Surface Density Function statistics in Hydrogen-air flames for different turbulent premixed combustion regimes

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ABSTRACT

The choice of reaction progress variable c on the statistical behaviour of the surface density function (SDF) and the strain rates, which govern the evolution of SDF, have been analysed using a detailed chemistry Direct Numerical Simulation (DNS) database of freely propagating statistically planar H_2 -air flames with an equivalence ratio of 0.7. The DNS database consists of three cases spanning the corrugated flamelets, thin reaction zones and broken reaction zones regimes of premixed turbulent combustion. For this analysis, the reaction progress variable is defined based on the mass fractions of H_2 , O_2 and H_2O . The mean variations of the SDF and the flame displacement speed S_d have also been found to be dependent on the choice of the reaction progress variable. The progressive weakening (strengthening) of the preferential alignment of the reaction progress variable gradient with the most extensive (compressive) principal strain rate with increasing Karlovitz number leads to changes in the behaviours of normal and tangential strain rates from one combustion regime to another. The differences in displacement speed statistics for different choices of reaction progress variable affect the behaviours of the normal strain rate due to flame propagation and curvature stretch. The relative thickening/thinning of the reaction layers of the major species has been explained in terms of the statistics of effective normal strain rate experienced by the c -isosurfaces for different choices of reaction progress variable.

Keywords: Premixed flame, Surface Density Function, normal strain rate, tangential strain rate, stretch rate

1. INTRODUCTION

The modelling of turbulent premixed combustion and especially the closures of generalised Flame Surface Density (FSD) (Boger *et al.*, 1998), $\Sigma_{gen} = \overline{|\nabla c|}$, and scalar dissipation rate (SDR) (Chakraborty *et al.*, 2011), $N_c = D \nabla c \cdot \nabla c$, depend on the statistics of the Surface Density Function (SDF) (Kollmann and Chen, 1998), $|\nabla c|$, where c is the reaction progress variable (RPV), D is the progress variable diffusivity and the overbar indicates Reynolds averaging or Large Eddy Simulation filtering operation, as appropriate. The evolution of the SDF and its strain rate and curvature dependence have been analysed by a number of researchers (Pope, 1988; Candel and Poinso, 1990; Chakraborty and Cant, 2005; Kim and Pitsch, 2007; Sankaran *et al.*, 2007; Chakraborty and Klein, 2008, 2009; Chakraborty *et al.*, 2008). Furthermore, the implications of ∇c alignment with local principal strain rates on the FSD and SDR transports have also been studied (Chakraborty and Swaminathan, 2007; Kim and Pitsch, 2007; Chakraborty *et al.*, 2009; Hartung *et al.*, 2008). A number of studies (Cifuentes *et al.*, 2014; Cifuentes *et al.*, 2015; Dopazo *et al.*, 2015a,b; Dopazo and Cifuentes, 2016; Dopazo *et al.*, 2017) have recently demonstrated the influences of strain rates arising from flame propagation on the SDF evolution based on simple chemistry Direct Numerical Simulation (DNS) data representing the flamelet regime of combustion. On the other hand, Wang *et al.* (2017) reported some important qualitative differences in high Karlovitz number flames in comparison to the findings reported in Cifuentes *et al.* (2014), Cifuentes *et al.* (2015) Dopazo *et al.* (2015a,b) and Dopazo and Cifuentes (2016).

To date, there has not been any analysis which compared the statistics of the SDF and the strain rates relevant to the SDF evolution for different regimes of turbulent premixed combustion. Moreover, in the context of detailed chemistry, the RPV cannot be defined uniquely and different definitions of c based on different major species may lead to different SDF statistics.

As such, the SDF statistics are expected to reflect the responses of different species reaction layers to the strain rate, depending on the definition of c . With the advances in computing power, researchers started to consider multiple species and solve individual scalar transport equations in the context of RANS (Fiorina *et al.*, 2005) and even LES (Li and Kong, 2008; Vermoral *et al.*, 2009). Hence it is essential to understand the sensitivity of the SDF statistics on the definition of RPV in order to ensure appropriate modelling of FSD and SDR transport. To address these issues in detail, the main objectives of this paper are:

- (a) to demonstrate the differences in the statistical behaviours of the SDF and the strain rates which affect the SDF evolution for different combustion regimes and different definitions of the RPV;
- (b) to provide physical explanations for the observed behaviours.

The rest of the paper will be organised as follows. The pertinent details about the mathematical background and numerical implementation are provided next section before the results are presented and discussed. The main findings will be summarised and conclusions are drawn at the end of this paper.

2. MATHEMATICAL BACKGROUND & NUMERICAL IMPLEMENTATION

The RPV can be defined as: $c = (Y_0 - Y)/(Y_0 - Y_\infty)$ where Y stands for the mass fraction of a chosen species, and the subscripts 0 and ∞ indicate values in the unburned and fully burned gases, respectively. Often the non-dimensional temperature $c_T = (\hat{T} - T_0)/(T_{ad} - T_0)$ (where $\hat{T}$, T_0 and T_{ad} are the dimensional, unburned gas and adiabatic flame temperatures respectively) is also considered as the RPV but local differential diffusion effects may lead to super-adiabatic temperature (i.e. $c_T > 1$) in H_2 -air flames and thus invalidates its use as the RPV. Accordingly, $|\nabla c_T|$ may not provide a suitable measure of flame thickness in turbulent H_2 -air flames and thus the SDF statistics based on c_T have not been considered here.

The evolution of the magnitude of the normal distance Δx of two adjacent c -isosurfaces is given by (Cifuentes *et al.*, 2014; Cifuentes *et al.*, 2015; Dopazo *et al.*, 2015a,b; Dopazo and Cifuentes, 2016; Dopazo *et al.*, 2017):

$$(\Delta x)^{-1}(d\Delta x/dt) = [N_i N_j (\partial u_i / \partial x_j) + N_j \partial S_d / \partial x_j] = a_N^{eff} \quad (1)$$

where u_i and $N_i = -(\partial c / \partial x_i) / |\nabla c|$ are the i^{th} components of fluid velocity and flame normal, respectively, $d(\dots)/dt = \partial(\dots)/\partial t + V_j^c \partial(\dots)/\partial x_j$ is the total derivative with respect to a reference frame attached with the flame with $V_j^c = (u_j + S_d N_j)$ being the j^{th} component of propagation velocity of a given c isosurface. In eq. 1, $a_N = N_i N_j \partial u_i / \partial x_j$ is the flame normal strain rate, $S_d = [\dot{w} + \nabla \cdot (\rho D \nabla c)] / \rho |\nabla c|$ is the displacement speed of a chosen c iso-surface, where ρ is the gas density, $\dot{w} = -\dot{w}_Y / (Y_0 - Y_\infty)$ is the normalised reaction rate of species Y . Moreover, $a_N^{eff} = a_N + N_j \partial S_d / \partial x_j$ is the *effective* normal strain rate which influences the evolution of $|\nabla c|$ in the following manner (Chakraborty and Cant, 2005; Kim and Pitsch, 2007; Sankaran *et al.*, 2007; Chakraborty and Klein, 2008,2009; Chakraborty *et al.*, 2008):

$$\partial |\nabla c| / \partial t + \partial (u_j |\nabla c|) / \partial x_j = a_T |\nabla c| - \partial (S_d N_j |\nabla c|) / \partial x_j + 2 S_d \kappa_m |\nabla c| \quad (2)$$

where $\kappa_m = 0.5(\partial N_i / \partial x_i)$ is the arithmetic mean of two principal flame curvatures and $a_T = (\delta_{ij} - N_i N_j)(\partial u_i / \partial x_j)$ is the tangential strain rate. Using chain rules on both left and right hand sides of eq. 2 yields:

$$\partial |\nabla c| / \partial t + V_j^c \partial |\nabla c| / \partial x_j = -a_N |\nabla c| - N_j \partial S_d / \partial x_j |\nabla c| \text{ or } |\nabla c|^{-1}(d|\nabla c|/dt) = -a_N^{eff} \quad (3)$$

A comparison between eqs. 1 and 3 reveals that an increase in a_N^{eff} increases the normal distance between c -iso-surfaces which leads to a decrease in $|\nabla c|$. In this context, it is also worthwhile to consider the evolution of the flame surface area A (Pope, 1988; Candel and

Poinsot, 1990; Cifuentes *et al.*, 2014; Cifuentes *et al.*, 2015; Dopazo *et al.*, 2015a,b; Dopazo and Cifuentes, 2016; Dopazo *et al.*, 2017):

$$A^{-1}(dA/dt) = (a_T + 2S_d\kappa_m) = [(\delta_{ij} - N_iN_j)(\partial u_i/\partial x_j) + 2S_d\kappa_m] = a_T^{eff} \quad (4)$$

In eq. 4, $2S_d\kappa_m$ is an additional contribution to the tangential strain rate due to flame propagation and a_T^{eff} is the *effective* tangential strain rate (Cifuentes *et al.*, 2014; Cifuentes *et al.*, 2015; Dopazo *et al.*, 2015a,b; Dopazo and Cifuentes, 2016; Dopazo *et al.*, 2017). The quantities a_T^{eff} and $2S_d\kappa_m$ are alternatively referred to as *stretch rate* and *curvature stretch*, respectively (Pope, 1988; Candel and Poinsot, 1990).

The statistics of $|\nabla c|$ and its evolution have been analysed here in terms of the statistical behaviours of a_N , a_T and S_d for RPVs based on H_2 , O_2 and H_2O mass fractions for freely propagating statistically planar atmospheric turbulent premixed H_2 -air flames with an equivalence ratio ϕ of 0.7. This choice of ϕ is motivated by the fact that H_2 -air premixed flames remain thermo-diffusively neutral in that the flame speed is insensitive to stretch (Chen and Im, 2002). A three-dimensional DNS (Arias *et al.*, 2016; Wacks *et al.*, 2016) database, employing a detailed chemical mechanism with 9 steps and 19 chemical reactions (Burke *et al.*, 2012), is considered here. The cases investigated here are representative of three regimes of combustion: case A: corrugated flamelets (CF) ($Ka < 1$), case B: thin reaction zones (TRZ) ($1 < Ka < 100$) and case C: broken reaction zones (BRZ) regime ($Ka > 100$) (Peters, 2000). The numerical implementation has been discussed elsewhere (Arias *et al.*, 2016; Wacks *et al.*, 2016) and thus will not be repeated here. Turbulent inflow and outflow boundaries are taken in the direction of mean flame propagation and transverse boundaries are periodic. The inflow values of normalised root-mean-square turbulent velocity fluctuation u'/S_L , turbulent length scale to flame thickness ratio l_T/δ_{th} , Damköhler number $Da = l_TS_L/u'\delta_{th}$, 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 1 where ρ_0 is the unburned gas density, 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 refers to unstrained laminar flame quantities.

The domain size is $20mm \times 10mm \times 10mm$ ($8mm \times 2mm \times 2mm$) in cases A and B (case C), which is discretised by a uniform Cartesian grid of $512 \times 256 \times 256$ ($1280 \times 320 \times 320$) ensuring 10 grid points across δ_{th} . Simulations have been carried out until a quasi-steady state in terms of flame surface area is obtained (Arias *et al.*, 2016; Wacks *et al.*, 2016), and the simulation time (i.e. $1.0l_T/u'$, $6.8l_T/u'$ and $6.7l_T/u'$ for cases A-C respectively) remains comparable to several previous analyses (Boger *et al.*, 1994; Cifuentes *et al.*, 2014; Charlette *et al.*, 2002; Han and Huh, 2008; Reddy *et al.*, 2012).

3. RESULTS & DISCUSSION

The distributions of c based on H_2 and H_2O mass fractions for cases A-C in $x_1 - x_3$ mid-plane are shown in Fig. 1. The isocontours of c remain parallel to each other in case A as energetic turbulent eddies do not penetrate into the flame. In contrast, eddies penetrate into the flame in cases B and C but the reaction zone in case B retains its quasi-laminar structure. In case C, turbulent eddies penetrate into both preheat and reaction zones and cause considerable flame distortion. Figure 1 shows that H_2 and H_2O based RPVs are different especially on the burned gas side in cases B and C.

The effect of turbulence on the flame thickness remains a controversial issue. The thickening of reaction layer in a mean sense under turbulent environment has been reported in previous experimental (O'Young and Bilger, 1997; Chen and Monsour, 1998; Chen and Bilger, 2002)

and DNS (Sankaran *et al.*, 2007; Wang *et al.*, 2017) analyses, while contradictory evidences are also found in DNS (Hawkes and Chen, 2004) and experimental (Soika *et al.*, 1998) studies. In this context, the flame thickness is commonly determined by the statistical average gradient in the RPV. To further examine this issue, the profiles of the mean values of $|\nabla c| \times \delta_L$ conditional on c for cases A-C are shown in Figs. 2a-c for RPVs based on H_2 , O_2 and H_2O mass fractions respectively. Here, $\delta_L = 1/\max|\nabla c|_L$ is the reference flame thickness based on a laminar unstretched flame solution. As such, the peak mean value of $|\nabla c| \times \delta_L$ indicates a propensity towards flame thinning (> 1) or thickening (< 1) in a mean sense relative to the reference laminar flame condition.

Figure 2 shows that the flame thickening versus thinning depends on the choice of the RPVs. For RPVs based on O_2 and H_2O , the peak mean value of $|\nabla c| \times \delta_L$ increases (thinner flame) from case A to case C. On the other hand, for H_2 -based RPV the flame thickens from case A to case C, and even becomes slightly thicker than the laminar flame condition in case C. While a detailed analysis will follow, this behaviour is heuristically attributed to the fact that the H_2 based flame thickness is larger due to the higher diffusivity, reaching out to farther upstream, thus being subjected to a stronger level of turbulence. This finding does not settle the open question because it is limited to the hydrogen-air flames for the flow conditions under study, but implies that a careful re-examination of the existing and new data is warranted by considering the sensitivity to the choice of the RPVs.

With this basic observation, Equations 2-4 provide a means to analyse the specific contributions from the statistical behaviours of S_d , a_N and a_T to the SDF, in order to explain why the reaction zone thicknesses for different species respond differently.

First, as for the aerodynamic strain components, the mean values of flow dilatation $\nabla \cdot \vec{u}$, normal strain rate a_N , and tangential strain rate a_T conditional upon c for different choices of RPV are shown in Figs. 3a-c, respectively. All quantities are normalized by the product with the flame time δ_{th}/S_L . The spatial distribution for all three quantities are seen to be distinct for the H₂-based RPVs. The mean values of $\nabla \cdot \vec{u}$ remain at substantial values for cases A and B, but are markedly smaller for case C. The dilatation rate assumes mostly positive values in premixed flames due to heat release, but the effect is attenuated in case C as energetic eddies enter into the reaction zone and distribute the chemical reaction more widely across the flame thickness.

The mean value of a_N remains predominantly positive in cases A and B, whereas it is negative throughout the flame for case C. The normal strain rate a_N can be expressed as $a_N = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma)$ where e_α, e_β and e_γ are the most extensive, intermediate and most compressive principal strain rates respectively and α, β and γ are the angles between ∇c and the eigenvectors associated with e_α, e_β and e_γ , respectively. It has been shown (Chakraborty and Swaminathan, 2007; Kim and Pitsch, 2007; Chakraborty *et al.*, 2009; Hartung *et al.*, 2008) that ∇c aligns strongly with e_α when the strain rate due to flame normal acceleration dominates over turbulent straining and this is highly probable for flames with $Da > 1$ (Chakraborty and Swaminathan, 2007; Chakraborty *et al.*, 2009). In contrast, ∇c preferentially aligns with e_γ when turbulent strain rate overcomes the strain rate arising from flame normal acceleration, which is highly probable for $Da < 1$ (Chakraborty and Swaminathan, 2007; Chakraborty *et al.*, 2009). Accordingly, ∇c preferentially aligns with e_α for cases A and B, and thus yielding a mean positive value of a_N , while ∇c aligns with e_γ in case C to give rise to negative mean values of a_N . Referring to eq. 3, this implies that the

normal flow strain has a net flame thickening effect for cases A and B, and thinning effect for case C. This qualitative behaviour is independent of the choice of the RPV species.

Regarding the effect on the flame surface, the mean value of $a_T = \nabla \cdot \vec{u} - a_N$ is determined by the relative magnitudes and signs of $\nabla \cdot \vec{u}$ and a_N . In case A, the mean values of $\nabla \cdot \vec{u}$ and a_N remain close to each other to yield a small positive mean value of a_T . The extent of the alignment of ∇c with e_α is relatively weaker in case B than in case A and that leads to smaller positive mean value of a_N in case B in comparison to that in case A. With $\nabla \cdot \vec{u}$ being comparable for cases A and B, this results in a greater value of $a_T = \nabla \cdot \vec{u} - a_N$ in case B than in case A. For case C, the large negative mean value a_N eclipses the reduced mean positive value of $\nabla \cdot \vec{u}$ to lead to a large positive mean value of $a_T = \nabla \cdot \vec{u} - a_N$. Referring to eq. 4, this implies that the aerodynamic tangential strain rate continues to increase from case A to C, leading to an increased flame surface area.

Next, the effects associated with the flame propagation are examined. The variations of mean values of S_d/S_L conditional upon c for cases A-C are shown in Figs. 4a-c for H_2 , O_2 and H_2O based RPVs respectively. All S_d related quantities have been shown for $0.05 \leq c \leq 0.95$ in Fig. 4 and subsequent figures to avoid singularities in the displacement speed evaluation. Figure 4 shows that S_d/S_L for H_2 based RPV increases from unburned to burned gas side before reaching a peak value close to $c \approx 1.0$. For O_2 and H_2O based RPVs, the peak mean value of S_d/S_L is obtained close to the middle of the flame-front but slightly skewed towards the burned gas side and this suggests $\rho S_d \neq \rho_0 S_L$ for these cases as ρ monotonically decreases with increasing c .

The differences in the mean behaviours of S_d/S_L for H_2 , O_2 and H_2O can be explained by examining the statistical behaviours of $S_d = S_r + S_n + S_t$ where $S_r = \dot{w}/\rho|\nabla c|$; $S_n = \vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho|\nabla c|$ and $S_t = -2D\kappa_m$, which are the reaction, normal diffusion and tangential diffusion components of S_d , respectively (Peters *et al.*, 1998; Echekki and Chen, 1999; Im and Chen, 2002). The variations of mean values of S_r/S_L , S_n/S_L and S_t/S_L conditional upon c are shown in Fig. 5 which reveals that the mean values of $(S_r + S_n)/S_L$ (not shown) and S_d/S_L remain close to each other because the mean contribution of $S_t = -2D\kappa_m$ is negligible in statistically planar flames. Figure 5 shows that the mean value of S_r/S_L remains positive throughout the flame-front, whereas the mean value of S_n/S_L assumes positive (negative) values towards the unburned (burned) gas side of the flame-front. However, the qualitative distributions of S_r/S_L and S_n/S_L are different for each species, which contributes to the differences in S_d/S_L for different RPVs.

To assess contributions from the flame propagation to the SDF as appearing in eq. 3, the mean values of $N_j \partial S_d / \partial x_j$, $N_j \partial (S_r + S_n) / \partial x_j$ and $N_j \partial S_t / \partial x_j$, normalised with δ_{th}/S_L , conditional upon c for different choices of RPV for cases A-C are shown in Figs. 6a-c respectively. For cases A and B, it is evident that the behaviour of $N_j \partial S_d / \partial x_j$ is dominated by $N_j \partial (S_r + S_n) / \partial x_j$, while the effect of $N_j \partial S_t / \partial x_j$ is minimal. Although not shown here, the mean values of $N_j \partial S_r / \partial x_j$ and $N_j \partial S_n / \partial x_j$ are close to each other at large magnitudes but opposite in sign, leading to the undulations in the net values. The average value across the entire region for c is negative as a net, and contributes to the overall flame thinning, as seen in Fig. 2.

In case C, however, the magnitudes of $N_j \partial S_t / \partial x_j$ and $N_j \partial (S_r + S_n) / \partial x_j$ remain comparable, with magnitudes much larger than in cases A and B. The positive mean values of $N_j \partial S_t / \partial x_j$

dominate over negative mean values of $N_j \partial(S_r + S_n)/\partial x_j$ to yield mean positive values of $N_j \partial S_d/\partial x_j$, leading to the flame thickening. Incidentally, as the c -isosurfaces are not parallel to each other in cases B and C, especially on the burned gas side (see Fig. 1), the spatial variation of κ_m along with high D leads to large magnitudes of $N_j \partial S_t/\partial x_j = -2N_j \partial(D\kappa_m)/\partial x_j$ towards the burned gas side in these cases. According to scaling arguments by Peters (2000), the contribution of S_t to S_d strengthens with increasing Ka and thus the contribution of $N_j \partial S_t/\partial x_j$ is likely to play a dominant role for $Ka \gg 1$ flames, consistent with the present observation in case C.

Figures 6d-f further shows the flame propagation effect coupled with the curvature stretch $2S_d\kappa_m$, i.e. the last term in eq. 2, which assumes predominantly negative values for all cases except some positive values towards the burned gas side. The mean contribution of $2(S_r + S_n)\kappa_m$ remains positive for all RPVs considered here. However, the deterministically negative mean contribution of $2S_t\kappa_m$ dominates over $2(S_r + S_n)\kappa_m$ to result in the mostly negative mean values of $2S_d\kappa_m$. The aforementioned strong κ_m variation and high values of D are responsible for large magnitudes of $2S_t\kappa_m = -4D\kappa_m^2$ towards the burned gas side of the flame-front. The differences in S_d statistics and c distributions contribute to the qualitative and quantitative differences in the mean behaviours of $N_j \partial S_d/\partial x_j$ and $2S_d\kappa_m$ for different RPV definitions.

The mean values of a_N^{eff} conditional upon c for different choices of RPV for cases A-C are shown in Fig. 7a-c. According to eq. 3, the effective normal strain rate assumes both positive and negative values within the flame-front for cases A and B, whereas the mean value of a_N^{eff} remains positive throughout the flame-front for case C. A comparison between Figs. 3 and 6 reveals that the undulations in mean values of a_N^{eff} originate due to the undulations of the mean

values of $N_j \partial S_d / \partial x_j$. The mean value of the resulting evolution of the SDF $|\nabla c|^{-1}(\partial|\nabla c|/\partial t)$ is also shown in Figs. 7a-c for all choices of c . A comparison between Figs. 2a-c and 7a-c reveals that mean $|\nabla c|^{-1}(\partial|\nabla c|/\partial t) \times \delta_{th}/S_L$ assumes positive values at the location of the peak mean value of SDF for O_2 and H_2O based RPVs, which is consistent with flame thinning observed in these cases. By contrast, the mean $|\nabla c|^{-1}\partial|\nabla c|/\partial t$ assumes a positive value at the location of the peak mean value of $|\nabla c|$ for cases A and B for H_2 based RPV, whereas a small negative value is obtained at the location of the peak mean value of $|\nabla c|$ in case C, which is also in accordance with the flame thinning (thickening) in cases A and B (case C) in Fig. 2.

Finally, Figs. 7d-f show the variation of the mean stretch a_T^{eff} conditional upon c for different choices of RPV for cases A-C, which indicate that the mean a_T^{eff} remains predominantly negative for case C, whereas the profile of the mean a_T^{eff} undulates between positive and negative values with a bias towards positive values for cases A and B. The small imbalance between comparable magnitudes of a_T and $2S_d\kappa_m$ is responsible for the undulations in the mean a_T^{eff} profiles in cases A-C. A similar behaviour was also reported in a recent simple chemistry based DNS analysis (Dopazo *et al.*, 2017). A positive (negative) value of a_T^{eff} is indicative of flame area generation (destruction). The volume-integrated heat release rate $\Omega = \int_V \dot{\omega}_T dV$ (where $\dot{\omega}_T$ is the heat release rate) in turbulent flames normalised by its corresponding laminar value assumes a value of about 3.5 for cases A and C and 5.0 for case B. Although Ω may not have a one-to-one relation with the flame surface area evaluated by the volume-integral of $|\nabla c|$ based on a single RPV definition in the context of multi-species systems, high values of flame surface area are still associated with high values of Ω . The greater probability of having positive values of a_T^{eff} in case B than in case C yields a higher value of Ω in case B. Moreover, the greater likelihood of positive values of a_T^{eff} in case A than in case

C leads to comparable values of Ω in these two cases in spite of case A having much smaller u'/S_L than in case C (see Table 1). The high values of u'/S_L in case C tend to produce highly wrinkled c isosurfaces, and a combination of Huygens propagation and flame-flame interaction tends to produce a flat flame surface and this is reflected in the negative mean value of a_T^{eff} .

4. CONCLUSIONS

The effects of the choice of RPV definition on the mean behaviours of the SDF (i.e. $|\nabla c|$) and the strain rates affecting $|\nabla c|$ transport have been analysed using a detailed chemistry DNS database of statistically planar H_2 -air premixed flames with an equivalence ratio of 0.7 spanning the CF, TRZ and BRZ regimes of combustion. For each case the SDF and strain rate statistics have been analysed for RPVs defined based on H_2 , O_2 and H_2O mass fractions. The differences in $|\nabla c|$ statistics for different definitions of RPV have been explained in terms of the statistics of strain rates in the flame normal and tangential directions. The dilatation rate effects weaken in the BRZ regime, and the alignment of ∇c with the most extensive (compressive) principal strain rate weakens (strengthens) from the CF to the TRZ regime to the BRZ regime. This leads to differences in the mean behaviours of normal and tangential strain rates from one case to another. The mean behaviours of S_d and its components for different choices of the RPV have been found to be qualitatively different. This leads to differences in the normal strain rate arising from flame propagation and the curvature stretch for different choices of RPV. The sensitivity of the statistics of SDF on the definition of RPV indicates that the sub-models of the FSD and SDR transports need to accurately capture the respective behaviours of the unclosed terms for different definitions of RPV in order to be applicable in a multi-species system.

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Table 1**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

FIGURE CAPTIONS

Fig. 1: Distributions of RPV based on H_2 (1st row) and H_2O (2nd row) mass fractions in the central $x_1 - x_3$ mid-plane for cases A-C (1st-3rd columns). The $c = 0.1 - 0.9$ (in steps of 0.1) isolines are shown by magenta line.

Fig. 2: Variations of mean values of $|\nabla c| \times \delta_L$ conditional on c for cases A-C for (a) H_2 , (b) O_2 and (c) H_2O based RPVs. Here and in the remaining figures c refers to the RPV defined based on the respective species mass fraction considered.

Fig. 3: Variations of $\nabla \cdot \vec{u}$ (solid line), a_N (line with circle) and a_T (dotted line), normalized with δ_{th}/S_L , conditional upon c for cases (a-c) A-C. The results for RPV definitions based on H_2 , O_2 and H_2O mass fractions are shown by purple, green and brown lines respectively in Figs. 3,6 and-7.

Fig. 4: Variations of mean values of S_d/S_L conditional upon c for cases A-C for (a) H_2 , (b) O_2 and (c) H_2O based RPVs.

Fig. 5: Variations of mean values of S_α/S_L (where $\alpha = r$ (solid line), n (broken line) and t (line with circle)) conditional upon c for cases A-C for (a) H_2 , (b) O_2 and (c) H_2O based RPVs. The same colour code as in Fig. 2 is used.

Fig. 6: Variations of (a-c) $N_j \partial S_\alpha / \partial x_j$ (1st column) and (d-f) $2S_\alpha \kappa_m$ (2nd column), normalized with δ_{th}/S_L , for (where $\alpha = d$ (solid line), $r+n$ (broken line) and t (line with circle)) conditional upon c for cases A-C (1st-3rd row).

Fig. 7: Variations of (a-c) a_N^{eff} , (solid line) $|\nabla c|^{-1}(\partial|\nabla c|/\partial t)$ (line with o) (1st column) and (d-f) a_T^{eff} (2nd column), normalized with δ_{th}/S_L , conditional upon c for cases A-C (1st-3rd row).

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Fig. 5: Variations of mean values of S_α/S_L (where $\alpha = r$ (solid line), n (broken line) and t (line with circle)) conditional upon c for cases A-C for (a) H_2 , (b) O_2 and (c) H_2O based RPVs. The same colour code as in Fig. 2 is used.

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