualitative nature of the distributions of Q^* and R^* in cases B and C is significantly different in comparison to case A: The distributions of Q^* and R^* in cases B and C exhibit much smaller length scales than in case A. Note that case B has much higher turbulent

Reynolds number Re_t than in case A and thus case B shows a larger range of length scales than in case A. Cases A and B have the same values of l_T , but case B shows smaller structures of turbulence in Q^* and R^* distributions due to larger scale separation arising from a higher value of Re_t . Case C has a smaller value l_T and a greater value of Re_t than in case A and thus case C exhibits much smaller turbulence structures in Q^* and R^* distributions than in case A due to the combination of higher Re_t and smaller l_T .

It is also seen from Fig. 2 that large nonzero values of P are concentrated within the flame because P is directly related to the dilatation rate (i.e., $P = -\nabla \cdot \vec{u}$) and the effects of thermal expansion and dilatation rate are strong only within the flame. Furthermore, focusing of heat gives rise to high magnitudes of positive $\nabla \cdot \vec{u}$ (i.e., negative values of P with high magnitude) at the locations where the flame is concave towards the reactants. In contrast, defocusing of heat leads to small positive and in some extreme cases negative values of $\nabla \cdot \vec{u}$ (i.e., small negative and positive values of P) at the locations where the flame is convex towards the reactants.¹

Both the strain rate and vorticity along with the dilatation rate (i.e., $-P$) contribute towards the value of Q since $Q_s = 0.5(P^2 - S_{ij}S_{ij})$ and $Q_w = W_{ij}W_{ij}/2$ according to $Q = Q_s + Q_w$ [see Eq. (1)]. The sign of Q is indicative of vorticity-dominated regions outside the flame (where $P \approx 0$ for low Mach number flows like the one considered here), for which $Q > 0$, and strain-dominated regions, for which $Q < 0$. Figure 2 shows that both vorticity-dominated and strain-dominated regions exist in all cases outside the flame, but the degree of intermittency is much greater in cases B and C than in case A. A comparison of the magnitudes of P and Q from Fig. 2 reveals that the magnitude of P^2 remains smaller than the magnitude of Q in most cases in the flow field and these quantities become comparable only within the flame. An increase in u'/S_L leads to an increase in the magnitude of Q : The maximum value of Q in case C is greater than that in case B, which is greater than that in case A.

Distinct modes of the flame-turbulence interaction are evident by comparing cases B and C in Fig. 2 by the evolution of the Q fields across the flame. The magnitude of Q drops significantly across the flame in case B (see the drop of the magnitude of Q across the $c_T = 0.1$ isosurface in case B in Fig. 2). In contrast, in case C the magnitude of the Q field remains significant throughout the flame front even beyond $c_T = 0.7$. Finally, the high values of Q are found close to the highly concave (to the reactants) regions in case A. This behavior arises due to focusing of heat in these regions, leading to an increased volumetric dilatation rate ($\nabla \cdot \vec{u}$) and subsequently Q due to high values of P^2 (since $P = -\nabla \cdot \vec{u}$) [see Eq. (1)].

The expression for R contained in Eq. (1) may be rewritten as the sum of the terms that play roles in dissipation rate generation ($-S_{ij}S_{jk}S_{ki}/3$) and enstrophy production ($PQ_w - \omega_i S_{ij} \omega_j/4$) in the following manner:

$$\begin{aligned} R &= \frac{1}{3}(-P^3 + 3PQ - S_{ij}S_{jk}S_{ki}) - \frac{1}{4}\omega_i S_{ij} \omega_j \\ &= \underbrace{\frac{1}{3}(-P^3 + 3PQ_s - S_{ij}S_{jk}S_{ki})}_{R_s} + PQ_w - \frac{1}{4}\omega_i S_{ij} \omega_j. \end{aligned} \quad (2)$$

Hence, R^* may assume high positive or negative values where there is an imbalance of the terms contributing to dissipation rate generation and production of enstrophy. It is evident from Fig. 2 that, in case A, this imbalance is most pronounced in the vicinity of the flame front, whereas in both cases B and C it is evident throughout the entire unburned gas region. In all three cases the magnitude of R^* is negligible in most of the burned gas region. Furthermore, in case A, the non-negligible values of R^* retain the same sign along most of the flame front shown here, whereas, in cases B and C, both positive and negative values of R^* coexist in the unburned gas region and within the flame front.

¹It is not clearly evident from the plane shown in Fig. 2, but this occurs on other planes.

FIG. 3. Log-linear variation of $P \times (\delta_{th}/S_L)$ with c_T for cases A (red), B (green), and C (blue).

Figures 3–6 show the variations of the normalized mean values of P , Q , and R and their constituent terms conditional on c_T . The dilatation rate $\nabla \cdot \vec{u} = -P$ remains predominantly positive in turbulent premixed flames, but it is possible to get some localized pockets of negative dilatation rate (i.e., $P > 0$) in the regions of the flame that are convex to the reactants (see Fig. 2). However, the probability of finding a negative dilatation rate remains smaller than obtaining positive $\nabla \cdot \vec{u}$ and thus the mean value of $P = -\nabla \cdot \vec{u}$ remains negative for all cases considered here (see Fig. 3). The magnitude of $P = -\nabla \cdot \vec{u}$ depends on the strength of chemical activity within the flame. Cases A and B exhibit similar variations of P across the flame, but the magnitudes are much less in case C. The flame thicknesses in cases A and B are smaller or comparable to the respective η such that the reaction zone remains quasilaminar and largely unaffected by turbulent fluctuations. Thus, although the turbulence intensity u'/S_L of case B is almost an order of magnitude greater than that in case A, the thermal expansion experienced in both cases is remarkably similar. In case C, however, the turbulent eddies enter into the inner reaction layer of the flame and disrupt the chemical processes, leading to enhanced heat loss to the preheat zone and a reduction in the reaction rate. For this reason the magnitude of $P = -\nabla \cdot \vec{u}$ observed in case C is much lower than that observed in cases A and B. The diminishing strength of dilatation rate $\nabla \cdot \vec{u} = -P$ with increasing Ka is consistent with the modeling assumption by Peters [26].

Figure 4 shows the variation of mean values of $Q \times (\delta_{th}/S_L)^2$ and its components $\{Q_S, Q_W\} \times (\delta_{th}/S_L)^2$, conditional on c_T . Both $\nabla \cdot \vec{u} = -P$ and $\sqrt{S_{ij}S_{ij}}$ influence the component $Q_S = (P^2 - S_{ij}S_{ij})/2$, whereas the component $Q_W = W_{ij}W_{ij}/2$ depends on enstrophy Ω (i.e., $W_{ij}W_{ij}/2 = \omega_i\omega_i/4 = \Omega/2$, where ω_i is the i th component of vorticity). Since the turbulence intensity u'/S_L in case A is low, the main nonzero contribution arises due to P as a result of thermal expansion. For case A, the mean value of Q_W is negligible and the mean variation of Q is

FIG. 4. Log-linear variation of $Q \times (\delta_{th}/S_L)^2$ (red), $Q_S \times (\delta_{th}/S_L)^2$ (green), and $Q_W \times (\delta_{th}/S_L)^2$ (blue) with c_T for cases A–C.

FIG. 5. Log-linear variation of $R \times (\delta_{th}/S_L)^3$ (red), $R_S \times (\delta_{th}/S_L)^3$ (green), $P Q_W \times (\delta_{th}/S_L)^3$ (blue), and $(-\omega_i S_{ij} \omega_j / 4) \times (\delta_{th}/S_L)^3$ (magenta) with c_T for cases A–C. All terms in case C are to be multiplied by 10^4 as indicated.

dominated by the mean value of Q_S , which assumes predominantly positive values except towards the burned gas side of the flame where the effects of P^2 are negligible due to the weak dilatation rate $\nabla \cdot \vec{u} = -P$. For case B, the mean value of Q_W remains nonzero and positive across the flame, whereas the mean value of Q_S remains negative for low and high values of c_T , indicating that $S_{ij} S_{ij}$ dominates over P^2 . This behavior originates from weak contributions of dilatation rate $\nabla \cdot \vec{u} = -P$ on both unburned and burned gas sides of the flame (see Fig. 3) and thus the contribution of $Q_S = (P^2 - S_{ij} S_{ij})/2$ is principally governed by $S_{ij} S_{ij}$ in these regions. However, P^2 assumes high values due to large values of dilatation rate $\nabla \cdot \vec{u} = -P$ close to the reaction zone (see Fig. 3) and thus P^2 dominates over $S_{ij} S_{ij}$ to give rise to positive mean value of Q_S for intermediate values of c_T in case B. Thus, the mean value of $Q \times (\delta_{th}/S_L)^2$ remains small at high and low values of c_T and attains its maximum values at $c_T \approx 0.2$, where the mean values of Q_S and Q_W are both positive. In contrast to cases A and B, the magnitude of Q and its components at $c_T \approx 0.0$ are far greater in case C. The mean contribution of $Q_S = (P^2 - S_{ij} S_{ij})/2$ remains negative throughout the flame in case C because in this case the effects of the dilatation rate $\nabla \cdot \vec{u} = -P$ are too weak to supersede the influences of $S_{ij} S_{ij}$ and thus in this case the behavior of Q_S is principally governed by $(-S_{ij} S_{ij})/2$.

The quantity Q_S can be expressed as $Q_S = Q_{S1} + Q_{S2} = P^2/3 - E/4\nu$, where $E = (\tau_{ij} \partial u_i / \partial x_j) / \rho$ is the dissipation rate of instantaneous kinetic energy (i.e., $u_i u_i / 2$) and ν is the kinematic viscosity. Hence, $Q_S > 0$ ($Q_S < 0$) corresponds to dilation- (dissipation-) dominated regions. Using $Q_{S1} = P^2/3 \sim \{\tau S_L / \delta_{th}\}^2$ [17,34] and $|Q_{S2}| = |-E/4\nu| \sim 1/\tau_\eta^2$ (where τ_η is the Kolmogorov time scale) leads to $Q_{S1}/|Q_{S2}| \sim \tau^2 \text{Ka}^{-2}$, where $\tau = (T_{ad} - T_0)/T_0$ is the heat release parameter. This suggests that the relative strength of Q_{S1} with respect to Q_{S2} weakens (strengthens) with increasing Ka (heat release). Thus, in case C (where $\text{Ka} \gg 1$), the mean behavior of Q_S is governed by $Q_{S2} = -E/4\nu$, whereas in case A (where $\text{Ka} < 1$) the mean behavior of Q_S is governed by the positive mean value of $Q_{S1} = P^2/3$ for the major part of the flame brush. In case B (where

FIG. 6. Log-linear variation of $\{-P^3/3\} \times (\delta_{th}/S_L)^3$ (red), $\{P Q_S\} \times (\delta_{th}/S_L)^3$ (green), and $\{-S_{ij} S_{jk} S_{ki} / 3\} \times (\delta_{th}/S_L)^3$ (blue) with c_T for cases A–C. The inset in case C shows variation of terms of smaller magnitude. All terms in case C are to be multiplied by 10^4 as indicated.

$Ka > 1$), Q_{S1} dominates over Q_{S2} to result in a mean positive value of Q_S only in the region of the flame where the effects of heat release are strong.

In summary, in case C the mean values of Q_S and Q_W largely balance each other, although the mean value of Q remains negative across the entire flame front, which is opposite to the behavior of cases A and B.

The third invariant R may be written as $R = R_S + PQ_W - \omega_i S_{ij} \omega_j / 4$, where $R_S = (-P^3 + 3PQ_S - S_{ij}S_{jk}S_{ki})/3$ contains a contribution to the dissipation rate generation (i.e., $S_{ij}S_{jk}S_{ki}$), while $(PQ_W - \omega_i S_{ij} \omega_j / 4)$ contributes to the enstrophy production rate [6,16]. Thus, $R > 0$ indicates that the enstrophy production rate dominates over the dissipation rate generation and vice versa [6,16]. The contributions of $PQ_W - \omega_i S_{ij} \omega_j / 4$ and R_S appear to balance across the flame front in cases A and B (see Fig. 5). In both cases the mean value of R_S attains its maximum value, whereas the mean value of PQ_W attains its minimum value, at $c_T \approx 0.25$. In case C, the mean value of R_S is largely balanced by the mean contribution of $-\omega_i S_{ij} \omega_j / 4$, which are both an order of magnitude greater than the mean values of PQ_W and R . The mean value of R attains its maximum value at $c_T \approx 0.0$, but also a local maximum is obtained at $c_T \approx 0.20$, and R remains positive across the flame, indicating that the enstrophy production rate dominates over the dissipation rate generation, unlike cases A and B where the mean $R \approx 0$ across the flame.

Finally, Fig. 6 shows the individual terms contributing to R_S : $-P^3/3$, PQ_S , and $-S_{ij}S_{jk}S_{ki}/3$. For cases A and B, all terms are approximately zero at $c_T \approx 0.0$ and $c_T \approx 1.0$. The mean value of $-P^3/3$ remains positive and is balanced by the mean contributions of PQ_S and $-1/3S_{ij}S_{jk}S_{ki}$, which are both negative in the region $0.15 < c_T < 0.35$ for cases A and B. In contrast, in case C, the mean contributions of $-P^3/3$, PQ_S , and $-S_{ij}S_{jk}S_{ki}/3$ are positive, but they are dominated by the mean value of $-S_{ij}S_{jk}S_{ki}/3$, which is related to the dissipation rate generation. One can express $(\nabla \cdot \vec{u})E$ as $(\nabla \cdot \vec{u})E = 4\nu(PQ_S - P^3/3)$. It can be seen from the mean values of PQ_S and $-P^3/3$ in Fig. 6 that the mean value of $PQ_S - P^3/3 = (\nabla \cdot \vec{u})E/4\nu$ remains positive throughout the flame. As the mean value of $\nabla \cdot \vec{u}$ remains positive and the correlation between $\nabla \cdot \vec{u}$ and E is not particularly strong, the positive mean value of $PQ_S - P^3/3$ in Fig. 6 indicates a positive mean value of $E = 2\nu(S_{ij}S_{ij} - P^2/3)$.

Figure 7 shows the joint probability density function (PDF) contours of the normalized second and third invariants $F(Q^*, R^*)$ for cases A–C on $c_T = 0.1, 0.5, 0.7$, where $Q^* = Q \times (\delta_{th}/S_L)^2$ and $R^* = R \times (\delta_{th}/S_L)^3$. The behavior on isosurfaces of higher c_T values is not shown here, since $Q^* \approx 0.0$ for higher values of c_T (see Fig. 4). The joint PDF exhibits a negative correlation between Q^* and R^* [2,5] for all c_T isosurfaces. As c_T is increased, the most probable value of the distribution moves towards the origin (i.e., $Q^* = 0$ and $R^* = 0$).

It is useful to examine the variation of the individual local topologies S1–S8 across the flame and to see how their variation changes from one case to another. Figures 8(a)–8(c) show the variation of the volume fraction (VF) of each topology as a function of c_T following the approach adopted by Cifuentes *et al.* [15,16]. Figure 8 reveals a noticeable difference in the distribution of the flow topology between cases A–C. For case A, both focal and nodal topologies show clear variation with c_T , with S1, S3, and S4 increasing and S2, S7, and S8 decreasing as moving from the unburned to the burned gas region. Such trends diminish from case A to case C such that each topology is more uniformly distributed across c_T in case C. In particular, for case C, the S8 nodal topology disappears entirely. The S8 topology is associated with high positive values of dilatation rate ($\nabla \cdot \vec{u} = -P \gg 0$) and thus its probability decreases for case C due to weakening of dilatation rate.

Figure 8(d) compares the distributions of volume fraction of total combined focal (i.e., S1, S4, S5, and S7) and nodal (i.e., S2, S3, S6, and S8) topologies between cases A–C. For case A nodal topologies are dominant in the unburned gas region and focal topologies in the burned gas region. This contrasts with the previous simple chemistry analyses [15,16], which showed that the VF of focal topologies decreases from the unburned gas to the burned gas side. The heat release parameter $\tau = (T_{ad} - T_0)/T_0$ for cases A–C is greater than that used in Refs. [15,16] (6 as opposed to 4) and thus the flame-induced turbulence is stronger in these cases than in the cases analyzed in

FIG. 7. Joint PDFs of $Q^* = Q \times (\delta_{th}/S_L)^2$ and $R^* = R \times (\delta_{th}/S_L)^3$, $F(Q^*, R^*)$, on $c_T = 0.1, 0.5, 0.7$ isosurfaces for cases A–C. The value of $F(Q^*, R^*)$ increases from blue to red color.

Refs. [15, 16], where the VF of vortical (focal) topologies decayed across the flame.² The strength of vortical structures within the flame front increases within the flame due to flame-induced turbulence in case A, which is reflected in the increase in the VF of focal (i.e., vortical) topologies within the flame. In case C, the flame does not significantly influence the background turbulent flow field and the focal topologies remain dominant across the entire flamefront.

The statistics of flame curvature plays a key role in order to understand the interrelation between the distributions of the flow and flame topologies. The topology of a c_T isosurface can be described in terms of its mean and Gauss curvatures κ_m and κ_g , respectively, following Dopazo *et al.* [7], where $\kappa_m = (\kappa_1 + \kappa_2)/2 = 1/2 \nabla \cdot (-\nabla c_T / |\nabla c_T|)$ and $\kappa_g = \kappa_1 \kappa_2$, in which κ_1 and κ_2 are the principal curvatures [7, 16]. In the $\kappa_m - \kappa_g$ plane, the region $\kappa_g > \kappa_m^2$ indicates complex curvatures and thus is nonphysical. Moreover, positive (i.e., $\kappa_m > 0$) curvature is associated with the wrinkles that are convex to the reactants, whereas negative (i.e., $\kappa_m < 0$) curvature represents wrinkles that are

²The generation of enstrophy due to baroclinic torque is indeed found to be comparable to the magnitude of viscous dissipation of enstrophy in case A, which leads to considerable enstrophy generation within the flame for this case. By contrast, the viscous dissipation of enstrophy dominates over baroclinic torque contribution in cases B and C, where the vortex-stretching and viscous dissipation remain the leading-order contributors.

FIG. 8. Variation of volume fractions of topologies $S1$ – $S8$ with c_T for (a)–(c) cases A–C: focal topologies $S1$ (red solid line), $S4$ (blue solid line), $S5$ (green solid line), and $S7$ (magenta solid line) and nodal topologies $S2$ (red dashed line), $S3$ (blue dashed line), $S6$ (green dashed line), and $S8$ (magenta dashed line). (d) Variation of VFs of total focal (solid lines) and nodal (dashed lines) topologies with c_T for cases A (tan), B (black), and C (olive).

concave to the reactants (see Fig. 2). The realizable part of $\kappa_m > 0$ ($\kappa_m < 0$) and $\kappa_g > 0$ represents cup convex (cup concave) flame topology. By contrast, $\kappa_m > 0$ ($\kappa_m < 0$) and $\kappa_g < 0$ represents saddle convex (saddle concave) flame topology. The combination of $\kappa_m > 0$ ($\kappa_m < 0$) and $\kappa_g = 0$ represents tile convex (concave) flame topology. Figure 9 shows a scatter plot of the mean versus Gaussian curvature for cases A–C conditional on one representative focal ($S7$) and one nodal ($S3$) topology. The plots in Fig. 9 are colored to highlight the highest concentrations of data points. It is apparent from Fig. 9 that the distribution of topologies $S3$ and $S7$ favors $\kappa_m, \kappa_g > 0$ ($\kappa_m < 0$ and $\kappa_g > 0$) for case A (for case C), whereas case B shows a more symmetric distribution. A similar

FIG. 9. Scatter of normalized mean and Gaussian curvatures colored by count for (from left to right) cases A–C. Topologies S3 and S7 are shown exemplarily. Magnitude increases with color from white to red. Green dots indicate the location of the maximum values.

trend is observed for topologies S1, S2, and S8. Topology S4 is more symmetric and for topologies S5 and S6 there were insufficient data. These results do not reveal any consistent trend between flow and flame topologies based on these results, and a more detailed analysis is needed in this respect.

Figure 1 shows that the topologies are associated with different types of generic flow structures. Thus, the contributions of these topologies to turbulent processes such as micromixing characterized by the scalar dissipation rate (SDR) $N_c = D \nabla c_T \cdot \nabla c_T$ (where D is the thermal diffusivity) and enstrophy $\Omega = \bar{\omega} \cdot \bar{\omega} / 2$ transport in turbulent premixed flames are of fundamental importance. The transport equations of N_c and Ω are given by [17,18,34,35]

$$\begin{aligned} \rho \frac{DN_c}{Dt} = & \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial N_c}{\partial x_j} \right) - 2D \frac{Dc_T}{Dt} \frac{\partial c_T}{\partial x_k} \frac{\partial \rho}{\partial x_k} - 2\rho D \underbrace{\frac{\partial c_T}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial c_T}{\partial x_j}}_{\Lambda} \\ & + 2D \frac{\partial \dot{\omega}_T}{\partial x_k} \frac{\partial c_T}{\partial x_k} - 2\rho D^2 \frac{\partial^2 c_T}{\partial x_k \partial x_i} \frac{\partial^2 c_T}{\partial x_k \partial x_i} + f(D), \end{aligned} \quad (3a)$$

$$\frac{D\Omega}{Dt} = \underbrace{\omega_i \omega_k \frac{\partial u_i}{\partial x_k}}_V - \epsilon_{ijk} \omega_i \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{kl}}{\partial x_l} + \frac{\epsilon_{ijk} \omega_i}{\rho} \frac{\partial^2 \tau_{kl}}{\partial x_j \partial x_l} - 2 \frac{\partial u_k}{\partial x_k} \Omega + \epsilon_{ijk} \frac{\omega_i}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k}, \quad (3b)$$

where ρ , p , $\dot{\omega}_T$, and τ_{ij} are the density, pressure, chemical source term, and viscous stress tensor, respectively, and $f(D)$ accounts for the contribution due to diffusivity gradients. The terms $-2\rho D \Lambda$ and V are referred to as the scalar-turbulence interaction and vortex-stretching terms, respectively [17,18,34,35]. The term Λ in Eq. (3a) can be written as $\Lambda = (\partial c_T / \partial x_i) (\partial u_i / \partial x_j) (\partial c_T / \partial x_j) = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma) \nabla c_T \cdot \nabla c_T = a_n \nabla c_T \cdot \nabla c_T$, where $a_n = N_i N_j \partial u_i / \partial x_j$ is the normal strain rate with $N_i = -(\partial c_T / \partial x_i) / |\nabla c_T|$ being the i th component of the flame normal vector [17]. This suggests that Λ takes a positive (negative) value for positive (negative) values of a_n [17]. The expression $\Lambda = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma) \nabla c_T \cdot \nabla c_T = a_n \nabla c_T \cdot \nabla c_T$ indicates that the behaviors of Λ and a_n are governed by the alignment of ∇c_T with local principal strain rates.

FIG. 10. Variation of the mean values of $\Lambda^* = \Lambda \times (\delta_{th}^3/S_L)$ (top row) and $V^* = V \times (\delta_{th}/S_L)^3$ (bottom row) conditional on c_T for cases A (left column), B (middle column), and C (right column): focal topologies S1 (red solid line), S4 (blue solid line), S5 (green solid line), and S7 (magenta solid line) and nodal topologies S2 (red dashed line), S3 (blue dashed line), S6 (green dashed line), and S8 (magenta dashed line). Results are omitted where the volume fraction is less than 0.01. The values of V^* in case C are to be multiplied by 10^5 as indicated.

As the flow topologies are associated with particular combinations of strain rate and vorticity distributions, they are likely to influence the statistical behaviors of terms Λ and V . These dependences of $\Lambda = (\partial c_T / \partial x_i)(\partial u_i / \partial x_j)(\partial c_T / \partial x_j) = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma) \nabla c_T \cdot \nabla c_T$ and $V = 2(e_\alpha \cos^2 \alpha' + e_\beta \cos^2 \beta' + e_\gamma \cos^2 \gamma') \Omega$ arise due to the alignment of ∇c_T and $\vec{\omega}$ with the most extensive (i.e., most positive), intermediate, and most compressive (i.e., most negative) strain rates (i.e., e_α , e_β , and e_γ), where α, β , and γ (α', β' , and γ') are the angles between ∇c_T ($\vec{\omega}$) and the eigenvectors associated with e_α , e_β , and e_γ , respectively.

The first row of Fig. 10 shows the contribution of different topologies to the mean values of Λ conditional on c_T .³ Cases A and B show positive mean contributions of Λ for all topologies except for S5 and S6 in case A and S3, S5, and S6 in case B. The mean value of Λ peaks at $c_T \approx 0.25$. In case A, S2 and S7 remain major contributors of Λ , closely followed by S4 and S8, whereas S8 is the primary contributor in case B, followed, in order, by S7, S2, S4, S1, and S3. The absence of contributions of S1 and S3 in case A is due to the scarcity of the corresponding samples at low values of c_T [see Fig. 8(a)]. Although case C also displays peak mean values of Λ for low c_T , the behavior of the topologies is vastly different: Mean contributions for S1–S7 are mostly negative, with the exception of S8. The peak magnitude of the negative mean value of Λ is obtained for S2 at $c_T \approx 0.15$. A non-negligible contribution is obtained from S5, although the sample size remains small [see Fig. 8(c)].

A preferential alignment between ∇c_T and e_α (e_γ), characterized by high probability of $\cos^2 \alpha \approx 1.0$ ($\cos^2 \gamma \approx 1.0$), leads to a positive (negative) Λ [17,34,36–39]. It has been shown elsewhere [17,34,36–39] that ∇c_T preferentially aligns with e_α when the strain rate induced by

³The components of Λ and V conditional on topology have not been shown because they deterministically show similar behavior. For example, the mean values of $(e_\alpha \cos^2 \alpha) \nabla c_T \cdot \nabla c_T$ and $2(e_\alpha \cos^2 \alpha') \Omega$ conditional on each topology will exhibit positive values due to positive value of e_α . By the same token, the mean values of $(e_\gamma \cos^2 \gamma) \nabla c_T \cdot \nabla c_T$ and $2(e_\gamma \cos^2 \gamma') \Omega$ conditional on topology will deterministically exhibit negative values for all cases. The magnitudes of these conditional mean values are expected to be different from one case to another because the strain rate magnitude will depend on u'/S_L and l_T/δ_{th} .

flame normal acceleration overcomes turbulence straining. In contrast, ∇c_T aligns with e_γ under the dominance of turbulent straining [17,34,36–39]. As the effects of heat release are stronger in the corrugated flamelets and thin reaction zone regime flames (e.g., cases A and B) than in the broken reaction zone regime flames (e.g., case C), ∇c_T shows strong alignment with e_α (e_γ) in cases A and B (case C), thus leading to a positive (negative) value of Λ . Although case C exhibits predominantly negative Λ , the S8 topology is associated with local high positive $\nabla \cdot \vec{u} = -P$ (see Fig. 1) and thus ∇c_T aligns locally with e_α to result in a positive Λ in this region.

A careful comparison reveals that the mean values of Λ conditional on c_T for S1–S4 topologies exhibit positive values due to predominant alignment of ∇c_T with e_α under the action of strong heat release in cases A and B. By contrast, predominant alignment of ∇c_T with e_γ due to weak influences of heat release in case C yields negative mean values of Λ conditional on c_T for S1–S4 topologies. As the flow topologies S5 and S6 are rare occurrences in premixed flames, a consistent trend is not expected for these topologies. The topologies S7 and S8 are associated with positive $\nabla \cdot \vec{u} = -P$ (see Fig. 1) and thus the effects of heat release are strongly felt in these topologies and as a result ∇c_T aligns locally with e_α to yield positive mean values of Λ conditional on c_T for these topologies in all three cases. However, the effects of heat release are weak towards the unburned gas side of the flame and thus the mean value of Λ conditional on c_T exhibits negative values even for the S8 topology in case C.

The second row of Fig. 10 shows the contribution of different topologies to the mean values of $V = 2(e_\alpha \cos^2 \alpha' + e_\beta \cos^2 \beta' + e_\gamma \cos^2 \gamma')\Omega$ conditional on c_T , which reveals that the mean value of V conditional on c_T for all topologies remain positive for all three cases. The predominant alignment of $\vec{\omega}$ with the intermediate and most extensive principal strain rates (i.e., e_β and e_α) in these cases, in accordance with previous findings [18,32,35], gives rise to a positive mean value of V for all cases considered here, but both the mean value and the qualitative behavior vary greatly between cases. In case A, S7 and S8 remain dominant contributors to V between $0.25 < c_T < 0.75$, but no clear peak in their mean contribution is evident. In case B, however, the contribution of S1 is dominant and its mean value shows a clear peak at $c_T \approx 0.25$. Finally, in case C, all nonzero topologies exhibit peak values at $c_T \approx 0.0$, with S4 and S7 attaining the highest mean values of V . Furthermore, in cases B and C, with the exception of S5 in case C, the contributions of all focal topologies of significant presence (i.e., S1, S4, and S7) attain higher values across the entire flame than for all significant nodal topologies (i.e., S2, S3, and S8).

The effects of flame-induced turbulence are the strongest for topologies that are associated with high positive $\nabla \cdot \vec{u} = -P$ in case A (e.g., S7 and S8). This trend weakens with increasing Ka. Thus, the focal topologies associated with positive Q [S1, S4, and S7 (see Fig. 1)] contribute more to V than the nodal topologies S2, S3, and S8. The topologies S4 and S7 are associated with the vortex stretching (see Fig. 1) and thus they exhibit a high positive mean contribution of V in case C. In the absence of significant flame-induced turbulence, Ω decreases within the flame in case C and the peak mean value of V is obtained at the unburned gas (i.e., $c_T \approx 0.0$) side of the flame front.

IV. CONCLUSION

The flow topology distributions in different regimes of premixed turbulent combustion were investigated using DNS data of statistically planar turbulent H₂-air flames with $\phi = 0.7$. The flow topologies were characterized in terms of the first, second, and third invariants (i.e., $P = -\nabla \cdot \vec{u}$, Q , and R) of the velocity gradient tensor $\partial u_i / \partial x_j$, where invariants Q and R are closely linked with vorticity and strain rates and also their generation rates. The mean value of $\nabla \cdot \vec{u} = -P$ decreases considerably in the broken reaction zone regime due to the severe disruption in chemical processes. The regime of combustion, especially the weakening of dilatation rate effects with increasing Karlovitz number, significantly affects the statistical behaviors of dilatation rate, enstrophy, and strain rate magnitude in addition to the generation rates of enstrophy and dissipation rate. These influences are reflected in the statistical behaviors of the second and third invariants (i.e., Q and R) of the velocity gradient tensor and their behavior across the flame.

Detailed explanations were provided for the observed combustion regime dependences of P , Q , and R , the flow topology distribution, and their influences on the scalar-turbulence interaction and vortex-stretching terms in the SDR and enstrophy transport equations, respectively. It was demonstrated that the influences of the combustion regime on P , Q , and R have important consequences on the distribution of those flow topologies that make dominant contributions to the scalar-turbulence interaction and vortex-stretching terms in the SDR and enstrophy transport equations, respectively. This analysis identified the flow topologies that make dominant contributions to Λ and V and thus the flow configurations responsible for the observed trends in different combustion regimes. This information can help in designing simplified experimental configurations for analyzing the statistical behaviors of the scalar-turbulence interaction and vortex-stretching terms.

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