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Statistics of vorticity alignment with local strain rates in turbulent premixed flames

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HIGHLIGHTS

- The statistics of alignment of vorticity with local principal strain rates have been analysed.
- Effects of regime of combustion and the global Lewis number have been investigated.
- Relative alignments with local principal strain rates are affected by Damköhler and Lewis numbers.
- Detailed physical explanations have been provided for the aforementioned observed behaviours.

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ABSTRACT

The instantaneous alignment of the vorticity vector with local principal strain rates is analysed for statistically planar turbulent premixed flames with different values of heat release parameter and global Lewis number spanning different regimes of combustion. It has been shown that the vorticity vector predominantly aligns with the intermediate principal strain rate in turbulent premixed flames, irrespective of the regime of combustion, heat release parameter and Lewis number. However, the relative alignment of vorticity with the most extensive and compressive principal strain rates changes based on the underlying combustion conditions. Detailed physical explanations are provided for the observed behaviours of vorticity alignment with local principal strain rates. It has been shown that heat release due to combustion significantly affects the alignment of vorticity with local principal strain rates. However, the mean contribution of the vortex-stretching term in the transport equation of enstrophy remains positive for all cases considered here, irrespective of the nature of the vorticity alignment.

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1. Introduction

The alignment of the vorticity vector with local principal strain rates is of fundamental importance for the understanding and modelling of turbulent fluid motion, as the alignment statistics directly affect the nature of the vortex-stretching mechanism [1]. It has been demonstrated in several previous studies that the vorticity vector instantaneously aligns with the intermediate eigenvector of strain rate tensor for non-reacting turbulence [2–12]. However, relatively limited attention was given to the analysis of alignment of vorticity with local strain rates in the case of turbulent reacting flows [13–15]. In many applications (e.g. Spark Ignition (SI) engines and industrial gas turbines), the fuel and oxidiser are homogeneously mixed prior to the combustion process (i.e. premixed combustion). Thus, the understanding of vorticity alignment with local principal strain rates is of fundamental interest for the development of high-fidelity models which can, in turn, contribute

to the design of new generation energy-efficient and environment-friendly combustion devices. The analysis of Nomura and Elghobashi [13], Boratov et al. [14] and Jaber et al. [15] concentrated on vorticity alignment with local principal strain rates for non-premixed flames where fuel and oxidiser are completely separated from each other prior to the combustion process. Recently, Hamlington et al. [16] analysed vorticity statistics in premixed combustion based on numerical solutions of reactive systems. The analysis by Nomura and Elghobashi [13] demonstrated that the vorticity vector aligns with the intermediate principal strain rate in non-premixed flames similar to non-reacting turbulent flows but vorticity in non-premixed flames shows appreciable probabilities of local alignment with the most extensive principal strain rate. The analysis by Boratov et al. [14] on non-premixed flame DNS data reveals that the extent of vorticity alignment with the most extensive principal strain rate increases in the regions where the magnitude of strain rate dominates over the vorticity magnitude. By contrast, vorticity shows preferential alignment with the intermediate principal strain rate in the regions where the vorticity magnitude dominates over the strain rate magnitude. The analysis by Jaber et al. [15] further demonstrated that the alignment of

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Nomenclature

Arabic

a	Acoustic velocity
a_{chem}	Strain rate induced by chemical reaction
a_{turb}	Turbulent straining
a_T	Tangential strain rate
A_i	i th wave associated with boundary
B	Pre-exponential factor
B^*	Normalised pre-exponential factor
c	Reaction progress variable
c^*	Reaction progress variable value indicating the flame surface
C_p	Specific heat capacity at constant pressure
C_v	Specific heat capacity at constant volume
D	Progress variable diffusivity
Da	Damköhler number
e_α	Most extensive principal strain rate
e_β	Intermediate principal strain rate
e_γ	Most compressive principal strain rate
e_θ	Principal strain rate
e_{ij}	Component of strain rate tensor
$\hat{e}_1, \hat{e}_2, \hat{e}_3$	Eigenvectors associated with eigenvalues e_α, e_β and e_γ respectively
E_{ac}	Activation energy
f_1	Terms involving viscosity gradients in the vorticity transport equation
f_2	Terms involving viscosity gradients in the enstrophy transport equation
k	Thermal conductivity
Ka	Karlovitz number
l	Integral length scale
L_i	i th wave amplitude variation
Le	Lewis number
N_i	i th component of flame normal vector
p	Pressure
p^{req}	Target value of pressure at the boundary
Pr	Prandtl number
q_{Ti}	Conduction heat flux in the i th direction
q_{Ci}	Diffusive mass flux in the i th direction
Q	General quantity
Re_t	Turbulent Reynolds number
S_d	Displacement speed
S_L	Unstrained laminar burning velocity
t	Time
t_{chem}	Chemical time scale
t_f	Initial turbulent eddy turnover time
t_{sim}	Simulation time
t_η	Kolmogorov time scale
T	Non-dimensional temperature
T_0	Unburned gas temperature
T_{ad}	Adiabatic flame temperature
T^{req}	Target value of non-dimensional temperature at the boundary
$\hat{T}$	Dimensional temperature
u_i	i th component of fluid velocity
u_i^{req}	Target value of i th component of fluid velocity at the boundary
u'	Root mean square turbulent velocity fluctuation magnitude
$\vec{u}$	Velocity vector
v_η	Kolmogorov velocity scale
V	Volume
$\dot{w}$	Chemical reaction rate

x_i	i th Cartesian co-ordinate
Y_R	Reactant mass fraction
Y_{RO}	Reactant mass fraction in unburned gases
$Y_{R\infty}$	Reactant mass fraction in fully burned gases

Greek

α_H	Heat release parameter
α	Angle between vorticity and the most extensive principal strain rate
α_p	Angle between pressure gradient and the most extensive principal strain rate
β	Angle between vorticity and the intermediate principal strain rate
β_p	Angle between pressure gradient and the intermediate principal strain rate
β_Z	Zel'dovich number
γ	Angle between vorticity and the most compressive principal strain rate
γ_p	Angle between pressure gradient and the most compressive principal strain rate
γ_G	Ratio of specific heat capacities
δ_{th}	Thermal flame thickness
Δ	DNS grid spacing
η	Kolmogorov length scale
λ	Thermal conductivity
λ_i	Wave velocity associated with i th wave amplitude variation L_i
Λ	Vortex-stretching term
μ	Dynamic viscosity
μ_0	Dynamic viscosity of the unburned gas
θ	Angle
φ_1	Function of Lewis number related to a_{chem}
φ_2	Function of Lewis number related to $\partial u_i / \partial x_i$
ρ	Gas density
ρ_0	Unburned gas density
σ_i	Relaxation factor associated with i th wave amplitude variation
τ	Heat release parameter
τ_{ij}	Components of viscous stress
ω_i	i th component of vorticity
$\vec{\omega}$	Vorticity vector
Ω	Enstrophy (i.e. $\Omega = \omega_i \omega_i / 2$)

Symbol

$\langle Q \rangle$	Ensemble averaged values of a general quantity Q conditionally averaged in bins of c values
$\vec{A} \bullet \vec{B}$	Scalar product between vectors $\vec{A}$ and $\vec{B}$

Acronyms

DNS	Direct Numerical Simulation
LES	Large Eddy Simulation
pdf	Probability density function
RANS	Reynolds Averaged Navier–Stokes

vorticity with the intermediate (most extensive) principal strain rate decreases (increases) due to chemical heat release in non-premixed flames. It is worth nothing that the analysis by Jaber et al. [15] was carried out for constant volume homogeneous turbulence but their findings were found to be qualitatively similar to the results by Nomura and Elghobashi [13] for non-premixed combustion in the presence of inhomogeneous turbulence. Moreover, Jaber et al. [15] showed that vorticity remains mostly perpendic-

ular to the most compressive principal strain rate in both reactive and non-reactive regions of non-premixed turbulent combustion. The computational analysis by Hamlington et al. [16] reveals that vorticity alignment with local principal strain rates in turbulent premixed flames is qualitatively similar to the previous findings in the context of non-premixed combustion (i.e. preferential alignment with the intermediate principal strain rate; negligible alignment with the most compressive principal strain rate and an increased alignment with the most extensive principal strain rate in the heat releasing zone). In general it has been found that the alignment of vorticity with the most extensive principal strain rate increases in the heat releasing zone in turbulent reacting flows [13–16]. Moreover, Hamlington et al. [16] demonstrated that the alignment of vorticity vector with local principal strain rates is expected to show a behaviour similar to a passive non-reacting isothermal turbulent flow when the root-mean-square (rms) velocity fluctuation u' remains much greater than the unstrained laminar burning velocity S_L . However, the statistical behaviour of vorticity alignment with local principal strain rate changes significantly in comparison to passive turbulent conditions when u' remains either small than or comparable to S_L . Detailed physical explanations for the u'/S_L dependence of vorticity alignment have also been provided by Hamlington et al. [16] who indicated that the alignment of vorticity with flame normal vector plays a key role and vorticity tends to align with local flame normal vector in the reaction zone for small values of u'/S_L , which in turn increases alignment of vorticity with the most extensive principal strain rate in the thin reaction zones regime flames with unity Lewis number Le (i.e. the ratio of thermal diffusivity to mass diffusivity).

The relative sizes of flame thickness, and the Kolmogorov length scale, significantly affect the nature of combustion process in turbulent premixed combustion [17,18]. Energetic turbulent eddies cannot penetrate into the flame structure for the regime of combustion where Kolmogorov length scale remains greater than the flame thickness. This regime is commonly referred to as the corrugated flamelets regime [17]. By contrast, energetic eddies can penetrate into the preheat zone and can perturb the reaction–diffusion balance when the flame thickness remains greater than the Kolmogorov length scale but the reaction zone thickness needs to be smaller than the Kolmogorov length scale to prevent flame extinction. This regime of combustion is referred to as the thin reaction zones regime of combustion [17]. The regime of combustion is often characterised by a non-dimensional number known as the Karlovitz number Ka , which scales as $Ka \sim \delta_{th}^2/\eta^2$ [17]. Thus $Ka < 1$ ($Ka > 1$) is associated with the corrugated flamelets (thin reaction zones) regime of combustion. Alternatively Ka can be taken to scale as $Ka \sim v_\eta^2/S_L^2$, which suggests that the velocity induced by thermal expansion due to heat release is likely to play an important role in the corrugated flamelets regime (where $Ka < 1$). By contrast, turbulent velocity fluctuations are likely to mask the effects of heat release in the thin reaction zones regime (where $Ka > 1$). Thus it can be expected that the regime of combustion is likely to have an appreciable effect on the vorticity statistics in turbulent premixed flames. The analysis of Hamlington et al. [16] concentrated on the regimes of premixed turbulent combustion with unity Lewis number (i.e. $Le = 1.0$) where δ_{th} remains greater than η (i.e. $Ka > 1$) but differences in vorticity alignment statistics between $Ka < 1$ and $Ka > 1$ combustion are yet to be analysed in detail. Moreover, the analysis by Hamlington et al. [16] was carried out based on implicit Large Eddy Simulations (LES) where the numerical scheme was responsible for the dissipation of sub-grid turbulent kinetic energy. In contrast to LES, which inherently allows for approximations, Direct Numerical Simulations (DNS) resolve all the relevant length and time scales of turbulence without any recourse to turbulence modelling. However, most of the relevant length scales are resolved in LES

and as a result the implications of modelling inaccuracies are much less severe than in Reynolds Averaged Navier–Stokes (RANS) simulations. Thus, the vorticity alignment with local principal strain rates reported by Hamlington et al. [16] based on LES is found to be consistent with the present DNS findings for the thin reaction zones regime flames with unity Lewis number (see Section 3).

A recent DNS analysis [19] indicates that the characteristic Lewis number Le of turbulent premixed combustion has significant influences on the alignment statistics of reactive scalar gradients and thus Le is expected to have appreciable effects on vorticity alignment statistics. The effects of the ratio of flame thickness to the Kolmogorov length scale (characterised by Karlovitz number $Ka \sim \delta_{th}^2/\eta^2$) and global Lewis number on vorticity alignment statistics have been analysed here using a DNS database of statistically planar turbulent premixed flames with a range of different intensities of heat release τ and global Lewis number Le . In this respect the main objectives of the present analysis are:

1. To indicate differences in vorticity alignment statistics between the typical flames representing the corrugated flamelets and thin reaction zones regimes of combustion.
2. To demonstrate the effects of global Lewis number on the alignment of vorticity with local principal strain rates in turbulent premixed flames.
3. To provide physical explanations for the observed differences in vorticity alignment statistics between the corrugated flamelets and thin reaction zones regimes of combustion.
4. To offer physical explanations for the observed differences in vorticity alignment in response to the variation of characteristic Lewis number Le .

The transport equation of the i th component of vorticity ω_i in turbulent premixed flames is given as:

$$\begin{aligned} \rho \frac{\partial \omega_i}{\partial t} + \rho u_j \frac{\partial \omega_i}{\partial x_j} = & \rho \omega_j \frac{\partial u_i}{\partial x_j} - \rho \omega_i \frac{\partial u_k}{\partial x_k} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \omega_i}{\partial x_j} \right) \\ & + \frac{\varepsilon_{ijk}}{\rho} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} - \frac{\varepsilon_{ijk} \mu}{\rho} \frac{\partial^2 u_k}{\partial x_i \partial x_l} \frac{\partial \rho}{\partial x_j} \\ & - \frac{\varepsilon_{ijk} \mu}{3\rho} \frac{\partial^2 u_m}{\partial x_k \partial x_m} \frac{\partial \rho}{\partial x_j} + f_1(\mu) \end{aligned} \quad (1)$$

where the repeated indices in Eq. (1) and subsequent equations implicitly indicate a summation process according to the standard tensor notation. The first term on the right hand side of Eq. (1) is the vortex-stretching term. The second term on the right hand side originates from the non-zero dilatation rate (i.e. $\nabla \cdot \vec{u} = \partial u_k / \partial x_k$) due to thermal expansion, whereas the third term denotes the molecular diffusion of vorticity. The fourth term on the right hand side depicts vorticity generation/destruction by baroclinic effects. The fifth and sixth terms originate due to density change caused by the chemical reaction, and the last term $f_1(\mu)$ involves the term involving spatial gradients of viscosity.

Multiplying Eq. (1) by ω_i yields the transport equation of $\Omega = \omega_i \omega_i / 2$, which is given by:

$$\begin{aligned} \rho \frac{\partial \Omega}{\partial t} + \rho u_j \frac{\partial \Omega}{\partial x_j} = & \rho \omega_j \frac{\partial u_i}{\partial x_j} \omega_i - \rho \omega_i \omega_i \frac{\partial u_k}{\partial x_k} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \Omega}{\partial x_j} \right) \\ & + \frac{\varepsilon_{ijk}}{\rho} \omega_i \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} - \frac{\varepsilon_{ijk} \mu}{\rho} \omega_i \frac{\partial^2 u_k}{\partial x_i \partial x_l} \frac{\partial \rho}{\partial x_j} \\ & - \omega_i \frac{\varepsilon_{ijk} \mu}{3\rho} \frac{\partial^2 u_m}{\partial x_k \partial x_m} \frac{\partial \rho}{\partial x_j} - \mu \frac{\partial \omega_i}{\partial x_j} \frac{\partial \omega_i}{\partial x_j} + f_2(\mu) \end{aligned} \quad (2)$$

where the penultimate term on right hand side (i.e. $-\mu(\partial \omega_i / \partial x_j)(\partial \omega_i / \partial x_j)$) is responsible for molecular dissipation of Ω , and $f_2(\mu)$ accumulates the terms involving spatial derivatives of viscosity.

The statistical behaviour of the first term on the right hand side (i.e. $\rho\omega_i\partial u_i/\partial x_j\omega_j$) originates due to vortex stretching, and the statistical behaviour of this term depends on the alignment of ω_i with strain rate tensor $e_{ij} = 0.5(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$, which can be verified from the following expression:

$$\rho\omega_i \frac{\partial u_i}{\partial x_j} \omega_j = \rho\omega_i e_{ij} \omega_j = \Lambda$$

$$= 2\rho\Omega(e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma) \quad (3)$$

It is evident from Eq. (3) that the magnitude and sign of $\rho\omega_i e_{ij} \omega_j$ depend on the statistical behaviours of $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$, and on the relative magnitudes of e_α , e_β and e_γ . The alignment of vorticity with local principal strain rates will be discussed in detail in Section 3 of this paper. The enstrophy Ω is closely related to the dissipation rate of turbulent kinetic energy [20], which plays a key role in the closure of turbulent Reynolds stresses [20], and serves as an input parameter to the turbulent combustion models [21,22]. Thus it is important to analyse the vorticity alignment statistics (e.g. vortex-stretching term in Eq. (3)) for the modelling dissipation rate of turbulent kinetic energy.

2. Mathematical background & numerical implementation

In the present analysis, the alignment statistics of vorticity have been studied based on three-dimensional DNS data of statistically planar freely propagating turbulent premixed flames. A well-known DNS database [23] has been used for analysing vorticity alignment in the corrugated flamelets regime. The simulations representing the thin reaction zones regime were carried out using a compressible DNS code called SENG [24]. Ideally, both the three-dimensionality of turbulence, and the detailed structure of the flame should be accounted for in combustion DNS studies. However, accounting for detailed chemical mechanism along with three-dimensionality of turbulent flow field remains extremely computationally expensive even by contemporary standards. Therefore, the chemical aspect of combustion in this analysis is accounted for by a single-step Arrhenius-type reaction (i.e. Reactants $\rightarrow$ Products). In the context of simplified chemistry, a reaction progress variable c uniquely represents the species field. The reaction progress variable c is defined in terms of the mass fraction of a suitable reactant Y_R (i.e. $c = (Y_{R0} - Y_R)/(Y_{R0} - Y_{R\infty})$) in such a manner that c rises monotonically from 0 to 1 from unburned gases to fully burned gases. The reaction rate of c takes the following form, under the assumptions of single-step chemistry:

$$\dot{w} = B^* \rho(1-c) \exp \left[-\frac{\beta_Z(1-T)}{1-\alpha_H(1-T)} \right] \quad (4)$$

where

$$T = \frac{\hat{T} - T_0}{T_{ad} - T_0}, \quad \tau = \frac{\alpha_H}{(1-\alpha_H)} = \frac{(T_{ad} - T_0)}{T_0} \quad (5)$$

$$\beta_Z = \frac{E(T_{ad} - T_0)}{RT_{ad}^2}, \quad B^* = B \exp \left[-\frac{\beta_Z}{\alpha_H} \right].$$

In the present study, the specific heats of all species are taken to be equal and independent of temperature, and Fick's law has been used for mass diffusion. The Soret and Dufour effects are neglected. Moreover, thermo-physical properties such as, viscosity μ , thermal conductivity k and the density-weighted mass diffusivity ρD are taken to be equal for all species, and independent of temperature, following several previous studies [24–27]. The initial values of normalised root-mean-square (rms) turbulent velocity fluctuation u'/S_L , integral length scale to flame thickness ratio l/δ_{th} , turbulent Reynolds number $Re_t = \rho_0 u' l / \mu_0$, Damköhler number

Table 1

List of initial simulation parameters and non-dimensional numbers for the present DNS database.

Case	u'/S_L	l/δ_{th}	Re_t	Da	Ka
A	1.41	9.64	56.7	6.84	0.54
B–G	7.5	2.45	47.0	0.33	13.17

$Le = 1.0$ (A, B, F) 0.34 (C), 0.6 (D), 0.8 (E) and 1.2 (G). $\tau = 2.3$ (A), 3.0 (B), 4.5 (C–G)

$Da = lS_L/u'\delta_{th}$ and Karlovitz number $Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$ are provided in Table 1, along with the values of heat release parameter $\tau = (T_{ad} - T_0)/T_0$ and Lewis number Le . The thermal flame thickness is defined as $\delta_{th} = (T_{ad} - T_0)/\text{Max}|\nabla \hat{T}|_L$ where the subscript L refers to the unstrained laminar flame quantities. Unstrained planar laminar flame simulation is performed on different grids to ensure grid-independent solution and the maximum value of $|\nabla \hat{T}|_L$ was evaluated based on these laminar flame simulations.

Table 1 suggests that case A represents the corrugated flamelets regime combustion (i.e. $Ka < 1$), whereas the other cases represent the thin reaction zones regime (i.e. $Ka > 1$) according to the regime diagram by Peters [17]. Among the cases considered here, the differential diffusion of heat and mass has been ignored in cases A, B and F, which is reflected in the unity value of Lewis number.

The rate of mass diffusion is taken to be faster (slower) than the thermal diffusion rate in cases C–E (case G), which is reflected in the $Le < 1$ ($Le > 1$) value in these cases. In a real combustion process, different species have different values of Lewis number but often the Lewis number of the deficient reactant is taken to be the characteristic Lewis number of the underlying combustion process [28]. In several previous studies [29–36], the characteristic Lewis number was modified independently of other parameters in order to analyse the effects of differential diffusion of heat and mass in isolation. The same approach has been adopted in this analysis.

It is evident from Table 1 that the initial values of turbulent Reynolds number Re_t are different but comparable for cases A and B–G. The difference between Re_t for cases A and B–G (i.e. $Re_t = 56.7$ in case A and $Re_t = 47.0$ in cases B–G) is not large enough to induce any major Reynolds number dependence. Cases B and F are identical to each other except the value of heat release parameter τ . If a comparison between the results for cases B and F reveals that a 1.5 fold increase τ (i.e. $\tau = 3.0$ in case B and $\tau = 4.5$ in case F) does not significantly modify the qualitative nature of vorticity dynamics in the thin reaction zones regime (which will be substantiated later in this paper), it can be inferred that the differences in vorticity alignment statistics between cases A and B originate due to differences in the combustion regimes because the difference in τ between cases A and B ($\tau = 2.3$ in case A and $\tau = 3.0$ in case B) is not expected to play a major role. There have been several previous analyses where either cases A, B and F or the simulations parameters similar to cases A, B and F have been used to demonstrate and analyse the fundamental differences in flame propagation [18], turbulent kinetic energy [37] and scalar dissipation rate [22] and Flame Surface Density [38,39] closures, scalar gradient alignment [40] and conditional velocity statistics [41] between the corrugated flamelets and thin reaction zones regimes and the same approach has been followed here.

For case A, inflow and outflow boundaries are specified in the direction of mean flame propagation and transverse directions are considered to be periodic. The inlet turbulent velocity field is specified by scanning a plane through a frozen turbulent velocity fluctuation field. The outflow boundary is specified using the Navier–Stokes Characteristic Boundary Conditions (NSCBC) outlined by Poinot and Lele [42]. The boundaries in the direction of the mean flame propagation (i.e. negative x_1 -direction in the

present configuration) for cases B–G are taken to be partially non-reflecting in nature, following NSCBC [42] technique, and transverse boundaries are considered to be periodic. According to NSCBC technique, the inviscid part of the Navier–Stokes equations is specified using a characteristic analysis based on a locally one-dimensional system $\partial A_i / \partial t + \lambda_i \partial A_i / \partial x_1 = \partial A_i / \partial t + L_i = 0$ (for $i = 1-5$) where $A_1 = p - \rho u_1 a$, $A_2 = p / \rho^\gamma$, $A_3 = u_2$, $A_4 = u_3$ and $A_5 = p + \rho u_1 a$, and the wave velocities λ_i are given by $\lambda_1 = u_1 - a$, $\lambda_2 = \lambda_3 = \lambda_4 = u_1$ and $\lambda_5 = u_1 + a$. The wave amplitude variations L_i directed into the domain need to be specified at the partially non-reflecting boundary and the wave amplitude variations for the outgoing waves are estimated from internal solutions. For the incoming waves the following expressions for L_i : $L_1 = \sigma_1(p - p^{req})$, $L_2 = \sigma_2(T - T^{req})$, $L_3 = \sigma_3(u_2 - u_2^{req})$, $L_4 = \sigma_4(u_3 - u_3^{req})$ and $L_5 = \sigma_5(u_1 - u_1^{req})$ were considered, where σ_i s are the relevant relaxation parameters [42]. The values of $\partial \tau_{ij} / \partial x_1$ (for $j = 1, 2$ and 3), $\partial q_{T1} / \partial x_1$ and $\partial q_{C1} / \partial x_1$ are considered to be zero at the partially non-reflecting boundaries [42], where $q_{T1} = -k(\partial \hat{T} / \partial x_1)$ and $q_{C1} = -\rho D \partial c / \partial x_1$ are the heat and mass fluxes respectively. Interested readers are referred to Ref. [42] for a more detailed discussion on boundary conditions. In DNS, the turbulent flow field is simulated without any physical approximation, and the grid spacing remains smaller than the Kolmogorov length scale. The grid size for DNS is chosen in such a manner that the grid spacing satisfies $\Delta \leq \min(\eta, \delta_{th} / 10)$. For all cases considered here the grid spacing is determined by the resolution of the flame, and at least about 10 grid points are kept within δ_{th} . As turbulence decays rapidly with the increase in kinematic viscosity in the burned gases (even in the present case due to the decrease in gas density in the burned gas), the flame-turbulence interaction is mainly characterised by the turbulent processes in the unburned gas side [25,26]. Thus, the findings based on constant thermo-physical properties are likely to be qualitatively valid even when temperature dependent properties are considered. This matter has been discussed earlier in detail by Poinso et al. [25] and Louch and Bray [26]. Standard values are taken for Zel'dovich number β_Z , Prandtl number Pr and the ratio of specific heats γ_G (i.e. $\beta_Z = 6.0$, $Pr = 0.7$, $\gamma_G = C_p / C_v = 1.4$).

The turbulent velocity fluctuation is initialised by a homogeneous isotropic incompressible flow field which is generated using a pseudo-spectral method [43] following the Batchelor–Townsend spectrum [44]. The flame is initialised using unstrained planar laminar flame simulations. In case A all the convective terms are time advanced in an explicit manner using a low-storage 3rd order Runge–Kutta scheme [45]. By contrast, all the diffusive/viscous terms in case A are time-advanced implicitly using the Crank–Nicolson scheme. For cases B–G all the terms are time-advanced in an explicit manner using a low-storage 3rd order Runge–Kutta scheme [45]. Similar procedure has been followed in several previous analyses [18,19,24,28–41,46–51]. In all cases flame-turbulence interaction takes place under decaying turbulence. Under decaying turbulence, simulations should be carried out for $t_{sim} \geq \text{Max}(t_f, t_c)$, where $t_f = l/u'$ is the initial eddy turn over time and $t_c = \delta_{th}/S_L$ is the chemical time scale. The simulation in case A was run for about 4 initial eddy turn over times ($t_{sim} \sim 4t_f \sim 4l/u'$), whereas cases B–G were run for a time equivalent to $3.34t_f$. The aforementioned simulation times remain either greater than (case A) or equal to (cases B–G) one chemical time scale $t_c = \delta_{th}/S_L$, and are comparable to several previous studies [18,19,24,28–41,46–51]. As the typical values of eddy turn over time t_f is much greater in case A than in cases B–G, the numerical treatment for case A is different in comparison to cases B–G for the purpose of computational economy.

The turbulent kinetic energy and its dissipation rate in the unburned gas ahead of the flame were not varying significantly with time when statistics were extracted. The values of u'/S_L in the

unburned reactants ahead of the flame at the time when statistics were extracted decreased by about 52% and 50% of its initial value in cases A and B–G respectively. The values of l/δ_{th} have increased from their initial values by a factor of about 1.10 and 1.7 for cases A and cases B–G respectively, but there are still enough turbulent eddies in each side of the computational domain. All the statistics presented in Section 3 correspond to $t = 4.0l/u'$ ($t = 3.34l/u'$) for case A (cases B–G) but the qualitative nature of the statistics was found to have remained unchanged since $t = 2.0l/u'$ for all cases.

3. Results & discussion

Distribution of vorticity

The distributions of vorticity magnitude $\sqrt{\omega_i \omega_i}$ in the $x_1 - x_2$ mid-plane are shown in Fig. 1 for all the cases considered here. The contours of c from $c = 0.1$ to 0.9 (from left to right) in steps of 0.1 are also shown in Fig. 1. It can be seen from Fig. 1 that the contours of c remain parallel to each other in case A where the flame thickness is smaller than the Kolmogorov length scale (i.e. $Ka < 1$). As a result of this, turbulent eddies cannot penetrate into the flame, and the flame gets wrinkled by the large-scale turbulent motion. For cases B–G, the flame thickness remains greater than the Kolmogorov length scale (i.e. $Ka > 1$), but the thickness of the reaction zone is smaller than the Kolmogorov length scale. Thus, turbulent eddies penetrate into the preheat zone in these cases, but cannot enter into the reaction zone. As a result of this, the preheat zone of cases B–G gets more distorted than the reaction zone, and the progress variable contours representing the preheat zone (i.e. $c < 0.5$) are more distorted and not parallel to the contours representing the reaction zone (i.e. $0.7 \leq c \leq 0.9$). It can be seen from the contours of c in Fig. 1c–g that the extent of flame wrinkling increases with decreasing Le . In $Le < 1$ flames reactants diffuse into the reaction zone at a faster rate than the rate at which heat is conducted out, which gives rise to simultaneous presence of high temperature and high reactants concentration. This eventually leads to enhanced burning rate and flame area generation in $Le < 1$ flames in comparison to the $Le = 1.0$ flame with same unburned gas turbulence and this tendency increases with decreasing Le . By contrast, heat diffuses faster than the rate of diffusion of fresh reactants in the reaction zone in $Le > 1$ flames, which in turn gives rise to simultaneous presence of low temperature and reactant concentration. This leads to reduced burning rate and flame area generation in $Le > 1$ flames than the corresponding $Le = 1.0$ flame. The global burning rate and flame area can be characterised by $\int_V \dot{w} dV$ and $\int_V |\nabla c| dV$ where dV is an infinitesimal volume element [32,34–36]. The values of $\int_V \dot{w} dV$ ($\int_V |\nabla c| dV$) in cases C–E and G are 7.5, 2.5, 1.4 and 0.82 (2.14, 1.44, 1.15 and 0.95) times that in case F respectively [36]. This is found to be consistent several previous analyses on the effects of non-unity Lewis number [19,29–36,52,53]. The enhanced (reduced) burning rate in the $Le < 1$ ($Le > 1$) flames give rise to strengthening (weakening) of dilatation rate and velocity jump across the flame in comparison to the corresponding unity Lewis number flame, and the effects of flame generated turbulence strengthen (weaken) with decreasing (increasing) Le . These effects were discussed elsewhere [19,35,36] in detail by this author (see Fig. 5 of Ref. [19] for the pdfs of $\partial u_i / \partial x_i$ for cases C, E and G. The values of $(\partial u_i / \partial x_i)$ and velocity jump across the flame for cases C–G are shown in Fig. 3b, e of Ref. [35]. The augmentation of flame generated turbulence with decreasing Le can be seen from Fig. 2 of Ref. [36]) and interested readers are referred to these papers for further information. It has also been demonstrated by the present author that the alignment of ∇c with local principal strain rates is also significantly affected by the enhanced heat release effects at small values of Le and interested readers are referred to Ref. [19] for more information.

Fig. 1. Distribution of vorticity magnitude $\sqrt{\omega_i \omega_i} \times \delta_{th}/S_L$ in the central $x_1 - x_2$ plane when the statistics were extracted for (a–g) cases A–G (see Table 1 for attributes of cases A–G). The white lines indicate reaction progress variable contours from $= 0.1$ to 0.9 from left to right in steps of 0.1 .

Fig. 1 shows that $\sqrt{\omega_i \omega_i}$ decays significantly in the burned gas in cases B, D–G due to strong viscous action as a result of increased kinematic viscosity. Moreover, dilatation rate $\partial u_i / \partial x_i$ within the flame also acts to suppress the vorticity within the flame (see second term on right hand side of Eqs. (1) and (2)). However, di-

latation rate assumes negligible magnitude in fully burned gas for low Mach number flows so viscous action is primarily responsible for the decay of vorticity magnitude in the completely burned gas. The relative contributions of the different terms of Eq. (2) are found to be qualitatively similar to the behaviour reported in

Fig. 2. Pdfs of the magnitude of the cosine of the angle between the vorticity vector and the most extensive principle strain rate (i.e. $|\cos \alpha|$) on the reaction progress variable $c =$ (a) 0.1, (b) 0.3, (c) 0.5, (d) 0.7 and (e) 0.9 isosurfaces, for cases A–G.

Jaberi et al. [15] (see Fig. 17 in Ref. [15]) and thus are not shown here for the sake of brevity.

It can be seen from Fig. 1a that there is a large separation between the vorticity magnitudes at the inlet boundary and within the flame in case A. In case A the turbulent velocity fluctuation values are much smaller than other cases whereas integral length scale is much larger than other cases (see Table 1). The dilatation rate $\partial u_i / \partial x_i$ can be scaled as $(\partial u_i / \partial x_i) \sim \tau S_L / \delta_{th} \sim \tau Da(u' / \lambda) / Re_t^{1/2}$ [18,19,40] and thus dilatation rate dominates over turbulent straining (which can be taken to scale with u' / λ [20]) in case A due to large values of Da . This is reflected in the preferential alignment of ∇c with e_α , which was demonstrated and discussed elsewhere [40]. The strong dilatation rate field suppresses the vorticity magnitude (see the second term of Eq. (2)) as the flow approaches towards the flame. However, there are localised spots where vorticity magnitude increases across the flame due to large velocity gradients induced by strong velocity jump across the flame (see Ref. [36]) in case A. It is also worth noting that $Ka \sim \delta_{th}^2 / \eta^2 < 1$ for case A, which indicates that this

flame is not expected to encounter energetic turbulent eddies, which can be substantiated from Fig. 1. By contrast, cases B–G has higher (smaller) values of $u' / S_L(l / \delta_{th})$ than in case A (see Table 1) and thus have much smaller Damköhler number than case A. This suggests that the effects of vorticity suppression due to dilatation rate are likely to be much weaker in the low Damköhler number $Le \approx 1.0$ flames (e.g. cases B, E–G). It has been shown in previous studies [19,25,36] that dilatation rate effects strengthen with decreasing Le but the effects of vorticity suppression due to dilatation rate are countered by strong velocity gradient induced by large velocity jump across the flame in these cases. This gives rise to localised augmentation of vorticity across the flame in cases C and D. Moreover, energetic turbulent eddies penetrate into the flame in cases B–G due to $Ka \sim \delta_{th}^2 / \eta^2 > 1$ and thus flames in cases B–G encounter large values of vorticity unlike case A. Smaller values of l / δ_{th} in cases B–G than in case A leads to more abundance of small scale structures in these cases than in case A. It is evident from Fig. 1 that the effects of flame-generated turbulence weaken with increasing Le .

Fig. 3. Pdfs of the magnitude of the cosine of the angle between the vorticity vector and the intermediate principle strain rate (i.e. $|\cos \beta|$) on the reaction progress variable $c =$ (a) 0.1, (b) 0.3, (c) 0.5, (d) 0.7 and (e) 0.9 isosurfaces, for cases A–G.

The flames with $Le \approx 1.0$ within the thin reaction zones regime (i.e. cases B, E–G) do not impart much influence on the vorticity field in the upstream of the flame. As the initial turbulent velocity field is the same in cases B, and E–G, and the thermo-chemistry is similar as well, they exhibit almost identical reaction progress variable and vorticity fields. However, the extent of wrinkling and burning increases with decreasing Le in the $Le \ll 1.0$ flames (e.g. cases C and D) due to thermo-diffusive instabilities [29–36,52,53]. The strong velocity jump across the flame and high dilatation rate magnitude due to high rate of heat release alter the vorticity field significantly in cases C and D in comparison to cases B, E–G. The flame-generated turbulence locally augments vorticity magnitude across the flame in the $Le \ll 1$ flames (e.g. cases C and D). The effects of turbulent combustion regime (i.e. Ka) and Lewis number Le on flame-generated turbulence (e.g. turbulent kinetic energy generation) have been analysed elsewhere [36,37], and will not be repeated here for the sake of conciseness.

Vorticity alignment with local principal strain rates

In turbulent premixed combustion the reacting scalar field is often characterised in terms of c and thus it is useful to present the vorticity alignment statistics for different values of c across the flame. In the context of single step chemistry the reaction zone is confined to the region given by $0.7 \leq c \leq 0.9$ [18,32]. Thus the effects of dilatation rate and heat release are particularly strong in the region given by $0.7 \leq c \leq 0.9$ [19]. As the alignment of the vorticity vector with local strain rates can be characterised by the magnitude of the cosines of the angles α , β and γ (see Eq. (3)), it is useful to analyse the probability density functions (pdfs) of $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$. The pdfs of $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$ for five different c isosurfaces across the flame are shown in Figs. 2–4 respectively. The predominant probability of finding $|\cos \theta| = 1$ indicates the perfect alignment with the principal strain rate e_θ , where $\theta = \alpha, \beta$ and γ as applicable. A comparison between Figs. 2–4 reveals the effects of combustion regime and global Lewis number Le on the local vorticity alignment behaviour.

Fig. 4. Pdfs of the magnitude of the cosine of the angle between the vorticity vector and the most compressive principle strain rate (i.e. $|\cos \gamma|$) on the reaction progress variable $c =$ (a) 0.1, (b) 0.3, (c) 0.5, (d) 0.7 and (e) 0.9 isosurfaces, for cases A–G.

Difference in vorticity alignment behaviour between the different regimes of combustion for unity Lewis number flames

The vorticity vector aligns predominantly with the intermediate principal strain rate e_β towards the unburned gas side of the flame (e.g. $c = 0.1$), irrespective of the heat release parameter τ , and the regime of combustion. This is consistent with previous findings in the context of non-reacting [2–12] and reacting [13–16] turbulent flows. However, the alignment of vorticity vector with e_α and e_γ changes within the flame and the vorticity alignment with local principal strain rates differs from one case to the other. The vorticity vector shows a significant extent of alignment with the most compressive principal strain rate e_γ for the major part of the flame, except the unburned gas side in the corrugated flamelets regime flame (i.e. case A) considered here, and this tendency increases towards the heat releasing zone of the flame (i.e. $0.7 \leq c \leq 0.9$). The vorticity vector does not align with the most extensive principal strain rate e_α throughout the flame in case A. This

preferential alignment of vorticity in case A with e_γ is contrary to the findings in the context of both reacting [13–16] and non-reacting flows [2–12]. It is worth noting that Hamlington et al. [16] demonstrated that the alignment of vorticity with local principal strain rates exhibits deviation from passive turbulent flow conditions (i.e. predominant vorticity alignment with e_β) for small values of u'/S_L , which is qualitatively consistent with the findings of Hamlington et al. [16]. However, Hamlington et al. [16] did not report preferential alignment of vorticity with e_γ as in case A, but the values of Da and Ka for case A are significantly different from the values considered in Ref. [16].

The vorticity vector preferentially aligns with e_β throughout the flame in cases B and F, which represent the thin reaction zones regime combustion but in case F vorticity shows a relatively higher level of alignment with the most extensive principal strain rate in the heat releasing zone (i.e. $0.7 \leq c \leq 0.9$) than in case B. The analysis of Hamlington et al. [16] demonstrated that the alignment

of vorticity with e_α decreases with weakening of heat release effects for unity Lewis number thin reaction zones regime flames, which is responsible for smaller extent of vorticity alignment with e_α in case B than in case F due to smaller value of τ in case B.

Jimenez [4] showed that vorticity tubes with high vorticity magnitude induce velocity field in such a manner that the most extensive and compressive principal strain rates occur on the planes orthogonal to the plane in which these vortex tubes are placed. Thus, the high vorticity regions are preferentially aligned with the intermediate principal strain rate e_β in non-reacting turbulent flows. This behaviour has been observed in all the flames in both unburned and burned gas sides of the flame for all cases. Moreover, in case B, where combustion is taking place in the thin reaction zones regime (i.e. $v_\eta \gg S_L$) for a small value of τ , the presence of the flame does not alter the vorticity alignment, in comparison to the familiar behaviour obtained in the context of non-reacting turbulent flows (i.e. preferential alignment of vorticity with e_β).

It can be seen from Figs. 2–4 that the variation of τ between cases B and F does not have any major influence on the qualitative behaviour of the alignment of vorticity with local principal strain rates in the thin reaction zones regime. By contrast, the vorticity alignments with local principal strain rates for cases A and B are markedly qualitatively different although the ratio of τ between cases B and A is comparable to the ratio of τ between cases F and B. As the turbulent Reynolds number Re_t for cases A, B and F are comparable to each other (Re_t in case A is 56.7, whereas this value is 47 in cases B and F), it is unlikely that this small variation of Re_t is responsible for the differences in vorticity alignment between cases A and B, F, and the observed differences in vorticity alignment statistics between these cases arise due to different combustion regimes (i.e. case A represents a typical corrugated flamelets regime flame, whereas cases B and F represent typical thin reaction zones regime flames).

Difference in vorticity alignment behaviour in response to global Lewis number Le

The alignment of vorticity with principal strain rates for the $Le = 0.8$ and 1.2 flames (i.e. cases E and G) remains qualitatively similar to that in the $Le = 1.0$ flame with same values of τ (i.e. case F). In the $Le = 0.34$ and 0.6 flames the vorticity vector also aligns predominantly with e_β throughout the flame. In the $Le = 0.34$ flame, the alignment of the vorticity vector with e_α decreases from the unburned gas side to the heat releasing zone of the flame. The extent of vorticity alignment with e_α was shown to increase in the heat releasing zone in the previous analyses on turbulent non-premixed [13–15] and premixed [16] combustion. Similar behaviour has been observed for the unity Lewis number flames within the thin reaction zones regime (i.e. cases B and F). It was shown in Ref. [19] that ∇c aligns with e_α in the reaction zone in cases E–G and a greater level of vorticity alignment with e_α is consistent with the findings of Hamlington et al. [16], which demonstrated that vorticity tends to show significant alignment with e_α in the regions of intense heat release where vorticity aligns with ∇c in the thin reaction zones regime flames with unity Lewis number. However, the alignment of vorticity with e_α (e_γ) decreases (increases) in the heat releasing zone for the high Damköhler number corrugated flamelets regime flame (i.e. case A) and in the thin reaction zones regime flames with $Le \ll 1$ (i.e. cases C and D). The alignment of vorticity with e_γ was not observed in the previous analyses [2–16]. The analysis of Hamlington et al. [16] ignored the effects of baroclinic torque on vorticity alignment behaviour under the conditions of intense heat release (see Eq. (25) in Ref. [16]) and it will be demonstrated later in the paper that baroclinic torque might play a key role in the vorticity alignment statistics in $Le \ll 1$ flames (e.g. cases C and D) and also in the flame representing the corrugated flamelets regime combustion (i.e. case A).

Fig. 5. Variation of the ratio of the mean values of dilatation rate to tangential strain rate (i.e. $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$) conditional on reaction progress variable c for cases A–G throughout the flame. The angled brackets indicate ensemble averaged values conditional on c isosurfaces.

A comparison between Figs. 2–4 reveals that the extent of vorticity alignment with e_α decreases with decreasing Le and this trend is particularly prevalent for flames with $Le \ll 1$ (e.g. cases C and D). By contrast, the extent of vorticity alignment with e_β and e_γ increases with decreasing Le in the reaction zone $0.7 \leq c \leq 0.9$ (see cases C–G in Figs. 3 and 4) but no major difference is observed in the preheat zone (i.e. $c \leq 0.5$) in response to Le . The physical explanations for the aforementioned vorticity alignment behaviour will be provided next in this paper.

Physical explanations for the observed vorticity alignment

Figs. 2–4 suggest that the regime of combustion and Lewis number have significant influences on the alignment of the vorticity vector with local principal strain rates. The most extensive principal strain rate e_α in turbulent premixed flames can be scaled with the strain rate induced by chemical reaction a_{chem} . The strain rate induced by flame normal acceleration due to thermal expansion is referred to as the strain rate induced by chemical reaction a_{chem} in this analysis. In an unstrained laminar flame the velocity jump across the flame (i.e. difference between velocities in products and reactants) is given by τS_L . As this velocity difference takes place over the flame thickness δ_{th} , the strain rate induced by chemical heat release can be scaled as $a_{chem} \sim \tau S_L / \delta_{th}$ [19,40]. It can be shown for low Mach number unity Lewis number flames $\partial u_i / \partial x_i$ can be expressed as $(\partial u_i / \partial x_i) = \tau (\rho S_d) |\nabla c| / \rho_0$ [18,32] where $S_d = (Dc/Dt) / |\nabla c|$ is the displacement speed (i.e. the speed with which the flame surface moves normal to itself with respect to an initially coincident material surface). Scaling $\rho S_d |\nabla c|$ by $\rho_0 S_L / \delta_{th}$ enables one to scale $(\partial u_i / \partial x_i)$ in the following manner $(\partial u_i / \partial x_i) \sim \tau S_L / \delta_{th}$. It has been shown in a previous analysis [19] that a similar scaling can also be applied to turbulent non-unity Lewis number flames in the following manner $a_{chem} \sim \varphi_1(Le) \tau S_L / \delta_{th}$ and $(\partial u_i / \partial x_i) \sim \varphi_2(Le) \tau S_L / \delta_{th}$ where the functions $\varphi_1(Le)$ and $\varphi_2(Le)$ increase with decreasing Le to account for strengthening of heat release effects with decreasing Le [19].

The strain rate induced by turbulence a_{turb} can be scaled with tangential strain rate $a_{turb} \sim a_T = (\delta_{ij} - N_i N_j) \partial u_i / \partial x_j$. In turbulent premixed flames the chemical strain rate can be scaled using the dilatation rate $\partial u_i / \partial x_i$ as: $a_{chem} \sim \partial u_i / \partial x_i$. Thus the ratio between a_{chem} to a_{turb} can be scaled as: $a_{chem} / a_{turb} \sim (\partial u_i / \partial x_i) / a_T$. The variations of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ with c across the flame are shown in Fig. 5 for all cases considered here. It is evident from Fig. 5 that $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ assumes values much greater than unity in cases A, C and D for the major part of the flame. In cases B,

E–G the quantity $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ assumes much smaller values than the values obtained in cases A, C and D. A comparison between cases B and F reveals an increase in τ yields a greater value of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$. This suggests that the differences between $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ values between cases A and B arise principally due to the differences in the combustion regimes. Fig. 5 suggests that $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ assumes higher values in the corrugated flamelets regime flame than in the thin reaction zones regime flames with comparable values of Re_t (see cases A, B and F). As Re_t scales as: $Re_t \sim Da^2 Ka^2$ in the $Le = 1.0$ flames [17], it can be inferred by comparing the values of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ in cases A, B and F that $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ strengthens with increasing Da (as Re_t remains comparable for cases A, B and F but $Ka < 1$ in case A and $Ka > 1$ in cases B and F). The strengthening of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ in the corrugated flamelets regime is consistent with earlier findings of Chakraborty and Swaminathan [40] in the context of alignment statistics of ∇c . Fig. 5 further indicates that the peak value of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ decreases with increasing Le , which is found to be consistent with previous findings of Chakraborty et al. [19].

A comparison between Figs. 2–5 reveals that the cases with large values of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ (e.g. cases A, C and D) exhibit mostly perpendicular alignment of vorticity with e_α . However, a one-to-one correspondence between the increase in $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$ and decreasing collinear alignment of vorticity with e_α on a given c isosurface may not always be achieved because Fig. 5 shows the ratio of mean quantities, whereas the pdfs in Fig. 2 show the instantaneous behaviour. In non-reacting turbulent flows vorticity does not show any preferential (either collinear or perpendicular) alignment with e_α . Moreover, a comparison between Figs. 2 and 5 indicates that the vorticity alignment with e_α shows similar qualitative behaviour as that of non-reacting turbulent flows for small values of $\langle \partial u_i / \partial x_i \rangle / \langle a_T \rangle$.

The effects of dilatation rate on vorticity alignment can further be elucidated by the variation of the mean values of $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$ conditional on dilatation rate $(\partial u_i / \partial x_i)$ within the progress variable range given by $0.1 \leq c \leq 0.9$, which are shown in Fig. 6a–g for cases A–G respectively. Fig. 6a–g show that vorticity alignment with e_α decreases in the regions of high magnitude of $(\partial u_i / \partial x_i)$ although this trend is relatively weak for the $Le = 1.2$ flame where the rate of burning is the weakest [19,29–36,52,53]. By contrast, the alignment of vorticity with e_γ increases at the regions of high dilatation rate. The extent of vorticity alignment with e_β also decreases with increasing $(\partial u_i / \partial x_i)$ for $Le = 0.8$ and 1.0 flames (i.e. cases A, B, E and F). However, no systematic trend has been observed between $|\cos \beta|$ and $(\partial u_i / \partial x_i)$ for $Le = 0.34, 0.6$ and 1.2 flames (i.e. cases C, D and G).

The mean values of $|\cos \alpha_p|$, $|\cos \beta_p|$ and $|\cos \gamma_p|$ conditional on dilatation rate $(\partial u_i / \partial x_i)$ within the progress variable range given by $0.1 \leq c \leq 0.9$ are shown in Fig. 7a–g for cases A–G respectively. It is evident from Fig. 7a–g that ∇p remains imperfectly aligned with both e_β and e_γ , and the extent of ∇p alignment with e_α increases for large values of $(\partial u_i / \partial x_i)$. The density gradient $\nabla \rho$ is closely related to ∇c (i.e. $|\nabla \rho| \sim \tau \rho^2 |\nabla c| / \rho_0$ and an equality holds for low Mach number unity Lewis number flames). Previous analyses [19,40,49,54] indicated that ∇c aligns preferentially e_α in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (e.g. cases A, C and D) where the effects of $(\partial u_i / \partial x_i)$ are particularly strong, so $\nabla \rho$ also predominantly aligns with e_α in these cases. This suggests that the cross product between ∇p and $\nabla \rho$ is expected to have significant contributions in the directions of e_β and e_γ in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (e.g. cases A, C and D), whereas a weak contribution is expected in the direction of e_α . Thus, the effects of the baroclinic torque (i.e. $\varepsilon_{ijk}(\partial \rho / \partial x_j)(\partial p / \partial x_k)(1/\rho)$) are likely to be weak in the direction of e_α in cases A, C and D. A comparison between Figs. 2–4

and 6 also reveals that vorticity aligns significantly with e_β and e_γ in the regions of flame where the vorticity alignment with e_α is weak in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (e.g. cases A, C and D).

It is worth noting that the intensity of heat release increases with decreasing Lewis number which in turn increases the magnitude of dilatation rate with decreasing Le (see Fig. 5 in Ref. [19] and Fig. 3b in Ref. [36]). However, dilatation rate is one of the major manifestations of thermal expansion and flame normal acceleration also strengthens with decreasing Le . This strengthening of flame normal acceleration and dilatation rate also acts to aid the flame-generated turbulence in premixed flames and this effect is particularly strong in $Le \ll 1$ flames (see Refs. [35,36]). Thus, the qualitative behaviours of the variation of $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$ ($|\cos \alpha_p|$, $|\cos \beta_p|$ and $|\cos \gamma_p|$) conditional on dilatation rate $(\partial u_i / \partial x_i)$ for cases C–G are not expected to be identical because dilatation rate also affects the flame-generated turbulence and turbulence intensity, which in turn have significant influences of the alignment behaviours of vorticity and pressure gradient with local principal strain rates.

Fig. 1 of Ref. [6] showed imperfect vorticity alignment between ∇p and e_β (and also with e_γ to some extent) for non-reacting turbulence and the present results are in qualitative agreement with that finding but the extent of alignment of ∇p with the eigenvectors corresponding to e_α , e_β and e_γ in turbulent premixed flames are significantly different in comparison to non-reacting turbulent flows. The analysis of Jaber et al. [15] demonstrated that $\nabla \rho$ and ∇p show predominant collinear alignment in reacting flows without heat release but $\nabla \rho$ and ∇p tend to show high probability of mutually perpendicular alignment in the presence of heat release. As the extents of ∇c and ∇p alignments with e_α increase for large values of $(\partial u_i / \partial x_i)$ (see Fig. 7 and Ref. [54]), both $\nabla \rho \sim (-\tau \rho^2 \nabla c / \rho_0)$ and ∇p show greater extent of collinear alignment in the premixed flames analysed here than in the non-premixed flames with heat release analysed by Jaber et al. [15].

Lee et al. [55] reported that the extent of vorticity alignment with all the principal strain rates (i.e. e_α , e_β and e_γ) decreases with increasing $(\partial u_i / \partial x_i)$ for non-reacting compressible flows, which is in contrast to the present observations. In non-reacting compressible flows $\nabla \rho$ does not have any preferential alignment with e_α unlike turbulent premixed flames. Thus the baroclinic torque does not remain weak in a preferred direction at high magnitudes of $(\partial u_i / \partial x_i)$ in non-reacting compressible flows. It is worth noting that dilatation rate effects on vorticity alignment has been observed here for small values of Mach number where the dilatation rate effects principally originate due to the thermal expansion as a result of highly exothermic chemical reaction. Moreover, dilatation rate is predominantly positive in turbulent premixed flames due to thermal expansion in contrast to non-reacting turbulent compressible flows (see Fig. 6a–g).

The pdfs of e_β / e_α for all cases are shown in Fig. 8 whereas the pdfs of the ratio of the most compressive principal strain rate to the most extensive principal strain rate (i.e. e_γ / e_α) for all cases are shown in Fig. 9. The probability of finding small values of e_β / e_α are prevalent in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (e.g. cases A, C and D), where vorticity shows weak alignment with e_α . The probability of finding high values of e_β / e_α decreases with decreasing Le .

An alignment of a vortex tube with e_α increases the vorticity magnitude significantly due to the conservation of angular momentum, and this effect is particularly strong where e_β / e_α shows high probability of finding small values. An increase in angular velocity due to alignment of vorticity with e_α increases the rate of dissipation rate of turbulent velocity fluctuations significantly. For the above reason, vorticity alignment with e_α is unstable in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis

Fig. 6. Variations of mean values of the magnitudes of the cosine between the vorticity vector and principal strain rates (i.e. $|\cos \alpha|$, $|\cos \beta|$ and $|\cos \gamma|$) conditional on normalised dilatation rate $\partial u_i / \partial x_i \times \delta_{th} / S_L$ in the region corresponding to the progress variable range $0.1 \leq c \leq 0.9$ for cases (a–g) A–G.

number $Le \ll 1$ flames (e.g. cases A, C and D) where the probability of obtaining small values of e_β / e_α is significant. However, vorticity vector can locally align with e_α in $Le \approx 1.0$ flames (e.g. cases B, E–G) where e_β / e_α assumes either moderate or relatively high values (i.e. the most probable value of e_β / e_α remains of the order of 0.1).

It can further be noticed from Eq. (2) that dilatation rate $(\partial u_i / \partial x_i) = (e_\alpha + e_\beta + e_\gamma)$ (which is predominantly positive in premixed flames due to thermal expansion) in reacting flows acts to suppress Ω . The pdfs of $|e_\beta| / e_\alpha$ and $|e_\gamma| / e_\alpha$ are shown in Figs. 10 and 11, which demonstrate that the probability of

Fig. 7. Variations of mean values of the magnitudes of the cosine between pressure gradient and principal strain rates (i.e. $|\cos \alpha_p|$, $|\cos \beta_p|$ and $|\cos \gamma_p|$) conditional on normalised dilatation rate $\partial u_i / \partial x_i \times \delta_{th} / S_L$ in the region corresponding to $0.1 \leq c \leq 0.9$ for cases (a–g) A–G.

finding $e_\alpha \gg |e_\beta|$ and $e_\alpha \gg |e_\gamma|$ are significant for high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (i.e. cases A, C and D), which indicates a significant probability of finding $(\partial u_i / \partial x_i) \approx e_\alpha$ (compare between Figs. 10 and 11) in these cases. The probability of $(\partial u_i / \partial x_i) \approx e_\alpha$

decreases with increasing (decreasing) $Le(Da)$. This can further be substantiated from Fig. 12 where the pdfs of $(\partial u_i / \partial x_i) / e_\alpha$ are shown. Fig. 12 shows that the probability of finding $(\partial u_i / \partial x_i) \approx e_\alpha$ is relatively smaller in low Damköhler number (i.e. $Da < 1$) flames with $Le \approx 1.0$ (i.e. cases B, E–G) than in high Da unity Lewis number

Fig. 8. Pdfs of the ratio of the intermediate principal strain rate to the most extensive principal strain rate (i.e. e_β/e_α) on the reaction progress variable $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces, for cases (a–g) A–G.

and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (e.g. cases A, C and D).

The vortex-stretching term $\rho \vec{\omega} \bullet \nabla \vec{u}$ in Eq. (1) can be expressed as: $\rho |\vec{\omega}| (e_\alpha \cos \alpha \hat{e}_1 + e_\beta \cos \beta \hat{e}_2 + e_\gamma \cos \gamma \hat{e}_3)$ where $\hat{e}_1, \hat{e}_2$ and $\hat{e}_3$ are unit eigenvectors in the directions associated with the

principal strain rates e_α, e_β and e_γ respectively. This indicates the component of $\rho \vec{\omega} \bullet \nabla \vec{u} - \rho (\nabla \bullet \vec{u}) \vec{\omega}$ in the direction of $\hat{e}_1$ is given by: $\rho |\vec{\omega}| [e_\alpha - (\partial u_i / \partial x_i)] \cos \alpha$. This suggests that the high probability of finding $e_\alpha \gg |e_\beta|$ and $e_\alpha \gg |e_\gamma|$ leads to negligible contribution

Fig. 9. Pdfs of the ratio of the most compressive principal strain rate to the most extensive principal strain rate (i.e. e_γ/e_α) on the reaction progress variable $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces, for cases (a–g) A–G.

to the vorticity transport due to $\rho |\vec{\omega}| [e_\alpha - (\partial u_i / \partial x_i)] \cos \alpha \approx \rho |\vec{\omega}| (e_\alpha - e_\alpha) \cos \alpha \approx 0$ in cases A, C and D.

The density gradient $\nabla \rho$ in turbulent premixed flames aligns with the reaction progress variable c gradient (i.e. $|\nabla \rho| \sim$

$\tau \rho^2 |\nabla c| / \rho_0$). It has been demonstrated earlier ∇c aligns preferentially e_α in high Da unity Lewis number and low Da (i.e. $Da < 1$) sub-unity Lewis number $Le \ll 1$ flames (i.e. cases A, C and D) [19,35,36]. This suggests that the baroclinic torque

Fig. 10. Pdfs of the ratio of the magnitude of the intermediate principal strain rate to the most extensive principal strain rate (i.e. $|e_\beta|/e_\alpha$) on the reaction progress variable $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces, for cases (a–g) A–G.

(i.e. $\varepsilon_{ijk}(\partial\rho/\partial x_j)(\partial p/\partial x_k)(1/\rho)$) effects in Eq. (1) are likely to be weak in the direction of e_α . This suggests that there is no major vorticity generating mechanism in the direction of e_α in cases A, C and D and thus vorticity does not align with e_α for the major portion of the flame in these cases. Therefore, vorticity alignment

with e_α remains unstable in cases A, C and D in the region of the flame where the probability of finding $(\partial u_i/\partial x_i) \approx e_\alpha$ is significant. Fig. 12 shows that the probability of finding $(\partial u_i/\partial x_i) \approx e_\alpha$ is overwhelming throughout the flame in high Da unity Lewis number combustion (e.g. case A) and thus vorticity does not align with e_α

Fig. 11. Pdfs of the ratio of the magnitude of the most compressive principal strain rate to the most extensive principal strain rate (i.e. $|e_\gamma|/e_\alpha$) on the reaction progress variable $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces, for cases (a–g) A–G.

for the major portion of the flame in case A. A comparison between Figs. 2 and 12 further shows that the extent of vorticity alignment of e_α decreases in the region of the flame where the probability of finding $(\partial u_i/\partial x_i) \approx e_\alpha$ is significant in $Le \ll 1$ flames (i.e. cases C and D). The order of magnitudes of e_α , e_β and e_γ remain comparable to each other in low Damköhler number flames with $Le \approx 1$

(i.e. cases B, E–G). It can be substantiated from Fig. 12 that the probability of finding $(\partial u_i/\partial x_i) \approx e_\alpha$ is relatively smaller in cases B, E–G than in cases A, C and D, so the high values of e_α are not necessarily associated with large magnitudes of $(\partial u_i/\partial x_i)$ in cases B, E–G. As a result of this, the effects of vorticity suppression in the direction of e_α are much weaker in cases B, E–G than in cases A, C and D.

Fig. 12. Pdfs of the ratio of dilatation rate to the most extensive principal strain rate (i.e. $(\partial u_i/\partial x_i)/e_\alpha$) on the reaction progress variable $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces, for cases (a–g) A–G.

The baroclinic torque plays a major contributor to the vorticity generation in reacting flows [15,16]. As the contribution of $\rho |\vec{\omega}| (e_\alpha - \nabla \bullet \vec{u}) \cos \alpha \approx \rho |\vec{\omega}| (e_\alpha - e_\alpha) \cos \alpha \approx 0$ and the baroclinic torque (i.e. $\varepsilon_{ijk}(\partial \rho/\partial x_j)(\partial p/\partial x_k)(1/\rho)$) is weak in the direction of e_α , only viscous diffusion of vorticity remains major

contributor in this direction in cases A, C and D. This further indicates that vorticity alignment is unstable in the direction of e_α in cases A, C and D. As both ∇p and $\nabla \rho$ assume large values in $Le \ll 1$ flames (e.g. cases C and D) [19,35,36], the effects of baroclinic torque in the directions of e_β and e_γ strengthen with

Table 2

Ratio of the magnitudes of the mean values of $e_\beta \cos^2 \beta$ to $e_\gamma \cos^2 \gamma$ (i.e. $|e_\beta \cos^2 \beta| / |e_\gamma \cos^2 \gamma|$) conditional on $c = 0.1, 0.3, 0.5, 0.7$ and 0.9 isosurfaces for cases A–G.

Case	$c = 0.1$	$c = 0.3$	$c = 0.5$	$c = 0.7$	$c = 0.9$
A	2.65	5.11	1.74	3.0	0.90
B	0.95	1.60	2.17	2.53	1.58
C	1.20	2.00	1.84	1.23	0.70
D	1.34	2.27	2.09	1.76	1.33
E	1.08	2.36	4.37	5.39	2.46
F	1.01	2.21	3.72	4.44	2.01
G	1.08	2.09	3.28	3.57	1.80

decreasing Le , which acts to yield an increasing extent of vorticity alignment with e_β and e_γ with decreasing value of Lewis number Le (compare cases C–G in Figs. 3 and 4).

It is worth noting that case A represents high Damköhler number (i.e. $Da \gg 1$) combustion, where the vorticity vector does not exhibit any appreciable alignment with e_α , so it can be expected that the flames in the corrugated flamelets regime (i.e. $Ka \sim Re_t^{1/2}/Da < 1$) will behave in a similar manner to case A, as $Re_t \gg 1$ in most practical engineering applications. However, it is theoretically possible to obtain $Da \gg 1$ even in the thin reaction zones regime combustion (i.e. $Ka \sim Re_t^{1/2}/Da > 1$), where the vorticity alignment is expected to qualitatively similar to that of case A. The qualitative nature of vorticity alignment in low Damköhler number (i.e. $Da < 1$) thin reaction zones regime combustion depends significantly on the global Lewis number Le , as demonstrated by cases C–G considered here. The effects of Lewis number on heat release rate and dilatation rate $\partial u_i / \partial x_i$ statistics are dependent on relative balances of thermal and mass diffusion and thus are mostly unaffected by the regime of combustion. As a result, the extent of alignment of vorticity with e_α (e_β and e_γ) is expected to decrease (increase) with decreasing Le in the corrugated flamelets regime as well.

Figs. 2–4 clearly demonstrate that the vorticity alignment behaviour changes with c for all the cases. In cases A, C and D the dilatation rate effects in the heat releasing region of the flame (i.e. $0.7 \leq c \leq 0.9$) are strong enough to alter the background turbulent flow field. However, the effects of dilatation rate are not strong for both unburned and burned gas side of the flame [19] and thus the vorticity alignment behaviour shows similarity to the well-known non-reacting turbulent flow alignment behaviour (i.e. preferential alignment with e_β) on both sides of the flame. In the thin reaction zones regime flames with $Le \approx 1.0$ (e.g. cases B, E–G) $v_\eta \gg S_L$ and thus these flames imparts relatively less influence on the background turbulent fluid motion in comparison to $Da > 1$ unity Lewis number combustion (e.g. case A). The effects of heat release are strong enough to influence the background fluid motion in $Le \ll 1$ flames even in the thin reaction zones regime.

The pdfs of e_β / e_α in Fig. 8 reveal that e_β / e_α predominantly assumes positive values throughout the flame, indicating predominantly positive values of e_β , as e_α is the most extensive (i.e. positive) principal strain rate. Eq. (3) suggests that the alignment of vorticity with e_α (e_γ) tends to yield positive (negative) values of Λ . The ratio of the mean values of the magnitudes of $e_\beta \cos^2 \beta$ to $e_\gamma \cos^2 \gamma$ (i.e. $|e_\beta \cos^2 \beta| / |e_\gamma \cos^2 \gamma|$) on five different c isosurfaces across the flame are presented in Table 2, which demonstrates that the magnitude of the mean contribution of $e_\beta \cos^2 \beta$ supersedes the magnitude of mean contribution of $e_\gamma \cos^2 \gamma$ for the major portion of the flame ensuring a positive mean contribution of Λ throughout the flame irrespective of the nature of vorticity alignment with local principal strain rates. This indicates that the mean contribution of the vortex-stretching term Λ in the transport equation of Ω remains positive, irrespective of the nature of vorticity alignment with local principal strain rates.

4. Conclusions

A three-dimensional simplified chemistry DNS database of statistically planar turbulent premixed flames, with a range of different values of Karlovitz number, heat release parameter and Lewis number, has been used to analyse the alignment of the vorticity vector with local principal strain rates. It has been found that vorticity aligns with the intermediate principal strain rate in all cases considered here, which is consistent with previous analyses for both non-reacting and reacting flows [2–16]. Moreover, vorticity vector also shows non-negligible alignment with the most extensive principal strain rate and this alignment increases in the heat releasing zone for high values of Karlovitz number (i.e. $Ka > 1$) for flames with $Le \approx 1.0$, which is consistent with previous analyses on turbulent reacting flows [13–16]. However, it has been found that the vorticity alignment with the most extensive principal strain rate is unstable for flames where the probability of finding $(\partial u_i / \partial x_i) \approx e_\alpha$ is significant, which can be realised for small values of Le and also for large (small) values of Da (Ka) in case of unity Lewis number flames. The absence of vorticity alignment with e_α in low Le and small Karlovitz number unity Lewis number flames, and alignment of vorticity with e_γ are in contrast to previous findings [13–16]. The intermediate principal strain rate predominantly assumes positive values, which makes the mean contribution of the vortex-stretching term in the transport equation of $\Omega = \omega_i \omega_i / 2$ to be positive for all cases considered here. The parameters such as the regime of combustion (which is characterised by Da and Ka), Lewis number Le and heat release parameter τ have major influences on the strength of the dilatation rate field in comparison to turbulent straining. The effects of dilatation rate on vorticity alignment statistics are significant in turbulent premixed flames even for small values of Mach number. The alignment of vorticity with the most extensive and intermediate principal strain rates decrease with increasing dilatation rate within the flame, which was observed in compressible non-reacting turbulent flows at much higher Mach number [55]. By contrast, the extent of alignment of vorticity with the most compressive principal strain rate increases at high dilatation rate locations in premixed turbulent flames unlike non-reacting compressible flows [55]. The dilatation rate effects strengthen significantly in comparison to the effects of turbulent straining with increasing Da and τ , and with decreasing Le . It has been found that there is a large probability of finding $(\partial u_i / \partial x_i) \approx e_\alpha$ for large (small) values of Da (Le), and under this situation vorticity ceases to align with e_α . One needs strong chemical reaction to have conditions given by $e_\alpha \gg |e_\beta|$ and $e_\alpha \gg |e_\gamma|$ so the vorticity alignment observed in high Da and $Le \ll 1$ flames are unlikely to be obtained for compressible non-reacting turbulent flows. Moreover, $(\partial u_k / \partial x_k)$ is identically zero for incompressible flows so the observed change in vorticity alignment with e_α cannot be seen in turbulent incompressible flows.

Hamlington et al. [16] analysed the effects of turbulence intensity on vorticity alignment statistics for unity Lewis number flames in the thin reaction zones regime. Given the similarity between the present findings and the results reported in Hamlington et al. [16], it can be expected that major qualitative differences in terms of the effects of turbulence intensity on vorticity alignment statistics are unlikely to be observed in unity Lewis number thin reaction zones regime flames. However, the vorticity alignment statistics in the corrugated flamelets regime and non-unity Lewis number flames show marked difference in comparison to the results reported in Hamlington et al. [16]. Thus, it necessitates further analyses of the effects of turbulence intensity of vorticity alignment with local principal strain rates in flames with $Le \neq 1$ and for flames representing the corrugated flamelets regime (i.e. $Ka < 1$). These analyses are beyond the scope of present study but will form the

basis for future investigations. Moreover, it should also be noted that the effects of detailed chemistry and transport are not considered in the present analysis, and therefore future research in these directions is necessary for a more comprehensive analysis of vorticity alignment characteristics.

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