DNS of a turbulent lifted DME jet flame

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Abstract

A three-dimensional direct numerical simulation (DNS) of a turbulent lifted dimethyl ether (DME) slot jet flame was performed at elevated pressure to study interactions between chemical reactions with low-temperature heat release (LTHR), negative temperature coefficient (NTC) reactions and shear generated turbulence in a jet in a heated coflow. By conditioning on mixture fraction, local reaction zones and local heat release rate, the turbulent flame is revealed to exhibit a “pentabrachial” structure that was observed for a laminar DME lifted flame [1]. The propagation characteristics of the stabilization and triple points are also investigated. Potential stabilization points, spatial locations characterized by preferred temperature and mixture fraction conditions, exhibit autoignition characteristics with large reaction rate and negligible molecular diffusion. The actual stabilization point which coincides with the most upstream samples from the pool of potential stabilization points for each spanwise location shows passive flame structure with large diffusion. The propagation speed along the stoichiometric surface near the triple point is compared with the asymptotic value obtained from theory [2]. At stoichiometric conditions, the asymptotic and averaged DNS values

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of flame displacement speed deviate by a factor of 1.7. However, accounting for the effect of low-temperature species on the local flame speed increase, these two values become comparable. This suggests that the two-stage ignition influences the triple point propagation speed through enhancement of the laminar flame speed in a configuration where abundant low-temperature products from the first stage, low-temperature ignition are transported to the lifted flame by the high-velocity jet.

Keywords:

direct numerical simulation (DNS), dimethyl ether (DME), negative temperature coefficient (NTC), low-temperature heat release (LTHR), lifted flame, diesel combustion

1. Introduction

Partially premixed combustion is prevalent in many combustion applications, for example, in the lift-off stabilization of a diesel jet flame. It nominally consists of fuel rich and fuel lean premixed flames and a trailing diffusion flame which consumes excess fuel and oxidizer originating from the premixed branches. This so-called triple flame structure is observed when the reactant temperature is sufficiently low so as to preclude the possibility of autoignition, in both stationary and non-stationary configurations [3]. While the structure is often masked in a turbulent flow due to significant strain and high mixing rates, its presence is revealed in mixture fraction and progress variable coordinates. The diesel engine is one such application where fuel and air are partially premixed. In diesel engine combustion, fuel is injected into a hot cylinder at a high velocity, and once the mixture is ignited a lifted

flame is established. As many studies have reported [4, 5, 6], the flame structure and stabilization of a lifted flame depends on a balance between mixing and chemical reaction modulated by large scale flow structure, which is difficult to generalize. For example, two previous direct numerical simulations of turbulent lifted hydrogen jet flames show very different flame structures [7, 8]. In addition to the competition between mixing, chemical reaction and global flow structure, there are additional complexities that can influence overall flame behavior in diesel combustion. The complexities arise due to the chemical kinetic characteristics observed in large hydrocarbon fuels, that is, the two-stage ignition and negative temperature coefficient (NTC). At sufficiently low injector temperatures diesel fuels undergo a two-stage ignition process comprised of low- and high-temperature ignition. The majority of the heat release is a result of the high-temperature ignition, similar to single-stage ignition fuels, whereas the low-temperature ignition is slightly exothermic, generating a small amount of low-temperature heat release (LTHR). The significance of low-temperature ignition, however, is that it also generates low-temperature species that could potentially influence the overall reactivity of the fuel mixture. Negative temperature coefficient regime is observed over a range of mixture temperatures, determined by the thermochemical condition. The ignition delay time increases with increasing temperature inside the NTC regime, whereas it decreases with increasing mixture temperature outside of this temperature range. The non-monotonic behaviour of ignition delay time could directly affect the lift-off length, particularly if the lifted stabilization mechanism is governed by autoignition [8]. NTC behaviour has the potential to further alter emissions and efficiency performance in a diesel

engine through its affect on the lift-off length [9, 10].

Recently, a parametric study of two-dimensional Direct Numerical Simulations (DNS) of shear-less laminar lifted dimethyl ether (DME) flames at a nominal engine pressure and temperatures has revealed the existence of a “*pentabrachial*” flame structure when a lifted flame is established under strong LTHR and NTC conditions with a relatively high oxidizer temperature [1]. A similar result is also reported in Ref. [11]. As explained in detail later in Sec. 3.1, the pentabrachial flame consists of two upstream flame branches due to LTHR and NTC in addition to a conventional triple flame further downstream. Also, the stabilization point of the lifted flame shifts towards fuel-lean conditions due to NTC. The existence of five flame branches may influence the overall flame behavior including the triple flame propagation speed. In turbulent flows, observation of such distinct flame branches established in partially premixed combustion is generally difficult due to strong turbulence–flame and flame–flame interactions [12, 4, 8], although a turbulent lifted hydrogen jet flame reported in Ref. [7] exhibits a clear triple flame structure in physical space.

In the present study, the focus is on the interactions between chemical reactions with LTHR and NTC, and sheared turbulence in a planar jet. Specifically, does a pentabrachial structure still exist under the presence of flame-flame and turbulent-flame interactions caused by strong turbulence? Moreover, what is the effect of two-stage ignition and NTC chemistry on the overall flame stabilization? Insights into these questions extend the previous understanding of laminar DME lifted flames [1]. For this purpose, a three-dimensional DNS of a turbulent lifted DME slot jet flame has been performed

at elevated pressure. Although the present pressure is still far from nominal engine conditions due to computational limitations, the fuel and oxidizer temperatures are carefully chosen to include LTHR and NTC effects.

The present paper is organized as follows: the numerical methods used to perform the present simulations are described in Sec. 2, followed by a detailed description of the DNS configuration and numerical and thermochemical conditions. The flame structure, the flame propagation characteristics and the effect of two-stage ignition are discussed in Sec. 3. The conclusions are made in Sec. 4.

2. Direct numerical simulations

The Sandia DNS code S3D [13] is used to simulate DME/air combustion. The code solves the fully-compressible conservation equations for mass, momentum, total energy and species continuity. The chemical reactions are described by a reduced mechanism for DME-air combustion involving 30 species developed in a previous study [14]. The present reduced mechanism is derived from a detailed chemical kinetic reaction mechanism [15], and includes key kinetic mechanisms for DME combustion. DME is primarily consumed by hydrogen abstraction by OH

but also by HO_2 under elevated pressure and intermediate temperature conditions

as reported previously [16, 17]. The CH_3OCH_2 radicals undergo oxygen addition at low temperature as

The equilibrium of this reaction is strongly temperature dependent, which favors methoxymethyl-hydroperoxy ($\text{CH}_3\text{OCH}_2\text{O}_2$) at low temperatures. Thus, $\text{CH}_3\text{OCH}_2\text{O}_2$ is a good marker for low-temperature chemical kinetics. Once the low-temperature process is suppressed by accumulated heat release due to LTHR, thermal decomposition of CH_3OCH_2 begins, which produces radicals that consume the remaining fuel and intermediates species, producing intense chemical reactions and heat. Nitrogen is inert in this context and therefore, NO_x formation reactions are not included. The species specific heats are modeled as polynomial functions of temperature as described in CHEMKIN and TRANSPORT, and mixture-averaged transport coefficients are used [18, 19]. Radiative heat transfer is not considered in the present simulations. Spatial derivatives are obtained using an eighth-order central finite difference scheme which gradually reduces to a third-order one-sided difference stencil on the open domain boundaries [20]. A tenth-order explicit spatial filter is applied to remove any spurious high-frequency fluctuation in the solution [20]. Time integration is achieved using a six-stage fourth-order explicit Runge-Kutta method [20].

2.1. Thermochemical condition

Diesel (surrogate) fuels are by nature highly reactive. In nominal diesel engine combustion conditions, the reactant mixture is even more reactive due to increased pressure and temperature. In an engine-relevant configuration,

Figure 1: High-temperature and low-temperature ignition delays, τ_H and τ_L , as a function of mixture fraction obtained from homogeneous SENKIN simulations. Low temperature ignition delay is denoted by square symbols, and high temperature ignition delay is denoted by circles. Two preferred mixture fractions for high-temperature ignition are highlighted by arrows at $\xi_1 = 0.04$ and $\xi = 0.57$.

a high speed jet (typically ~ 400 m/s issuing from the injector) yields a large lift-off length typically ~ 100 times the nozzle diameter, even in such a highly reactive environment. In partially premixed combustion, especially at engine conditions, a reactant mixture is exposed to several turbulence/combustion phenomena as it proceeds towards its lift-off position. They include mixing of reactants with high-temperature oxidizer due to strong velocity and scalar gradients and LTHR that creates radical pools for subsequent high-temperature reactions. Some of these conditions require immense computational resources that are not currently feasible for DNS. For example, a highly reactive fuel at high pressure yields very thin reaction layers that require extraordinarily fine spatial resolution (small mesh size Δx). Similarly, a large jet velocity close to sonic Ma that generates large velocity gradients also imposes fine turbulence scales. One way to alleviate the enormous spatial resolution requirements is through fuel dilution, which also permits a sufficient lift-off length for mixing and LTHR to occur and to achieve strong turbulence-flame interactions within a feasible DNS domain length considerably shorter than 100 nozzle diameters.

The mixture in the present fuel and oxidizer stream, respectively consists of 0.1DME+0.9N₂ and 0.21O₂+0.79N₂. Comparing previous DME jet flames in Ref. [1] the present fuel stream is heavily diluted. This results in a larger stoichiometric mixture fraction, $\xi_{st} = 0.42$, shifted well into the fuel jet stream. Under the present moderately elevated pressure of 5 atm, the high level of dilution results in a spatial resolution governed by comparable minimum reaction layer thickness and the Kolmogorov scale (discussed in Sec. 2.4), and hence, maximizing turbulence-flame interaction while main-

taining a feasible computational cost. Also, the temperature for each stream is carefully chosen to achieve both LTHR and NTC; they are chosen to be 500 K and 1000 K for the fuel and oxidizer streams, respectively. With these mixture compositions and temperatures for the present fuel and oxidizer streams, zero-dimensional homogeneous ignition simulations are performed at constant pressure using SENKIN [21]. The ignition delays for low-temperature and high-temperature ignition are plotted versus mixture fraction ξ in Fig. 1. Here, the mixture fraction is based on Bilger’s formula-tion [22] and ignition delay is defined based on the location of maximum heat release rate. The initial temperature is also a function of mixture fraction. The low-temperature ignition delay (square symbols in Fig. 1) increases with the amount of fuel in the mixture. However, the high-temperature ignition delay is non-monotonically dependent on ξ and has two local minima that are annotated in the figure. These characteristics are a consequence of the NTC behavior consistent with Ref. [1]. The homogeneous results ensure that the present mixture exhibits both LTHR and NTC characteristics.

Under the present dilution condition, however, the ignition delay for LTHR is too lengthy for strong flame-turbulence interactions since the sheared turbulence would decay significantly by the time the mixture establishes LTHR. Thus, to perform DNS for the present objectives, the evolution of turbulence is treated separately from LTHR processes while maintaining overall consistency. For this purpose, and also to minimize the computational requirements, the present combustion DNS is divided into three sequential stages—a one-dimensional mixing-reacting DNS; a three-dimensional temporally-evolving jet DNS; and, a three-dimensional turbulent lifted jet

Figure 2: Spatial variations of mixture fraction (a), temperature (b) and heat release rate (c) at $t_{step1} = 5.4$ ms and temporal evolution of maximum low-temperature species mass fraction, $Y_{CH_3OCH_2O_2}$ (d). Grey dashed line in (a, b) shows initial condition. The vertical dashed line in (d) shows $t = t_{step1}$.

flame DNS—that are described in detail in the following subsections.

2.2. Step 1: One-dimensional mixing–reacting DNS

The first step is to simulate a one-dimensional reaction–diffusion problem between the DME and air streams. Spatial profiles of initial mixture fraction and temperature are shown in Figs. 2a and 2b. The fuel stream is located between $-H/2 \leq y < H/2$, where H denotes the slot jet width chosen as $H = 0.6$ mm and y is the transverse distance. Here, the initial mixture fraction variation is imposed using hyperbolic tangent functions as:

$$\xi(y) = \{\tanh[(y + H/2)/\delta] - \tanh[(y - H/2)/\delta]\} / 2, \quad (1)$$

Table 1: Turbulence parameters in the temporally evolving turbulent jet at $t = t_{step2}$. $\tilde{u}$: mean streamwise velocity, u' : root-mean-square velocity, l_E : large eddy turbulent length scale, λ : Taylor microscale, η : Kolmogorov length scale, Re_{l_E} : Reynolds number based on l_E , Re_λ : Reynolds number based on λ , Da : Damköhler number, Ka : Karlovitz number.

	$\tilde{u}$ (m/s)	u' (m/s)	l_E (mm)	λ (μ m)	η (μ m)	Re_{l_E}	Re_λ	Da	Ka
$y = 0$	104	27.4	0.85	46.4	3.6	1430	79	0.81	48
$\tilde{\xi} = \xi_{st}$	19.4	19.8	0.64	48.3	4.7	715	54	0.85	34

where $\delta = 6.25 \times 10^{-3}H$ in the present study. Subsequently, the species mass fractions and temperature variations are specified based on $\xi(y)$. The velocity is initially taken to be zero, but evolves as low-temperature chemistry produces heat. The boundary conditions on the both sides are set to be non-reflecting outflow implemented with the NSCBC method [23, 24]. After the initialization, the low-temperature ignition starts producing low-temperature species and heat at the interfaces of the fuel and oxidizer streams. The simulation in Step 1 continues until $t_{step1} = 5.4$ ms when sufficient mixing between fuel and oxidizer is achieved through the scalar gradient, and intense heat release rate commences at $y = 0$ as shown in Figs. 2c and 2d. At $t = t_{step1}$, just after the mixture experiences peak LTHR, the instantaneous scalar fields are used for initialization in Step 2.

2.3. Step 2: Three-dimensional temporally evolving jet DNS

The second step involves a 3D non-premixed temporally evolving jet DNS using the results from Step 1 to initialize the scalar fields. This step is performed to obtain consistent scalar and turbulence coupling in the presence of

Figure 3: DNS results of low-temperature ignition in a temporally evolving slot jet. Temporal evolution of (a) velocity derivative skewness components, (b) mean streamwise velocity and its RMS at $y^+ = 0$, and (c) logarithm of heat release rate $\log(Q)$ J/m³/s (color) and ξ_{st} (dashed line) at $t = t_{step2}$. The dashed line in (a) and (b) denotes the time of sampling of feed data ($t = t_{step2}$). Note that only a portion of the DNS domain is shown in (c).

continual LTHR. The DNS conditions and configuration are briefly described here. A detailed description of the DNS configuration is reported in Ref. [14].

The DNS domain is a cuboid of dimensions $L_x \times L_y \times L_z = 24 \times 12 \times 3$ mm³ which is discretized using $N_x \times N_y \times N_z = 3024 \times 896 \times 384$ mesh points. The initial 3D temporally evolving jet DNS domain consists of a slot jet stream and oxidizer stream with a streamwise jet velocity, $u_j = 138$ m/s, at the center of the jet and a streamwise coflow velocity, $u_{cof} = 3$ m/s, outside of it, respectively. The velocity field is initialized using the same tanh profile as in Eq. (1). Turbulent fluctuations initialized using a synthetic homogeneous isotropic turbulence spectrum are superimposed on top of the mean jet velocity. The jet width is taken to be H . The species mass fractions, temperature and density fields from Step 1 are mapped onto the DNS domain to initialize the scalar fields. This initialization produces an inconsistent jet width between the velocity and scalar fields since the scalar fields were already evolved for t_{step1} in Step 1 via molecular diffusion and reaction due to the imposed scalar gradient, resulting in a larger “fuel core” width than the jet in practice. However, having a larger fuel core width than the momentum layer of the jet is a strategy often utilized in turbulent combustion DNS involving shear flows. This strategy maximizes turbulence–flame interaction while minimizing the effect of artificial turbulence on the interaction [8, 14, 25], and this approach is also employed in the present DNS. Based on these jet parameters and the partially premixed reacted mixture, the jet Reynolds number is 5400. The boundary conditions are periodic in the streamwise (x) and spanwise (z) directions, and non-reflecting outflow in the transverse direction (y) which are implemented based on the NSCBC

[23, 24] method.

After initialization, the DNS is continued for $t_{step2} = 40\mu s$ before a snapshot is taken serving as feed data for the combustion DNS in Step 3. The temporal evolution of the center-line velocity derivative skewness in the three directions is shown in Fig. 3a, which converges to an almost constant value of ~ -0.5 after $t = t_{step2}$. The temporal evolution of the mean streamwise velocity $\tilde{u}^+$ and Root-Mean-Square (RMS) velocity u'^+ is shown in Fig. 3b. Here, the superscript “+” denotes normalization using jet parameters, H and u_j . For example, length L and velocity U are normalized as L/H and U/u_j . Also, “ $\sim$ ” denotes a density-weighted mean. The RMS velocity peaks just before $t = t_{step2}$ due to the initial laminar–turbulence transition of the velocity shear layers while the mean velocity continues to decrease. An instantaneous snapshot of heat release rate at $t = t_{step2}$ is shown in Fig. 3c. The small heat release ($\sim 10^8$ J/m³/s) observed in the figure is produced through LTHR involving low-temperature species such as $CH_3OCH_2O_2$. Other important turbulence parameters at $t = t_{step2}$ are summarized in Table 1 at the $y^+ = 0$ centerline and stoichiometric locations. These parameters form the turbulence conditions for the present DNS case. The Damköhler and Karlovitz numbers are computed respectively as $Da = (S_L/u')/(\delta_F/l_E)$ and $Ka = (l_E/\delta_F)^{-0.5}(u'/S_L)^{1.5}$, where $S_L = 0.63$ m/s is the laminar flame speed and $\delta_F = \nu/S_L = 24$ μm is the diffusive thickness. Here, ν is the kinematic viscosity which is obtained from the corresponding stoichiometric laminar flame. The large-eddy lengthscale l_E , Taylor microscale λ and Kolmogorov

Table 2: Computational parameters for the DNS involved in Steps 1–3.

Step	$L_x^+ \times L_y^+ \times L_z^+$	$N_x \times N_y \times N_z$	$t_{step1,2}$	x	y	z
1: 1D mixing–reacting	–	–	5.4 ms	–	out	–
2: 3D temporal jet	$40 \times 20 \times 5$	$3024 \times 896 \times 384$	$40 \mu s$	peri	out	peri
3: 3D lifted jet	$20 \times 20 \times 5$	$1512 \times 896 \times 384$	–	in/out	out	peri

length scale η are, respectively, computed as:

$$l_E = u'^3/\epsilon ; \lambda = \frac{1}{3} \sum_{i=1}^3 \sqrt{\widetilde{u_i''^2}/(\partial u_i''/\partial x_i)^2} ; \eta = (\nu^3/\epsilon)^{1/4}, \quad (2)$$

where ϵ is the turbulent kinetic energy dissipation rate and u_i'' denotes a Favre velocity fluctuation.

2.4. Step 3: Three-dimensional turbulent lifted jet flame DNS

The last step corresponds to performing a spatially-evolving DNS of a turbulent lifted reacting DME jet flame. The domain size for the reacting DME DNS is $L_x^+ \times L_y^+ \times L_z^+ = 20 \times 20 \times 5$ which is discretized using $N_x \times N_y \times N_z = 1512 \times 896 \times 384$ mesh points. The mesh is uniform in the streamwise and spanwise directions, while it is non-uniform in the transverse direction. In the transverse direction a uniform mesh spacing of $\Delta y = 8 \mu m$ ensures at least 8 mesh points exist across the thinnest scalar thickness. The fine mesh exists across the flame brush and shear zone, $-4 < y^+ < 4$, where locally rich and stoichiometric premixed flame elements reside. Also, based on the smallest Kolmogorov length scale η_{min} and maximum wave number resolved in the current simulation k_{max} , $k_{max}\eta_{min} = 1.4$, the small scale turbulent

Figure 4: Contour line of $a = 0.999t$ (black) and contour line of $Y_{\text{OH}} = 0.2Y_{\text{OH,max}}$ (blue) overlaid on the normalized age variable field, a/t , (color) in the spanwise mid plane at $t = 0.279$ ms.

Figure 5: Instantaneous volume rendering of the turbulent DME lifted jet flame showing the coordinate system and a low-temperature heat release marker, $Y_{\text{CH}_3\text{OCH}_2\text{O}_2}$ and a high-temperature flame marker, Y_{OH} .

motion is resolved as well. The algebraic expression for the transverse non-uniform mesh is provided in a previous study [8]. The boundary conditions are specified as inflow boundary at $x = 0$, non-reflecting outflow at $x = L_x$ and in the transverse direction, and periodic in the spanwise direction. These open boundaries are implemented based on the NSCBC [23, 24] method. The computational parameters are summarized in Table 2 for the DNS cases involved in Steps 1–3.

The initial field is constructed by mapping the instantaneous turbulence and scalar fields taken from the temporally evolving slot jet DNS at $t = t_{step2}$ onto the spatially-developing combustion DNS domain. The same fields also issue from the $x = 0$ inflow boundary as feed data for the velocity, temperature and species mass fraction fields during the simulation. A flame ignition source is also introduced by smoothly imposing a high temperature (1700K) region downstream at $6 < x^+ < 20$ and $-1 < y^+ < 1$. Because of the “super-adiabatic” initial condition, the flame initially propagates upstream until $t \sim 70 \mu s$. Subsequently, the stabilization point, which will be defined later, begins to drift downstream at an average speed of 15 m/s after the super-adiabatic effect of the ignition source decreases. Sampling occurs between $t = 215 \mu s$ (2.5 jet-flow-through times) and $420 \mu s$ (4.8 flow-through times) when the initial mixture has disappeared from the combustion region, determined from examining an “age” variable a [26, 27] whose transport equation (Eq. (3)) is solved with the other governing equations during the DNS:

$$\frac{\partial a}{\partial t} + \mathbf{u} \cdot \nabla a = \frac{1}{\rho} \nabla \cdot (\rho D \nabla a), \quad (3)$$

where the diffusivity for N_2 is used. The age variable corresponds to the

mixture averaged residence time of the local mixture, and the variable does not influence the DNS results. Using the age variable, a criterion of $a < t$ can be used to ensure that the local mixture had not experienced initialization, and $a < t$ is guaranteed for most of the reaction zones after $t = 215 \mu\text{s}$. In the present study, the statistics shown are collected at $t = 279 \mu\text{s}$. Figure 4 shows variation of the age variable in the spanwise mid plane at $t = 279 \mu\text{s}$, and clearly shows that the reaction zones represented by $Y_{\text{OH}} > 0.2Y_{\text{OH,max}}$ (described in Sec. 3.1) consist of “fresh” mixture. Once the initial transient is swept out of the domain, there are two types of flames remaining in the domain. The first corresponds to a low-temperature flame, and the second to a high-temperature flame identified by using $\text{CH}_3\text{OCH}_2\text{O}_2$ and OH mass fractions, respectively, as shown in Fig. 5.

3. Results

3.1. Laminar pentabrachial flame structure

First, a laminar “pentabrachial” flame, originally reported in Ref. [1], is briefly explained in Fig. 6a where the oxidizer stream is on the left and the fuel stream is on the right. As the name suggests, there are five flame branches, two upstream and three downstream. The downstream flame branches (labelled as (1)–(3) in Fig. 6a) correspond to conventional “triple” flames which are rich premixed, lean premixed and trailing diffusion flames. One of the upstream flames located towards the rich side (labelled as (4) in Fig. 6a) is the low-temperature flame branch due to low-temperature ignition. The second upstream branch ((5) in Fig. 6a) is a high temperature flame generated by the high-temperature oxidizer stream and NTC behaviour. Clearly,

Figure 6: The logarithmic heat release rate ($\text{J}/\text{m}^3/\text{s}$) field of a laminar pentabrachial flame reported in Ref. [1] showing (1)–(3): the downstream flame branches correspond to conventional “triple” flames which are rich premixed, lean premixed and trailing diffusion flames, (4): upstream flame branch due to low-temperature ignition, and (5): the second upstream flame branch generated by the high-temperature oxidizer stream and NTC (a). The square symbol indicates the location of the stabilization point while the triangle symbol indicates the location of the triple point. Instantaneous stoichiometric mixture fraction (black) and $Y_{\text{OH}} = 0.2Y_{\text{OH,max}}$ (blue) iso-contour lines overlaid on the logarithm of heat release rate (b) and methoxymethyl-peroxy mass fraction, $Y_{\text{CH}_3\text{OCH}_2\text{O}_2}$ (c) from the present spatially-developing reacting DNS in the spanwise mid plane at $t = 0.279$ ms.

the upstream low-temperature flame is located on the rich side reflecting the fact that low-temperature ignition is observed where $\xi > \xi_{st}$ (e.g. see Fig. 1). However, the stabilization point, defined here as the most upstream location where $Y_{OH} = 0.2Y_{OH,max}$, is located on the lean side, unlike a conventional lifted flame where the stabilization point is located at $\xi \sim \xi_{st}$. Here, the same threshold has been used in a previous study [1] and the present results are insensitive to the choice of the threshold value. Between the streamwise distances of the stabilization point and triple point in Fig. 6a (approximately at $x^+ = 6$), there are two types of flames that are a subset of the downstream rich premixed (1) and lean premixed (3) flame branches: lean and ultra-lean flames. The lean flame, which serves as a bridge between the stabilization and triple points with a heat release rate, $\log_{10} Q \sim 12.5$ (J/m³/s), is a subset of the rich premixed flame. The ultra-lean flame is the beginning of the lean premixed flame branch extending from the stabilization point. Such lean stabilization and presence of lean and ultra-lean premixed flames originating from the lean stabilization point are unique characteristics of flames with strong NTC chemistry.

3.2. Flame structure of the turbulent lifted DME flame

Figures 6b and 6c show the fields of heat release rate and mass fraction of methoxymethyl-peroxy $Y_{CH_3OCH_2O_2}$, respectively, at $t = 0.279$ ms corresponding to the beginning of sampling. At this time, the streamwise location of the mean stabilization point of the left flame wing ($y^+ < 0$) is $\bar{x}_{stb}^+ = 8.2$ and its standard deviation is $\sigma_{x_{stb}}^+ = 0.3$. Here the mean location and its

Figure 7: Mean logarithm of the heat release rate, $\log[Q(\text{J/m}^3/\text{s})]$ (a), species mass fraction of methoxymethoxy-peroxy radicals $Y_{\text{CH}_3\text{OCH}_2\text{O}_2}$ (b), and Flame Index weighted by Q (c) conditioned on mixture fraction at $x^+ = 1$ (blue dash), 6 (gray solid), 7 (gray dash), 8 (red dash), 10 (gray dot-dash) at $t = 0.279$ ms. Vertical lines show standard deviation for $x^+ = 1$ and 8. Note $x^+ = 8$ (red dash) location corresponds to the stabilization point.

standard deviation are defined as:

$$\bar{x}_{stb}^+ = \frac{1}{N_z} \sum_{k=1}^{N_z} x_{stb}^+(z_k); \quad \sigma_{x_{stb}}^+ = \frac{1}{N_z} \sqrt{\sum_{k=1}^{N_z} [x_{stb}^+(z_k) - \bar{x}_{stb}^+]^2}, \quad (4)$$

where $x_{stb}^+(z)$ is the normalized instantaneous streamwise distance of the left stabilization point at a given spanwise location z . Also, the reader should be careful not to confuse x_{stb}^+ or $\bar{x}_{stb}^+$ as a lift-off length, since the jet issues not at $x^+ = 0$ in the present combustion DNS domain, but from an initial field obtained from the temporally-evolving jet DNS domain described in Step 2 (Sec. 2.3).

Since the low-temperature ignition had already begun in Step 1 (Sec. 2.2) and Step 2 (Sec. 2.3), LTHR and the low-temperature species are observed in the upstream region. These processes related to low-temperature chemistry are confined in the fuel rich mixture, and gradually decrease with streamwise distance. Once the low-temperature process diminishes sufficiently, high temperature chemistry commences, which is denoted by intense heat release rate occurring transversely outwards of the substantial low-temperature species (compare Figs. 6b and 6c). However, neither conventional triple flames nor pentabrachial flames are observed when the heat release rate field or any scalar fields are examined in physical coordinates, unlike the laminar lifted DME flame reported in Ref. [1].

The unique feature of a pentabrachial flame structure is the existence of an additional two upstream flame branches consisting of a high-temperature flame due to NTC and a low-temperature flame due to first-stage, low-temperature ignition. Therefore, the upstream flame structure is investigated first. Figure 7 shows the mean heat release rate, low-temperature species

mass fraction and Flame Index weighted by heat release rate conditional on mixture fraction ξ . Here, the Flame Index is a metric for the mixing mode defined using fuel and oxidizer mass fractions (Y_F and Y_O) as [28]:

$$FI = \frac{|\nabla Y_F| \cdot |\nabla Y_O|}{|\nabla Y_F| |\nabla Y_O|}. \quad (5)$$

A positive value of Flame Index indicates premixed mode, and non-premixed mode, otherwise. A fully premixed (non-premixed) flame yields $FI = 1$ (-1). Also, an average of any quantity q weighted by heat release rate Q conditional on mixture fraction ξ , $\langle q|\xi \rangle^*$, is computed as:

$$\langle q|\xi \rangle^* = \langle Qq|\xi \rangle / \langle Q|\xi \rangle. \quad (6)$$

The conditional averages are constructed at different x locations including the location of the mean stabilization point, using the instantaneous snapshot at $t = 0.279$ ms. For each x , the samples are collected from a slab having dimensions of $(H/2, L_y/2, L_z)$ for $y < 0$ (left flame wing).

At a location close to the inflow boundary (e.g. $x^+ = 1$ in Fig 7), the heat release rate monotonically increases with increasing ξ in the conditional space shown in Fig. 7a. The substantial heat release rate at large mixture fraction, i.e. $\xi > 0.3$, is due to the low-temperature reaction, as indicated by the relatively large mass fraction of the low-temperature species at the same ξ in Fig. 7b. Also, these upstream samples show negative Flame Index of ~ -1 in Fig. 7c, indicating the mixture is overall non-premixed. Thus, there is one upstream non-premixed flame branch associated with low-temperature chemistry.

At $x^+ = 6$ and 7 where the locations are still upstream of the stabilization point, a substantial amount of heat release rate relevant to low-temperature

reaction continues to occur at large values of mixture fraction. Additionally, there is a peak which significantly deviates from the $x^+ = 1$ plot at lean conditions, $\xi \sim 0.05$. Comparing the conditional averages of heat release rate (Fig. 7a) and low-temperature species (Fig. 7b), the peaks in the lean side at $x^+ = 6$ and 7 do not involve low-temperature species. Rather, a high-temperature flame due to NTC behaviour exists and constitutes one of the upstream branches described in Sec. 3.1. This is also validated by the results from the zero-dimensional ignition simulation in Fig. 1 showing that the local minimum of the high-temperature ignition delay due to NTC is located at $\xi \sim 0.05$. Moreover, the mixture forming the high-temperature flame becomes increasingly more premixed as seen by the increasing value of the Flame Index in Fig. 7c at $\xi \sim 0.05$. Therefore, the two upstream flame branches, consisting of high-temperature partially-premixed flames due to NTC and low-temperature non-premixed flame on par with the ones reported in Ref. [1], exist in a turbulent environment, and are clearly observed conditional on mixture fraction.

Downstream of the mean stabilization location, the conditionally-averaged heat release rate increases by an order of magnitude relative to its value upstream, indicating the presence of strong flames, while the low-temperature reaction persists on the rich side. However, a clearly delineated triple flame structure similar to what was observed downstream in the laminar case described in Sec. 3.1 is not observed, even conditional on mixture fraction. The relatively large standard deviation of Flame Index at $x^+ = 8$ suggests that samples include both premixed and non-premixed flames which cannot occur separately, unlike in the laminar case shown in Fig. 6a. This is a consequence

Figure 8: Samples (black) extracted by the maximum heat release rate ridge method overlaid on the heat release rate iso-contours ($\log[Q(\text{J/m}^3/\text{s})]$) in the spanwise mid-plane at different x , y locations (a, b), and the cross-sectional heat release rate plotted along the white dashed line in (a) with extracted samples (circle) (c).

of the intense flame-turbulence and flame-flame interactions that obscure the flame structure [12]. Thus, delineating the flame structure downstream of the stabilization point requires a different approach.

To reveal the downstream flame structure, local reaction zones are extracted from the instantaneous snapshot to eliminate the effect of samples with a small reaction rate compared to neighboring samples, which are not of interest in the acquired statistics. The locations of local reaction zones are defined as isolated local maxima (ridges) of heat release rate field for each z plane. The x - y heat release rate field is scanned in the x and y directions to locate mesh points that constitute ridges, and these locations are identified with sub-pixel accuracy using a fifth order Lagrangian interpolation. Using this method, samples forming both 2D and 3D “ridges” are extracted. Ide-

ally, only 3D ridges should be extracted to eliminate effects of samples that are not part of the reaction zones for the investigation. Also, there is a possibility that samples forming a ridge across multiple z -planes are not extracted, if they do not form a ridge in the x - y plane. However, the present 2D method eliminates a sufficient number of samples that are not reaction zones, and the results discussed here are not unduly biased by inclusion of such erroneous samples. The locations of the samples extracted by this method are overlaid on the x - y heat release rate field in Figs. 8a and 8b. A cross-sectional 1D heat release rate plot with extracted samples is also shown in Fig. 8c. Note that a few samples at $y^+ \sim -2.5$ in Fig. 8c are extracted since they form local peaks in the out-of-plane (x direction) variations. As observed in the figure, samples having local heat release maxima with intense heat release rate are successfully identified, although there still exist a few number of erroneous samples that are not completely eliminated.

Constructing statistics from the samples related to the local reaction zones retains only samples with moderate or intense heat release rate compared with neighboring points. The method also includes samples constituting complex flame topology such as interacting flames since the present method identifies local heat release peaks which persist even during the dynamic event of flame–flame interactions [29]. Using only samples obtained from the local reaction zone segmentation, the probability density function (PDF) of heat release rate at different axial locations for $y^+ < 0$ (left flame wing) is shown in Fig. 9. Also shown in Fig. 9 are the mean mixture fraction and Flame Index conditional on heat release rate.

First, the PDF and conditional averages constructed using samples lo-

Figure 9: PDF of the logarithm of release rate (top), and mean mixture fraction (middle) and Flame Index (bottom) conditioned on heat release rate constructed using samples forming local reaction zones at $t = 0.279$ ms. The plots are constructed at upstream locations of $x^+ = 7$ (dash line), 9 (solid line) and 11 (dash-dot line) (a) and downstream locations of $x^+ = 14$ (dash line), 16 (solid line) and 18 (dash-dot line) (b). Standard deviation $\pm\sigma$ is shown for $x^+ = 9$ (a) and 16 (thin solid line). The vertical solid lines show the standard deviation of the plots at $x^+ = 9$ (a) and 16 (b). The horizontal thin dash line indicates ξ_{st} (middle) and $FI = 0$ (bottom). Note that heat release rate is shown in logarithmic coordinates.

cated in the vicinity of $\bar{x}_{stb}^+$ are discussed in Fig. 9a. The $x^+ = 7$ plot is constructed just upstream of $\bar{x}_{stb}^+$, and the $x^+ = 9$ and 11 plots are located downstream of $\bar{x}_{stb}^+$. Upstream ($x^+ = 7$), the PDF is distributed broadly and its tail attains a value slightly greater than $\log_{10}[Q_{max}(\text{J/m}^3/\text{s})] \approx 10$. The conditionally-averaged mixture fraction indicates these samples are overall lean. A similar plot of low-temperature species mass fraction $Y_{\text{CH}_3\text{OCH}_2\text{O}_2}$ (not shown) shows two to three orders of magnitude smaller values than the values shown in Fig. 7b, ensuring that the local low-temperature flames are effectively eliminated by the process of identifying local reaction zones described above. The value of the Flame Index varies from -1 to 0.5, indicating these upstream samples related to the high-temperature reaction are partially premixed at this location, consistent with the discussion in Fig. 7c. At $x^+ = 9$ and 11, just downstream of $\bar{x}_{stb}^+$, the PDF starts to exhibit two peaks at $\log_{10}[Q(\text{J/m}^3/\text{s})] \sim 9$ and 10.5. These peaks, respectively, correspond to the ultra-lean and lean reaction zones as observed in the conditional average of ξ . Also, the Flame Index over the range of $\log_{10}[Q(\text{J/m}^3/\text{s})]$ exhibits positive values, suggesting these ultra-lean and lean reaction zones are premixed, forming a flame base that is observed in the laminar case as discussed in Sec. 3.1 (see Fig. 6a at $x^+ \sim 6$ for such ultra-lean and lean flames).

The flame structure further downstream of the stabilization point shown in Fig. 9b is discussed next. These plots are constructed using the identified local reaction zones at $x^+ = 14, 16$ and 18, far downstream from the mean stabilization point at $\bar{x}_{stb}^+$. At $x^+ = 14$, the PDF distribution is broad and the maximum value of the heat release rate is $\log_{10}[Q_{max}(\text{J/m}^3/\text{s})] \sim 11$, indicating the presence of strong flames directly observed in Fig. 6b at this

location. The mixture fraction spans from rich to lean and the Flame Index is positive, with no evidence of distinct tribrachial flames at this location. At $x^+ = 16$ and 18, however, the PDF shows three distinct peaks at $\log_{10}[Q(\text{J}/\text{m}^3/\text{s})] \sim 8.5, 9.5$ and 10.5. These peaks respectively correspond to lean, near stoichiometric and rich mixture fractions as shown in the ξ plots in Fig. 9b. Comparing this with the Flame Index plots, it is clear that both lean and rich reaction zones located at $\log_{10}[Q(\text{J}/\text{m}^3/\text{s})] \sim 8.5$ and 10.5 have positive Flame Indices while the reaction zones with $\xi \sim \xi_{st}$ at $\log_{10}[Q(\text{J}/\text{m}^3/\text{s})] \sim 9.5$ are negative. Thus, with proper conditioning, a tribrachial flame structure is identified downstream of the stabilization point. In combination with the upstream branches discussed in Figs 7 and 9, reaction zones with a pentabrachial flame structure exist even in a turbulent lifted flame.

3.3. Effects of two-stage ignition and NTC on triple point and stabilization point propagation speed

Section 3.2 revealed the existence of a pentabrachial flame structure in the present turbulent flame which includes two topologically significant points—the triple point and the stabilization point. In the present pentabrachial flames, the heat release rate is an order of magnitude higher in the vicinity of the triple point than it is at the stabilization point (see Fig. 6a for laminar and Fig. 7a for the turbulent lifted flames). Yet, the stabilization point is located upstream of the triple point. Thus, the mechanism that sustains these points is discussed in this section.

Figure 10 shows the conditional averages of Flame Index and displacement speed constructed from samples along the $\xi = \xi_{st}$ surface (Figs. 10a and 10b),

Figure 10: Mean Flame Index and flame displacement speed conditional on temperature (a, c, d) and mass fraction of CO+CO₂ (b). Flame displacement speed is computed based on Eq. (9) (a, c, d) and Eq. (10) (b). The conditional averages are constructed on $\xi = \xi_{st}$ iso-surfaces (a, b), $\xi = \xi_{stb}$ iso-surfaces (c) and at stabilization points (d) using a snapshot at $t = 0.279$ ms. The highlighted section in (c) indicates samples having preferred temperature and mixture fraction conditions to be stabilization points, defined as potential stabilization points. The vertical thin solid line indicates the standard deviation of S_d .

along the $\xi = \xi_{stb}$ surface (Fig. 10c) and from samples near the stabilization points (Fig. 10d). Here, ξ_{stb} is the spatially averaged mixture fraction at the left stabilization point at t obtained as:

$$\xi_{stb} = \frac{1}{N_z} \sum_{k=1}^{N_z} \xi(x_{stb}(z_k), y_{stb}(z_k), z_k, t), \quad (7)$$

and $\xi_{stb} = 0.2$. The density weighted displacement speed S_d is defined based on the material derivative:

$$S_d = \frac{\rho}{\rho_0} \frac{Dq}{Dt} / |\nabla q|, \quad (8)$$

where ρ_0 is the unburnt mixture density of the respective ξ iso-surface [30, 31]. The quantity q can be taken to be either temperature or the sum of CO and CO₂ mass fractions $Y(=Y_{CO+CO_2})$ and S_d , so defined, is shown in Fig 10. Also shown are the reaction $S_{d,R}$, normal diffusion $S_{d,N}$ and tangential diffusion $S_{d,T}$ terms and a term associated with different heat capacities $S_{d,cp}$, respectively computed as in Eqs. (9) and (10) [30]. The flame normal defined based on either CO+CO₂ or temperature is pointed towards the unburnt mixture.

$$S_d^T = \underbrace{\frac{Q}{\rho_0 c_p |\nabla T|}}_{S_{d,R}^T} + \underbrace{\frac{\mathbf{n} \cdot \nabla (\lambda \mathbf{n} \cdot \nabla T)}{\rho_0 c_p |\nabla T|}}_{S_{d,N}^T} + \underbrace{\frac{\lambda}{\rho_0 c_p} \nabla \cdot \mathbf{n}}_{S_{d,T}^T} - \underbrace{\frac{\rho}{\rho_0 c_p} \nabla T \cdot \left(\sum_{k=1}^N c_{p,k} D_k \frac{W_k}{W} \nabla X_k \right)}_{S_{d,cp}^T}; \quad \mathbf{n} = \frac{\nabla T}{|\nabla T|}. \quad (9)$$

$$S_d^Y = \underbrace{\frac{\omega_Y}{\rho_0 |\nabla Y|}}_{S_{d,R}^Y} + \underbrace{\frac{\mathbf{n} \cdot (\rho D \mathbf{n} \cdot \nabla Y)}{\rho_0 |\nabla Y|}}_{S_{d,N}^Y} + \underbrace{\frac{\rho D}{\rho_0} (\nabla \cdot \mathbf{n})}_{S_{d,T}^Y}; \quad \mathbf{n} = \frac{\nabla Y}{|\nabla Y|}. \quad (10)$$

The conditional mean Flame Index and the temperature based S_d^T along $\xi = \xi_{st}$ are shown in Fig. 10a. At a temperature below 1000 K the Flame Index is negative and it attains positive values between 1000 K < T < 2000 K, suggesting that the partially premixed flame base, on average, is located in this temperature range. The triple point, where a trailing diffusion flame extends from the premixed flame base, coincides with a location where the Flame Index changes from positive to negative values at $T = 1600 \sim 2000$ K in Fig. 10a. Among the four terms in Eq. 9, $S_{d,cp}^T$ is negligible in general (not shown), while the contribution of the reaction term $S_{d,R}^T$ is the largest. A comparison between the normal $S_{d,N}^T$ and tangential $S_{d,T}^T$ diffusion contributions shows that $S_{d,N}^T$ is much larger than $S_{d,T}^T$, suggesting that the curvature of the T iso-surface is small compared to the normal temperature gradient at $\xi = \xi_{st}$. The displacement speed S_d^T attains its peak value of 2 m/s near the temperature of the triple point. The S_d^Y plot based on Y_{CO+CO_2} in Fig. 10b also shows qualitatively similar features.

Similarly, S_d^T constructed along the $\xi = \xi_{stb}$ iso-surfaces using Eq. (9) is shown in Fig. 10c. The stabilization points $(x_{stb}(z), y_{stb}(z))$ at this time are likely to be formed at $T = 1710(= T_{stb})$ K on average with a standard deviation of $\sigma_{T,stb} = \pm 106$ K highlighted in Fig. 10c. Since the samples with $\xi = \xi_{stb}$ and $T \sim T_{stb}$ thermo-chemically have the potential to form stabilization points, they are called “potential stabilization” points here. From these samples, only one sample that is positioned most upstream on a given z plane is the actual stabilization point. At the potential stabilization points, the Flame Index is close to zero resulting from the partially-premixed, high-temperature flame branch upstream as discussed in Fig. 7c. The displacement

speed components at $T = T_{stb}$ are $S_{d,R}^T = 0.26$, $S_{d,N}^T \sim 0$ and $S_{d,T}^T = -0.01$ yielding a value of $S_d^T = 0.23$ m/s ($S_{d,cp}^T = -0.02$). Unlike the results at the triple point, the tangential diffusion contribution generally equals or outweighs the normal diffusion at the potential stabilization point, suggesting the reaction zones at this location are highly convoluted. The prevalence of high tangential diffusion resulting from large surface curvature continues at $T \sim 1800$ where the displacement speed at $\xi = \xi_{stb}$ peaks. Although $S_{d,R}^T \gg |S_{d,N}^T + S_{d,T}^T|$ suggesting an autoignition-advection dominated balance at the locations of potential stabilization points, the magnitudes of $S_{d,N}^T$ and $S_{d,T}^T$ contributions are comparable to $S_{d,R}^T$ at the location where the reaction contribution $S_{d,R}^T$ peaks (located just upstream of x_{stb} at $T \sim 1500$ K along $\xi = \xi_{stb}$) or at the location where S_d^T peaks (located just downstream of x_{stb} at $T \sim 1800$ K along $\xi = \xi_{stb}$). Thus, the potential stabilization point which is a continuation from the upstream high-temperature flame branch is undergoing autoignition while its neighboring mixture is sustained by a balance of reaction rate and diffusion, indicating flame propagation. Owing to intense turbulent strain and advection, complex mixed combustion modalities—autoignition and flame propagation—at potential stabilization points can exist in close proximity in both physical and phase space. This is in contrast to the conceptual stabilization mechanism for a laminar lifted DME flame [1] shown in Fig. 6a where autoignition is solely responsible for flame stabilization. This difference could be due to the following reasons. As observed from the laminar pentabrachial flame in Fig. 6a, the stabilization point is located on the lean side due to NTC, and this point is an intersection of the upstream high-temperature flame branch due to NTC and the

ultra-lean and lean flame branches. In the middle of this flame intersection (or flame–flame interaction), the scalar gradient is reduced while reaction rate remains intense as in a single flame, resulting in autoignition dominated behavior [29, 32]. In the turbulent case, however, the samples constituting the conditional average include these distinct high-temperature flames due to strong flame convolution generated by turbulent strain, resulting in the presence of locally-propagating flames at some locations in Fig. 10c. Lastly, a similar conditional average is shown, which is constructed based on samples at the stabilization points (most upstream “potential stabilization point” sample on each z plane) in Fig. 10d. To obtain a sufficient sample size, samples are also collected at ± 2 grid points from each stabilization point. As the figure shows, $S_{d,R} \ll |S_{d,N} + S_{d,T}|$ resulting in a negative S_d , clearly indicating a passive flame structure.

The triple flame propagation speed along the stoichiometric surface is given as:

$$S_{ref} = \sqrt{\frac{\rho_0}{\rho_1}} S_L \quad (11)$$

based on an asymptotic analysis [2], where ρ_0 , ρ_1 and S_L are maximum and minimum densities along the stoichiometric surface and the laminar flame speed of the stoichiometric mixture, respectively. Here, the mixture temperature is taken to be the temperature at $\xi = \xi_{st}$, $T_{st,f}$, determined by frozen mixing of fuel (500 K) and oxidizer (1000 K). In the present turbulent flame DNS, $\sqrt{\rho_0/\rho_1} = 1.94$ and the present thermochemical condition gives $S_L = 0.63 (= S_{L,0})$ m/s, yielding a smaller propagation speed of $S_{ref} = 1.2$ m/s than for the turbulent flame shown in Figs. 10a and 10b of approximately 2 m/s. Since the mixture that the triple point burns

Figure 11: (a): S_{ref} with different t_p . Circle symbols: one-dimensional laminar premixed flame speeds simulated using the partially-reacted mixtures taken at various t_p from SENKIN simulations shown in Fig. 1. Square symbols: Reference speed S_{ref} of a triple flame obtained using Eq. (11) at various t_p . The dashed line shows the peak S_d^T in Fig. 10a. (b): Variations of DME mass fraction of the simulated laminar premixed flames in (a).

is the partially-reacted reactants from the low-temperature ignition reactions (including radicals and intermediates with slightly elevated temperature, $T > T_{st,f}$), the effect of low-temperature products on the propagation speed is assessed. A normalized time corresponding to the progress of low-temperature reaction t_p at time t is defined as $t_p = (t - \tau_1)/(\tau_2 - \tau_1)$, where τ_1 and τ_2 are low-temperature and high-temperature ignition delays for $\xi = \xi_{st}$ shown in Fig. 1, respectively. The normalized ignition progress, t_p , varies between zero and unity as the mixture state is prepared for high-temperature ignition; thus it represents the degree of completion, or residence time, for low-temperature chemistry.

Figure 11a shows the one-dimensional laminar premixed flame speed based on the fuel consumption speed for the partially-reacted mixtures simulated using 1D DNS with a 0.01 m domain. The partially-reacted mixture composition and temperature, used in the 1D flame simulation, are obtained from a SENKIN homogeneous simulation result at various t_p . Note that the mixture is partially reacting and no unique S_L is obtained if the mixture ignites inside the domain. However, the present domain size ensures that the residence time of the mixture is much shorter than the autoignition delay time and meaningful S_L can be obtained under the present configuration [33]. Variations of DME mass fraction of the simulated one-dimensional flames are also shown in Fig. 11b for mixtures with different residence times, t_p . Clearly, for a large t_p (near the high-temperature ignition delay time), the flame speed rapidly increases and the flame characteristics approach autoignition. For moderate t_p (e.g. $0.1 < t_p < 0.8$) where the simulated flames are not too autoignitive, the flame speed ranges from $1.3S_{L,0}$ to $1.8S_{L,0}$, yield-

ing an enhanced triple flame propagation speed, S_{ref} , ranging between 1.6 to 2.2 m/s, comparable to the DNS results. This effect of low-temperature reaction on propagation is specific to flame configurations involving high velocity jets: in statistically one-dimensional planar turbulent flames, enhancement of the propagation speed is limited by a relatively small influx of production rates of low-temperature species (i.e. the increased propagation speed cannot be sustained if the consumption rate of low-temperature species at the flame front exceeds the production rate of such species in the LTHR region prior to intense heat release). In a configuration such as the present one, a high velocity jet provides an abundant pool of low-temperature species in the domain despite its small production rate and narrow jet exit. Although the present simulation considers a moderate Reynolds number and diluted reactant mixture, relevant scales between flame and turbulence are comparable to typical IC engine conditions as manifested in the non-dimensional parameters, Da and Ka in Table. 1 [34]. Since they are the key parameters that influence the turbulent flame structure and propagation characteristics discussed above, the results obtained in the present study may also apply to practical combustion devices utilising reactants with NTC and LTHR.

3.4. Implications for turbulent combustion modeling

The present investigation regarding flame structure and propagation characteristics identified five distinct types of flame branches that interact with turbulence, and the local flame propagation speed was found to depend on the concentration of radicals and intermediate species produced through low-temperature reactions. Clearly, modeling of turbulent combustion as in the present case needs to incorporate these additional complexities due to multi-

Figure 12: (a, b) conditional averages of Y_{OH} and Y_{HO_2} conditional on mixture fraction obtained at $x^+ = 1, 6, 7, 8 (= \bar{x}_{stb}^+)$ and 10; (c, d) doubly conditional means and standard deviation of Y_{OH} and Y_{HO_2} conditional on mixture fraction scalar dissipation rate and mixture fraction; (e, f) doubly conditional means and standard deviation of Y_{OH} and Y_{HO_2} conditional on temperature and mixture fraction. The vertical bars in (a, b) show the standard deviation for $x^+ = 8$ (a, b). All doubly conditional statistics are obtained at $x^+ = \bar{x}_{stb}^+$ (c-f).

stage, multi-mode ignition and combustion.

Figures 12a and 12b show typical conditional means of Y_{OH} and Y_{HO_2} conditioned on the mixture fraction at $x^+ = 1, 6, 7, 8 (= \bar{x}_{stb}^+)$ and 10, respectively. Similar conditional mean statistics for the low-temperature species $Y_{\text{CH}_2\text{OCH}_2\text{O}_2}$ was already discussed in Fig. 7b. While the low-temperature species shows very small fluctuation about the mean when conditioned on mixture fraction (Fig. 7b), representative species for high-temperature combustion reveal relatively large fluctuations as shown in Figs. 12a and 12b. The ratio of the maximum fluctuation to the conditional mean, $\langle Y_i'' | \xi \rangle_{\text{max}} / \langle Y_i | \xi \rangle_{\text{max}}$, is 1.2 for OH and 0.98 for HO₂. Such large fluctuations clearly suggest that the conditioning based on mixture fraction alone is insufficient to capture high-temperature flame characteristics, and an additional conditioning variable is required. Gordon et al. [35] reported fluctuations of lift-off height and attributed these possibly to the fluctuation of the scalar dissipation rate [36, 37]. The fluctuations in OH and HO₂ about the mean values are slightly reduced when the scalar dissipation rate of mixture fraction, N , is introduced as an additional conditioning scalar as shown in Figs. 12c and 12d in the mean and standard deviation. With this conditioning, the ratio of the fluctuation to the mean, $\langle Y_i'' | \xi, \log_{10} N \rangle_{\text{max}} / \langle Y_i | \xi, \log_{10} N \rangle_{\text{max}}$, is 0.52 for OH and 0.59 for HO₂. The multi-stage ignition results in high-temperature flames comprised of both premixed and non-premixed flames locally. Therefore, to capture the nature of the premixed flame branches a second conditioning scalar is chosen as a progress variable, which can be defined based on either species, sensible enthalpy or temperature [38, 39]. In the present analysis, temperature T is used as the second conditioning scalar. Figures 12e and 12f show doubly

conditional mean $\langle Y_i | \xi, T \rangle$ and fluctuations $\langle Y_i'' | \xi, T \rangle$ for OH and HO₂ at $x \sim \bar{x}_{stb}^+$. The ratio of the fluctuation to the mean, $\langle Y_i'' | \xi, T \rangle_{\max} / \langle Y_i | \xi, T \rangle_{\max}$, is 0.14 for OH and 0.22 for HO₂. Clearly, the doubly-conditional values show much smaller fluctuations compared to the mean and to $\langle Y_i'' | \xi, \log_{10} N \rangle$, and this trend holds for other x locations and other high-temperature species as well. Thus, an approach such as doubly-conditional moment closure may be suitable to model multi-stage, multi-mode combustion and the complexities associated with low-temperature chemistry discussed in Sec. 3.3.

4. Conclusions

A three-dimensional DNS of a turbulent lifted DME slot jet flame has been performed at elevated pressure to study interactions between chemical reactions with LTHR and NTC behavior and shear generated turbulence. Although the present pressure is far lower than nominal engine conditions due to computational limitations, the fuel and oxidizer temperatures are carefully chosen to include LTHR and NTC effects. Due to the presence of strong flame-turbulence and flame-flame interactions, the present turbulent flame does not exhibit a clear pentabrachial flame structure in physical coordinates, which was observed in a laminar flame with similar thermochemical conditions as the present case. However, by conditioning on mixture fraction, local reaction zones and local heat release rate, the turbulent flame structure is revealed, and is comprised of five distinct branches: (1) an upstream low-temperature flame branch with low-temperature species, (2) an upstream high-temperature flame branch due to NTC and (3)–(5) rich and lean premixed and trailing diffusion flame branches downstream, with a lean

stabilization point. Therefore, the pentabrachial flame is a unique flame structure for combustion in fuel jets with a high-temperature oxidizer coflow for conditions where the fuel undergoes two-stage ignition and exhibits NTC characteristics, even in the presence of highly unsteady non-uniform flow such as in sheared turbulence.

The propagation characteristics of both the stabilization and triple points are investigated by examining the conditional statistics of the budget for the displacement speed of a pertinent isoscalar. Potential stabilization points, which have preferred temperature and mixture fraction conditions exhibit autoignition characteristics with significant reaction rate and negligible diffusion. The stabilization point, identified as the most upstream samples forming the potential stabilization points for a given spanwise plane z reveals a passive flame structure with large diffusion and small reaction rate. At both points, tangential diffusion (curvature) is, on average, relatively large compared to normal diffusion, and the Flame Index nearly vanishes, which is consistent with the conditional mean in mixture fraction.

Finally, the propagation speed along the stoichiometric surface is compared with the asymptotic value. When a stoichiometric mixture constructed from the present fuel and oxidizer mixture compositions is considered, the asymptotic and averaged DNS values deviate by a factor of 1.7. However, by accounting for the effect of low-temperature species on the flame speed enhancement, the two values becomes comparable. Therefore, two-stage ignition influences the triple point propagation speed through enhancement of the laminar flame speed in a configuration where abundant low-temperature intermediate species are transported by a high-velocity jet. Thus, engineering

large-eddy or RANS simulations of two-stage autoignition in a turbulent flow configuration where fuel issues from a high velocity jet need to employ a turbulent combustion model that accommodates complex chemistry to includes this effect, or alternatively explicitly include the enhancement of propagation speed in algebraic form. With proper conditioning, doubly conditional moment closure seems to adequately capture both the low-temperature and multi-mode high-temperature combustion flame and ignition structure.

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