A Direct Numerical Simulation analysis of turbulent V-shaped flames propagating into droplet-laden mixtures

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ABSTRACT

Three-dimensional Direct Numerical Simulations (DNS) data has been used to analyse the gaseous phase combustion behaviour in a V-shaped flame configuration where fuel is supplied in the form of droplets such that an overall (i.e. liquid+gaseous) equivalence ratio of unity is maintained in the unburned gas. The analysis has been carried out for different initially mono-sized droplet diameters. A gaseous premixed V-shaped flame with the same flow conditions has been utilised to compare the flame propagation in V-shaped spray flames with a corresponding gaseous premixed flame case. It has been found that combustion in the gaseous phase mainly takes place under fuel-lean mode and the probability of finding fuel-lean burning increases with increasing droplet diameter. However, the mean equivalence ratio of the predominantly fuel-lean mixture increases with increasing axial distance from the flame holder. The presence of droplets has been found to give rise to dimples on the reaction progress variable isosurfaces, and the effects of droplet-induced flame wrinkling are reflected by the widening of the curvature probability density functions for large droplets. The heat release has been found to arise mainly from the premixed mode of combustion. Detailed analysis of reaction progress variable transport has been used to explain the mean variations of consumption speed and density-weighted displacement speed with the axial distance from the flame holder. The mean values of consumption speed, density-weighted displacement speed and turbulent burning velocity have been found to decrease with increasing droplet diameter. The flame speed statistics have been utilised to explain that the enhancement of the burning rate cannot be equated to the enhancement of the flame surface area in turbulent droplet-laden V-shaped flames.

Keywords: Droplet combustion, V-shaped flame, Equivalence ratio, Displacement speed, Consumption speed, Direct Numerical Simulations

1. INTRODUCTION

The V-shaped flame is one of the most commonly used laboratory-scale configurations, which has been extensively investigated in previous experimental (Smith and Gouldin, 1978; Veynante et al., 1994, 1996; Gouldin, 1996; Shepherd, 1996; Sattler et al., 2002; Vena et al., 2011, 2015; Sponfeldner et al., 2015; Letty et al., 2013) and numerical (Alshaalan and Rutland, 1998; Domingo et al., 2005; Bell et al., 2005; Wu et al., 2011; Dunstan et al., 2011, 2012) studies. Smith and Gouldin (1978) proposed an experimental methodology to measure turbulent flame speed in V-shaped turbulent methane-air flames with different equivalence ratios and turbulence intensities. Veynante et al. (1994, 1996) used experimental data of turbulent premixed propane-air V-flames to analyse flame surface density transport statistics. Gouldin (1996) and Shepherd (1996) investigated the burning and flame propagation rates by measuring the flame surface area in turbulent premixed V-shaped flames. Shepherd (1996) compared a stagnation point flame with a V-shaped flame and identified important differences in flame structure and burning rate between the two flames. A similar conclusion was drawn by Dunstan et al. (2011) based on Direct Numerical Simulations (DNS). Sattler et al. (2002) observed a linear increase in the mean flamelet area with downstream distance by taking measurements at several axial distances from the stabilizing rod for turbulent premixed methane/air V-flames. The flame topology and flame brush thickness for turbulent V-flames at different turbulence intensities have been experimentally investigated by Kheirkhah and Gulder (2014). Vena et al. (2011,2015) experimentally analysed flame topology and heat release rate statistics for turbulent V-flames for stratified iso-octane/air mixtures. It was shown by Vena et al. (2011) that equivalence ratio gradients have significant effects on flame wrinkling in comparison to the corresponding fully premixed reference flame. Sponfeldner et al. (2015) concentrated on the statistical behaviours of principal strain-rates and the local flamelet normal vector in their experimental analysis of premixed turbulent V-flames.

Advancements of high-performance computing enabled detailed and parametric analyses of V-shaped flames using DNS. Alshaalan and Rutland (1998) performed a three-dimensional DNS analysis with a single-step chemical mechanism to analyse the adiabatic and non-adiabatic flame-wall interactions in a V-flame configuration. Domingo et al. (2005) utilised two-dimensional DNS and Large Eddy Simulations (LES) of turbulent premixed V-flames for development and validation of Flame Surface Density-Probability Density Function (FSD-PDF) closures in the context of LES. Bell et al. (2005) carried out three-dimensional DNS for a laboratory-scale turbulent premixed V-shaped flame and reported a good agreement in the mean flame structure and the mean axial and transverse velocities between DNS results and experimental data. Wu et al. (2011) investigated the ignition and propagation of a V-shaped premixed ethylene-air turbulent flame using LES and an increase in flame angle is observed relative to the laminar cases. Dunston et al. (2011, 2012) performed an extensive three-dimensional DNS analysis with single-step chemistry for premixed turbulent V-flames under different turbulence intensities. The expression derived for the turbulent displacement speed showed a similar trend with the turbulent consumption speed in the downstream of the flame. However, qualitative differences between the turbulent displacement and consumption speeds originate due to turbulent and molecular diffusion (Dunstan et al., 2011).

Despite significant practical relevance of turbulent combustion of droplet-laden mixtures, the V-flame configuration has rarely been used (Letty et al., 2013) for the analysis of spray combustion. Although several previous analytical (Polymeropoulos, 1984; Silverman et al., 1993; Greenberg et al., 1993), experimental (Burgoyne and Cohen, 1954; Mizutani and Nishimoto, 1972; Hayashi et al., 1977; Szekely and Faeth, 1983; Ballal and Lefebvre, 1981; Lawes and Saat, 2011) and computational (Reveillon and Vervisch, 2000; Nakamura et al.,

2005; Wang and Rutland, 2005; Watanabe et al., 2007; Reveillon and Demoulin, 2007; Sreedhara and Huh, 2007; Xia and Luo, 2010; Fujita et al., 2013; Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012; Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b) studies investigated flame propagation in droplet-laden mixtures in conventional canonical configurations (e.g. statistically planar and spherical flames), a relatively limited effort (Letty et al., 2013) has been directed to the investigations on spray flames in relatively more complex laboratory-scale configurations such as V-shaped flames. Letty et al. (2013) carried out experiments to understand the combustion behaviour of V-shaped flames in heptane droplet-laden mixtures. They compared temperature distributions between droplets and gaseous phase mixture and indicated that the presence of droplets significantly alters the temperature of the gaseous mixture. However, the flame propagation statistics for droplet-laden mixtures in a V-shaped flame configuration are still incompletely understood due to the complex interaction between droplets, flame and the background fluid flow. To address this gap in the existing literature, three-dimensional carrier phase Direct Numerical Simulations (DNS) with modified single-step chemistry (Ozel-Erol et al., 2019b) have been performed in this analysis for three different droplet diameters for an overall (liquid+gaseous) equivalence ratio of unity in the unburned droplet-laden mixture. The variations of gaseous equivalence ratio ϕ_g , flame curvature κ_m and flame displacement and consumption speeds have been presented at different axial locations, which have been explained based on physical principles. In this respect, the main objectives of this paper are:

1. To demonstrate the evolution of the gaseous reacting mixture composition within the flame at different axial locations from the flame holder for V-shaped flames propagating in droplet-laden mixtures.
2. To explain the influences of droplet diameter on the reaction zone structure and flame propagation characteristics at different axial locations from the flame holder and to explain the

differences in flame structure arising from supplying the fuel in liquid form by comparing to a turbulent gaseous stoichiometric premixed V-shaped flame.

3. To indicate implications of the above findings in the context of modelling of turbulent combustion of droplet-laden mixtures.

The mathematical background and numerical implementation pertaining to this analysis are presented in the next section. This will be followed by the presentation of the results and their subsequent discussion. The main findings are summarised and conclusions are drawn in the final section of this paper.

2. MATHEMATICAL BACKGROUND

A modified single-step Arrhenius-type chemical mechanism (Tarrazo et al., 2006) has been adopted to keep the computational demand within reasonable limits. This chemical mechanism provides a realistic ϕ_g dependence of the unstrained laminar burning velocity $S_{b(\phi_g)}$ and adiabatic flame temperature $T_{ad(\phi_g)}$ in hydrocarbon-air flames. For further information on this behaviour in hydrocarbon-air flames, the interested readers are directed to Malkeson and Chakraborty (2010). Comparisons between the laminar flame speed of n-heptane from experiments (Kumar et al., 2007), simulations with detailed chemical mechanism (Chaos et al., 2007) and modified single step chemistry used in this study are presented in Fig 1. The variations of $S_{b(\phi_g)}/\{S_{b(\phi_g)}\}_{max}$ and $T_{ad(\phi_g)}$ with ϕ_g for the present thermo-chemistry have been found to exhibit good agreements with previous experimental data (Swaminathan and Bray, 2011) and the results obtained from a detailed chemical mechanism. Note that, single step chemistry has been used to analyse the turbulent spray flames in several previous studies (Reveillon and Demoulin, 2007; Sreedhara and Huh, 2007; Xia and Luo, 2010; Wang and

Rutland, 2005; Wandel, 2014) which offered valuable physical insights while being consistent with experimental observations. For example, the findings of simple chemistry DNS by Ozel-Erol et al. (2018, 2019) have been found to be qualitatively consistent with the experimental findings (Hayashi et al., 1977; Lawes and Saat, 2011). To date, the majority of the DNS based analyses on droplet combustion have been conducted using simple chemical mechanisms (Nakamura et al., 2005; Reveillon and Vervisch, 2005; Wang and Rutland, 2005; Reveillon and Demoulin, 2007; Schroll et al., 2009; Watanabe et al., 2007; Sreedhara and Huh, 2007; Wandel et al., 2009; Wandel, 2014; Wacks et al., 2016; Haruki et al., 2018; Pillai and Kurose, 2018, 2019). It is also worth noting that it has been demonstrated in several previous analyses that the flame propagation statistics extracted from simple chemistry DNS (Chakraborty and Cant, 2004, 2005; Jenkins et al., 2006; Klein et al., 2016; Chakraborty, 2007; Han and Huh, 2008) are at least qualitatively similar to those obtained from detailed chemistry DNS (Echekki and Chen, 1996; Chen and Im, 1998; Peters et al., 1998; Hawkes and Chen, 2004; Hawkes and Chen, 2005; Chakraborty et al., 2008) data.

Figure 1. Variations of the (a) normalised laminar burning velocity $S_b(\phi_g)/\{S_b(\phi_g)\}_{max}$ and (b) normalised adiabatic flame temperature $T_{b(\phi_g)} = (T_{ad(\phi_g)} - T_0)/(T_{ad(\phi_{g=1})} - T_0)$ with equivalence ratio ϕ_g for n-heptane obtained from modified single step chemistry (Tarrazo et al., 2006), detailed chemical mechanism (Chaos et al., 2007) and experimental (Kumar et al., 2007) data.

In this analysis, the Lewis numbers of all species are assumed to be unity and all species in the gaseous phase are taken to be perfect gases. Standard values have been considered for the ratio of specific heats ($\gamma = C_p^g/C_v^g = 1.4$, where C_p^g and C_v^g are the gaseous specific heats at constant pressure and constant volume respectively) and Prandtl number ($Pr = \mu C_p^g/\lambda = 0.7$ where μ is the dynamic viscosity and λ is the thermal conductivity of the gaseous phase). The position $\vec{x}_d$, velocity $\vec{u}_d$, diameter a_d and temperature T_d of the individual droplets are transported in the following manner using a Lagrangian approach (Reveillon and Vervisch, 2000; Reveillon and Demoulin, 2007; Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012; Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b):

$$\frac{d\vec{x}_d}{dt} = \vec{u}_d; \frac{d\vec{u}_d}{dt} = \frac{\vec{u}(\vec{x}_d, t) - \vec{u}_d}{\tau_d^u}; \frac{da_d^2}{dt} = -\frac{a_d^2}{\tau_d^p}; \frac{dT_d}{dt} = \frac{\hat{T}(\vec{x}_d, t) - T_d - B_d L_v / C_p^g}{\tau_d^T} \quad (1)$$

In the transport equations, $\hat{T}$ is the gaseous phase temperature, L_v is the latent heat of vaporization and τ_d^u , τ_d^p and τ_d^T stand for the relaxation timescales for droplet velocity, diameter and temperature, respectively, which can be expressed as (Reveillon and Vervisch, 2000; Reveillon and Demoulin, 2007):

$$\tau_d^u = \frac{\rho_d a_d^2}{(18C_u\mu)}; \tau_d^p = \frac{\rho_d a_d^2}{4\mu} \frac{Sc}{Sh_c \ln(1+B_d)}; \tau_d^T = \frac{\rho_d a_d^2}{6\mu} \frac{Pr}{Nu_c \ln(1+B_d)} \frac{C_p^L}{C_p^g} \quad (2)$$

where, ρ_d is the droplet density, Sc is the Schmidt number, C_p^L is the specific heat for the liquid phase. The liquid fuel properties used in the analysis are summarised in Table 1. In Eq. 2, $C_u = 1 + Re_d^{2/3}/6$ is the corrected drag coefficient, Re_d is the droplet Reynolds number, B_d is the Spalding number, Sh_c is the corrected Sherwood number and Nu_c is the corrected Nusselt number, which are defined as (Reveillon and Vervisch, 2000; Reveillon and Demoulin, 2007):

$$Re_d = \frac{\rho |\vec{u}(\vec{x}_d, t) - \vec{u}_d| a_d}{\mu}; B_d = \frac{[Y_F^s - Y_F(\vec{x}_d, t)]}{(1 - Y_F^s)}; \quad (3)$$

$$Sh_c = Nu_c = 2 + \frac{0.555 Re_d Sc}{(1.232 + Re_d Sc^{4/3})^{1/2}}$$

where Y_F^s is the value of fuel mass fraction Y_F at the droplet surface. The Clausius–Clapeyron equation is used to evaluate the partial pressure of the fuel vapour at the droplet surface p_F^s , which is in turn used to calculate the Spalding number B_d , which leads to the following expressions (Reveillon and Vervisch, 2000; Reveillon and Demoulin, 2007):

$$p_F^s = p_{ref} \exp\left(\frac{L_v}{R} \left[\frac{1}{T_{ref}^s} - \frac{1}{T_d^s}\right]\right); Y_F^s = \left(1 + \frac{W_g}{W_F} \left[\frac{p(\vec{x}_d, t)}{p_F^s} - 1\right]\right)^{-1} \quad (4)$$

where R is the gas constant, T_{ref}^s is the boiling point of the fuel at a pressure p_{ref} and T_d^s is assumed to be T_d , and W_g and W_F are the molecular weights of gaseous mixture and fuel, respectively. The liquid fuel droplets are coupled with the surrounding gaseous mixture with additional source terms in the gaseous transport equations as follows (Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012; Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b):

$$\frac{\partial(\rho\varphi)}{\partial t} + \frac{\partial(\rho u_j \varphi)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[R_\varphi \frac{\partial \varphi_1}{\partial x_j} \right] + \dot{\omega}_\varphi + \dot{S}_g + \dot{S}_\varphi \quad (5)$$

where $\varphi = \{1, u_i, e, Y_F, Y_O\}$ and $\varphi_1 = \{1, u_i, \hat{T}, Y_F, Y_O\}$ for the conservation equations of mass, momentum, energy, and mass fractions, respectively and $R_\varphi = \rho\nu/\sigma_\varphi$ is the generalised diffusion coefficient associated with $\varphi = \{1, u_i, Y_F, Y_O\}$ whereas R_φ is given by $R_\varphi = \lambda$ for $\varphi = e$, and u_i is the fluid velocity in the i^{th} direction. The term $\dot{\omega}_\varphi$ corresponds to the reaction rate contribution, $\dot{S}_g$ refers to an appropriate gaseous phase source term and $\dot{S}_\varphi$ is the appropriate source term due to the coupling between Lagrangian particulate and Eulerian carrier phases, which is tri-linearly interpolated from the droplet's sub-grid position, $\vec{x}_d$, to the eight surrounding nodes. Here, ν is the kinematic viscosity, and σ_φ is an appropriate Schmidt number corresponding to φ .

A reaction progress variable c , based on oxygen mass fraction, Y_O and mixture fraction, $\xi = (Y_F - Y_O/s + Y_{O\infty}/s)/(Y_{F\infty} + Y_{O\infty}/s)$, can be written in the following manner (Wacks et al., 2016; Wacks and Chakraborty, 2016):

$$c = \frac{[(1 - \xi)Y_{O\infty} - Y_O]}{[(1 - \xi)Y_{O\infty} - \max(0, \{\xi_{st} - \xi\}/\xi_{st})Y_{O\infty}]} \quad (6)$$

where $Y_{O\infty} = 0.233$ is the oxygen mass fraction in air and $Y_{F\infty} = 1.0$ is the fuel mass fraction in the pure fuel stream. Considering n-heptane, C_7H_{16} as the fuel in the analysis, $s = 3.52$ denotes the stoichiometric mass ratio of oxygen to fuel and $Y_{Fst} = 0.0621$ and $\xi_{st} = 0.0621$ represent the corresponding stoichiometric fuel mass fraction and stoichiometric mixture fraction, respectively.

The transport equation of the reaction progress variable, c is given by (Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b):

$$\rho \frac{\partial c}{\partial t} + \rho u_j \frac{\partial c}{\partial x_j} = \nabla \cdot (\rho D \nabla c) + \dot{w}_c + \dot{S}_{liq,c} + \dot{A}_c \quad (7)$$

where D is the molecular diffusivity, $\dot{w}_c$ indicates the reaction rate of reaction progress variable, $\dot{S}_{liq,c}$ represents the source/sink term arising due to droplet evaporation and $\dot{A}_c$ is the cross-scalar dissipation term arising due to mixture inhomogeneity. The reaction rate of the reaction progress variable $\dot{w}_c$ can be expressed as (Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b):

$$\dot{w}_c = -\xi_{st}\dot{w}_O/[Y_{O\infty}\xi(1 - \xi_{st})] \text{ for } \xi \leq \xi_{st} \text{ and } \dot{w}_c = -\dot{w}_O/[Y_{O\infty}(1 - \xi)] \text{ for } \xi > \xi_{st} \quad (8)$$

where $\dot{w}_O$ is the reaction rate of oxygen (Wacks et al., 2016; Wacks and Chakraborty, 2016).

The term associated with droplet evaporation $\dot{S}_{liq,c}$ is calculated as (Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b):

$$\dot{S}_{liq,c} = -\xi_{st}[\xi\dot{S}_O + (Y_{O\infty} - Y_O)\dot{S}_\xi]/[Y_{O\infty}\xi^2(1 - \xi_{st})] \text{ for } \xi \leq \xi_{st} \quad (9)$$

$$\text{and } \dot{S}_{liq} = -[(1 - \xi)\dot{S}_O + Y_O\dot{S}_\xi]/[Y_{O\infty}(1 - \xi)^2] \text{ for } \xi > \xi_{st}$$

where $\dot{S}_\xi = (\dot{S}_F - \dot{S}_O/s)/(Y_{F\infty} + Y_{O\infty}/s)$ is the droplet source/sink term in the mixture fraction transport equation, $\dot{S}_F = \Gamma_m(1 - Y_F)$ and $\dot{S}_O = -\Gamma_m Y_O$ are the droplet source/sink terms in the mass fraction transport equations for fuel and oxygen, respectively and Γ_m is the source term in the mass conservation equation due to evaporation (Wacks et al., 2016; Wacks and Chakraborty, 2016). The term associated with mixture inhomogeneity $\dot{A}_c$ is given as (Wacks et al., 2016; Wacks and Chakraborty, 2016):

$$\dot{A}_c = 2\rho D \nabla \xi \cdot \nabla c / \xi \text{ for } \xi \leq \xi_{st} \text{ and } \dot{A}_c = -2\rho D \nabla \xi \cdot \nabla c / (1 - \xi) \text{ for } \xi > \xi_{st} \quad (10)$$

Alternatively, Eq. 7 can be rearranged in the kinematic form for a given c isosurface as (Wacks et al., 2016; Wacks and Chakraborty, 2016):

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = S_d |\nabla c| \quad (11)$$

where S_d represents the displacement speed, which can be expressed as (Wacks et al., 2016; Wacks and Chakraborty, 2016):

$$S_d = \frac{[\nabla \cdot (\rho D \nabla c) + \dot{w}_c + \dot{S}_{liq,c} + \dot{A}_c]}{\rho |\nabla c|} \quad (12)$$

Using Eq. 12, the density-weighted displacement speed can be defined as $S_d^* = \rho S_d / \rho_0$ where ρ_0 is the unburned gas density. Another alternative flame speed, known as the consumption speed S_c , can be defined as (Ozel Erol et al., 2019b; Poinso et al., 1992; Haworth and Poinso, 1992):

$$S_c = \rho_0^{-1} \int \dot{w}_c dn \quad (13)$$

where dn is the elemental distance in the local flame normal direction.

Table 1. Liquid fuel properties used in this analysis

Liquid specific heat at constant pressure, C_p^l	2296.45 J/kgK
Latent heat of vaporization, L_v	315 kJ/kg
Liquid density, ρ_d	684 kg/m ³
Liquid temperature at the inlet, T_0	300 K

3. NUMERICAL IMPLEMENTATION

Simulations of the V-shaped flames propagating in droplet-laden mixtures are carried out using a three-dimensional compressible code SENG+ (Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012; Wacks et al., 2016; Wacks and Chakraborty, 2016; Ozel Erol et al., 2018, 2019a, 2019b). The governing equations of mass, momentum, energy and species of the gaseous phase are spatially discretised using a 10th order central difference scheme for the internal grid points, but the order of differentiation gradually decreases to a one-sided 2nd order scheme at the non-periodic boundaries. The time advancement is achieved by employing an explicit low-storage 3rd order Runge-Kutta scheme (Wray, 1990). Boundary conditions in the stream-wise direction (x –direction) are considered to be inflow and outflow according to the Navier-Stokes Characteristic Boundary Conditions (NSCBC) technique, whereas the remaining (i.e. y and z) directions are assumed to be periodic. The computational domain is taken to be a cube of $L_x = L_y = L_z = 30\delta_{st}$ where $\delta_{st} = (T_{ad}(\phi_{g=1}) - T_0)/\max|\nabla T|_L$ is the thermal flame thickness of the unstrained stoichiometric laminar premixed flame. The simulation domain is discretised by a uniform Cartesian grid of 384^3 , which ensures about 10 grid points within δ_{st} . A commercial software COSILAB (Rotexo-Softpredict-Cosilab) is used to initialise the reacting flow field for three different initial values of droplet diameter a_d (i.e. $a_d/\delta_{st} = 0.04, 0.05$ and 0.06) for an overall equivalence ratio ϕ_{ov} of unity (i.e. $\phi_{ov} = 1.0$). The V-flame is subjected to a moderate level of inlet turbulence (i.e. $u'/S_{b,st} = 2.0$), with a mean inlet velocity of $u_{mean}/S_{b,st} = 5.0$ and a

normalised longitudinal integral length scale of $l_t/\delta_{st} = 2.5$. The turbulent Reynolds number $Re_t = \rho_0 u' L_t / \mu_0$ (where $L_t = k^{1.5}/\varepsilon$ is the integral length scale based on turbulent kinetic energy k and its dissipation rate ε) for the flames considered here is about 35.0. It is admitted that the value of Re_t remains small but comparable to experiments by Vena et al. (2011, 2015) (where u' at the inlet varied from 0.19m/s to 0.33m/s, the hydraulic diameter of the burner exit is 0.024m, the integral length scale can be estimated as 7% of the hydraulic diameter, and the kinematic viscosity is given by $1.8 \times 10^{-5} m^2/s$). Moreover, the turbulent Reynolds number Re_t value of these simulations remains comparable to turbulent premixed V-flame simulations of Dunstan et al. (2011,2012). However, these V-shaped spray flame simulations are considerably more expensive than turbulent premixed V-flame DNS (Dunstan et al., 2011, 2012) because individual droplets are tracked in addition to accounting for gaseous phase combustion. A small value of $u'/S_{b,st}$ is considered in this study because the analysis of the flame-droplet interaction is one of the focal points of this paper and the flame-droplet interaction (e.g. curvature and strain effects) is eclipsed by flame-turbulence interaction for large values of $u'/S_{b,st}$ (Hayashi et al., 1977; Lawes and Saat, 2011; Ozel-Erol et al., 2018,2019).

Table 2. Simulation parameters considered in the analysis.

Initial droplet diameter, a_d/δ_{st}	0.04, 0.05, 0.06
Overall Equivalence ratio, ϕ_{ov}	1.0
Heat release parameter, $\tau = (T_{ad}(\phi_{g=1}) - T_0)/T_0$	6.54
Unburned gas temperature at the inlet, T_0	300 K
Mean velocity at the inlet, $u_{mean}/S_{b,st}$	5.0
Inlet turbulence, $u'/S_{b,st}$	2.0
Integral length scale, l_t/δ_{st}	2.5
Prandtl number $Pr = \mu C_p^g / \lambda$	0.7
Lewis number, Le	1.0
Ratio of specific heats $\gamma = C_p^g / C_v^g$	1.4
Stokes number, St	0.13

The steady state laminar spray flame simulation using the methodology adopted by Neophytou and Mastorakos (2009) has been used for obtaining reacting scalar fields under laminar V-flame conditions, which is used as initial conditions for turbulent flame simulations. A plane scans through a frozen field of homogeneous isotropic turbulence to specify turbulent velocity fluctuations at the inlet plane with the help of Taylor's hypothesis. Interested readers are referred to Chakraborty and Cant (2004) and Dunstan et al. (2011,2012) for further discussion on inlet boundary condition specification. The flame holder is placed at approximately $10\delta_{st}$ from the inlet plane. The radius of the flame holder is $0.3\delta_{st}$ and the statistics are presented at three different axial distances (i.e. position A, B and C) from the flame holder (i.e. $9\delta_{st}$, $13\delta_{st}$ and $17\delta_{st}$) after $2.0t_{flow}$ where $t_{flow} = L_x/u_{mean}$ is the flow through time. The reactant mass fractions (i.e. Y_F and Y_O) and the non-dimensional temperature of gaseous phase T are imposed using a Gaussian weighting function $g(r) = A\exp[-r^2/2\zeta^2]$ at the flame holder following Dunstan et al. (2011,2012) where A and ζ are adjustable constants to obtain the desired flame holder radius (i.e. $r = 0.3\delta_{st}$). The important simulation parameters are summarised in Table 2.

The initial droplet number density ρ_N varies between $1.23 \leq (\rho_N)^{1/3}\delta_{th} \leq 1.85$ in the unburned gas and the liquid volume fraction remains well below 0.01. The point-source assumption, which is widely used for DNS of diluted spray flames (Reveillon and Vervisch, 2005; Fujita et al., 2013; Neophytou et al., 2012, 2010; Schroll et al., 2009; Wandel, 2014; Wandel et al., 2009; Wang and Rutland, 2005) is employed here to evaluate the position, mass, velocity and temperature of individual droplets in a Lagrangian sense. By contrast, the conservation laws for the gas phase conservation equations are treated in the Eulerian frame of reference. The point source assumption is applicable for droplets, which are smaller than the Kolmogorov length scale and the grid size in DNS. However, these resolution requirements

restrict this approach for large droplets. The ratio of initial droplet diameter to the Kolmogorov length scale is $a_d/\eta = 0.09, 0.11, 0.13$ for the cases of $a_d/\delta_{st} = 0.04, 0.05, 0.06$ respectively for the inlet turbulence intensity (i.e. $u'/S_{b,st} = 2.0$) considered here. The ratio of the initial droplet diameter to grid spacing used here remains comparable to several previous analyses (Wang and Rutland, 2005; Sreedhara and Huh, 2007; Fujita et al., 2013; Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012). Furthermore, the diameter of the droplets interacting with the flame in the reaction zone (i.e. the most reacting place in the flame) has been found to be at least 50% smaller than the initial size due to the relatively high volatility of n-heptane. It is worth noting that Eulerian-Eulerian approaches, which can resolve both gaseous and liquid phases, also have some limitations (i.e. to capture the polydispersity and droplet crossing). Moreover, fully resolved dispersed phase simulations (Eulerian-Eulerian methods) for reacting flows are still not in a mature state and need further validation. As a reference, de Chaisemartin et al. (2009) compared the combustion of polydisperse droplets in a two-dimensional free jet using DNS with point source assumption and fully Eulerian methodologies. It was indicated that the Eulerian description of droplets yields a smoother gaseous mass fraction field in comparison to the Lagrangian description. However, the simulations with fully Eulerian approach were reported 10 times more expensive than those with point source assumption and it may require a huge parallelisation capability for 3D simulations. The Stokes number $St = \tau_p \sqrt{k}/l_t = \rho_d a_d^2 \sqrt{k}/(18C_u \mu l_t)$ (where $\tau_p = \rho_d a_d^2/18C_u \mu$ is the particle time scale and $l_t/\sqrt{k}$ is the turbulent time scale) remains smaller than 0.13 for the cases considered here. Alternatively, the Stokes number $St' = \tau_p S_{b,st}^2/\alpha_{T0} = \rho_d a_d^2 S_{b,st}^2/(18C_u \mu \alpha_{T0})$ can be estimated based on the chemical time scale $\alpha_{T0}/S_{b,st}^2$ and the maximum value of St' remains smaller than 0.27 for the largest droplets considered in this analysis. The mean normalised inter-droplet distance s_d/η ranges between 1.64 and 2.47 for

the inlet turbulence intensity considered here.

A group number, $G = 3(1 + 0.276Re_d^{1/2}Sc^{1/3})LeN^{2/3}(a_d/s_d)$ (where Le and Sc are the Lewis and Schmidt numbers, respectively, s_d is the distance between droplets, N is the number of droplets in a specified volume) can be defined following Chiu and Liu (1977) in order to distinguish between individually burning droplets ($G \ll 1.0$) and external sheath combustion ($G \gg 1.0$). All droplet cases considered in the current study come under the category of external sheath combustion (i.e. G remains much greater than unity). In the case of the small value of G pyrolysis takes place at the fuel-rich core due to extremely high temperature, whereas the temperature values in the external sheath combustion are usually not high enough to give rise to a significant amount of pyrolysis (Kuo and Acharya, 2012). For the present configuration, the burned gas temperature remains either comparable or smaller than the adiabatic flame temperature of the stoichiometric mixture, and thus the effects of pyrolysis are expected to be minimal. Moreover, thermochemistry for the present analysis involves a modified single-step Arrhenius-type chemical mechanism for the computational economy, and this chemical mechanism is not adequate for the analysis of the pyrolysis process. A similar assumption was made in several previous analyses (Wang and Rutland, 2005; Sreedhara and Huh, 2007; Fujita et al., 2013; Schroll et al., 2009; Wandel et al., 2009; Wandel, 2014; Neophytou et al., 2010, 2012) and the same approach has been adopted here. A recent DNS analysis by Zhou et al. (2019) demonstrated with the help of the Kerstein-Law parameter that either group combustion or individual burning is unlikely to occur under conditions which are comparable to the conditions analysed here.

Figure 2. Instantaneous distributions of (a) reaction progress variable, c (b) gaseous equivalence ratio, ϕ_g and (c) fuel reaction rate magnitude $|\dot{w}_F| \times \delta_{st}/\rho_0 S_b(\phi_g=1)$ on the central x-y midplane for initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ at $t = 2.0t_{flow}$. Blue lines show $c = 0.1, 0.5$ and 0.9 contours from outer to inner periphery and grey dots show the droplets residing on the plane (not to the scale).

4. RESULTS AND DISCUSSION

The contours of reaction progress variable, c , gaseous equivalence ratio, ϕ_g and fuel reaction rate magnitude $|\dot{w}_F| \times \delta_{st}/\rho_0 S_b(\phi_g=1)$ on the central x-y mid-plane at $t = 2.0t_{flow}$ are shown in Fig. 2 for initial droplet diameters $a_d/\delta_{st} = 0.04, 0.05, 0.06$. The droplets residing on the plane are illustrated by grey dots. It can be seen from the reaction progress variable distribution shown in Fig. 2 that the background fluid turbulence creates wrinkling on the flame surface. It is worth noting that fuel is supplied in the form of liquid droplets at the inlet which is placed on the left-hand side of the domain. Liquid fuel droplets, distributed randomly but statistically

uniform in space at the inlet plane, are introduced with a temperature of $T_0 = 300K$. The mass flux of liquid fuel at the inlet plane is estimated based on the values of u_{mean} and ϕ_{ov} . These droplets shrink in size due to evaporation as they approach the flame (see insets in Fig. 2) and the combustion of the evaporated gaseous fuel sustains the V-shaped flame. It can be seen from Fig. 2 that small droplets with initial $a_d/\delta_{st} = 0.04$ mostly complete their evaporation by halfway in the streamwise direction due to their high evaporation rate, whereas large droplets with initial $a_d/\delta_{st} = 0.05$ and 0.06 survive longer due to their lower evaporation rate and interact more with the flame than smaller droplets. Although an overall stoichiometric fuel-air mixture is provided in the unburned gas (note that fuel in the gaseous phase is absent at the inlet), the evaporation ahead of the flame is not sufficient to produce a gaseous stoichiometric mixture (i.e. $\phi_g = 1.0$) and this tendency is particularly prevalent for the case with initial $a_d/\delta_{st} = 0.06$. Although the gaseous phase combustion in V-flames takes place under $\phi_g < 1.0$ for all droplet cases, the likelihood of finding fuel-air mixture corresponding to $\phi_g \approx 1.0$ is comparatively higher for the initial $a_d/\delta_{st} = 0.04$ case. This behaviour arises due to the faster evaporation of smaller droplets. Some of the droplets penetrate the flame structure in the $a_d/\delta_{st} = 0.06$ case and they eventually evaporate in the reaction zone and in the burned gas to produce local islands of fuel-rich (i.e. $\phi_g > 1.0$) mixtures. It is worth noting that the evaporation of droplets leads to higher availability of fuel vapour, which in turn gives rise to local islands of high reaction rate magnitude $|\dot{w}_F| \times \delta_{st}/\rho_0 S_b(\phi_g=1)$ as can be seen from Fig. 2c where the magnified views of the regions with $\phi_g \approx 1.0$ are shown. The latent heat of evaporation L_v affects the temporal evolution of droplet temperature dT_d/dt through the Spalding number B_d . Most droplets complete their evaporation process in the reaction zone and thus the latent heat of evaporation acts to reduce the temperature and reaction rate magnitude but the availability of the fuel vapour due to evaporation tends to increase reaction rate

magnitude. The relative strengths of these two competing effects determine the net effect of the latent heat on the reaction zone. However, the extraction of the latent heat reduces the temperature of the gas within the preheat zone which acts to reduce the most probable burned gas temperature in comparison to the adiabatic flame temperature of the stoichiometric mixture. This was discussed earlier by Nakamura et al. (2005) and Wacks et al. (2016) and the qualitatively similar behaviour has been observed in the flames considered here and thus are not explicitly shown here.

Figure 3. PDFs of ϕ_g in the region corresponding to $0.01 \leq c \leq 0.99$ at different locations A, B and C (top to bottom) for initial $\alpha_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

In order to illustrate the composition of the gaseous phase mixture within the flame, the

probability density functions (PDFs) of the gaseous phase equivalence ratio ϕ_g within the region given by $0.01 \leq c \leq 0.99$ at three different axial locations (i.e. at distances $x/\delta_{st} = 9$, 13 and 17 from the flame holder, which are indicated as locations A, B and C, respectively) are presented in Fig. 3. It is evident from Fig. 3 that combustion predominantly takes place under fuel-lean mode for all locations and droplet diameters. However, the cases with small droplets (i.e. initial $a_d/\delta_{st} = 0.04$ and 0.05 cases) show a considerable likelihood of finding $\phi_g \approx 1.0$, especially at locations B and C. Furthermore, the PDF of ϕ_g for large droplets with initial $a_d/\delta_{st} = 0.06$ shows a mild peak at $\phi_g = 1.0$ at all locations but the probability of obtaining $\phi_g < 1.0$ remains greater than that of finding $\phi_g \geq 1.0$ in all cases. The probability of having a fuel-lean mode of combustion decreases in the downstream direction due to increased availability of fuel vapour as a result of evaporation of droplets. For example, the droplet number density $(\rho_N)^{1/3}\delta_{th}$ in the region corresponding to $0.01 \leq c \leq 0.99$ drops by 30%, 4% and 1.14% at location C in comparison to location A for cases with initial $a_d/\delta_{st} = 0.04$, 0.05 and 0.06, respectively. Therefore, the flame at plane A is leaner than in plane C, which can be substantiated from the fact that the time-averaged values of ϕ_g for $a_d/\delta_{st} = 0.04$ are 0.88, 0.89 and 0.90, for $a_d/\delta_{st} = 0.05$ are 0.83, 0.85 and 0.87, for $a_d/\delta_{st} = 0.06$ are 0.74, 0.77 and 0.79, at locations A, B and C, respectively. It is worth noting that the PDFs of ϕ_g in Fig. 3 are shown only for $0.01 \leq c \leq 0.99$ and a comparison between Figs. 2a and 2b reveals that it is possible that there are local islands of highly fuel-rich mixtures in the fully burned regions because of the mixing of evaporated vapour from the neighborhood and also due to small number of droplets which escape through the flame due to turbulent motion and complete the evaporation in the high temperature zone in the region with $c = 1.0$. Some of these unburned fuel-pockets eventually diffuse into the flame and mix with the air diffusing from the unburned gas side to give rise to local diffusion mode of burning, which will be discussed later in this

paper. Moreover, a close inspection of Fig. 3 reveals that the peak value of the PDF of ϕ_g at location C is found close to $\phi_g = 1.0$ (i.e. most probable value of ϕ_g is going to be close to 1.0). This clearly indicates that the PDF of ϕ_g within the flame is likely to see a peak at $\phi_g = 1.0$ and a mean value of ϕ_g close to unity in the case of $a_d/\delta_{st} = 0.04$ at a location which is further away from the flame holder than the location C. This behaviour can also be discerned from the distributions of ϕ_g in Fig. 2b. It is worth noting that the fuel-lean nature of the gaseous reacting mixture is qualitatively consistent with previous findings for laminar flame calculations (Neophytou and Mastorakos, 2009), statistically planar turbulent spray flames (Wacks et al, 2016) and spherically expanding turbulent spray flames Ozel-Erol et al. (2018). Thus, this fuel-lean nature of the gaseous phase combustion for globally stoichiometric (i.e. $\phi_{ov} = 1.0$) spray flames has been found to be mostly independent of the flame configuration but is influenced by the liquid droplet size, turbulence intensity and number density of liquid droplets (Wacks et al., 2016; Ozel-Erol et al., 2018). However, droplets interact with both statistically planar and spherically expanding flames at all stages of their propagation into the unburned gas but in turbulent V-spray flames, droplets travel in the mean flow direction during the evaporation process. As a result, the frequency of flame-droplet interaction decreases and the mean value of ϕ_g increases in the downstream direction.

It is worth noting that droplets do not evaporate instantly and the evaporated fuel vapour does not immediately homogeneously mix to produce a mixture with $\phi_g = 1.0$ even when the overall equivalence ratio ϕ_{ov} takes a value of 1.0. Thus the limiting case for small diameter is a gaseous stratified mixture flame but not a premixed flame, but this stratification cannot be a priori characterised. It has been shown in previous analyses on stratified combustion (Hélie and Trouvé, 1998; Malkeson and Chakraborty, 2010) that the burning rate and flame front thickness

for stratified mixture with a mean equivalence ratio of $\phi_g = 1.0$ can be smaller than in the stoichiometric premixed flames due to smaller burning rates of $\phi_g < 1.0$ and $\phi_g > 1.0$ mixtures.

Table 3: Variation of the mean droplet diameter normalised by its initial value $a_{d,m}/a_d$ in the unburned gas region at locations A, B, C.

		$a_d/\delta_{st} = 0.04$	$a_d/\delta_{st} = 0.05$	$a_d/\delta_{st} = 0.06$
A	$0 \leq c < 0.1$	0.36	0.60	0.74
	$0.1 \leq c < 0.3$	0.25	0.45	0.64
	$0.3 \leq c < 0.5$	Absent	0.33	0.54
B	$0 \leq c < 0.1$	0.29	0.54	0.70
	$0.1 \leq c < 0.3$	0.20	0.39	0.59
	$0.3 \leq c < 0.5$	Absent	0.29	0.49
C	$0 \leq c < 0.1$	0.23	0.49	0.67
	$0.1 \leq c < 0.3$	0.15	0.32	0.54
	$0.3 \leq c < 0.5$	Absent	0.27	0.43

The mean droplet diameters for $0 \leq c < 0.1$, $0.1 < c \leq 0.3$ and $0.3 < c \leq 0.5$ at locations A, B and C are shown in Table 3. It is worth noting that only few droplets survive for $c > 0.5$ so the statistical average based on limited samples are not meaningful. It can be seen from Table 3 that the mean droplet size decreases due to evaporation as c increases but the differences in mean diameter size increase within the flame because smaller droplets evaporate faster. It can also be seen from Table 3 that the mean droplet size in the region corresponding to $0 \leq c < 0.1$ remains comparable to the initial values of a_d/δ_{st} for large droplets, whereas smaller droplets are mostly evaporated when they reach location A as shown in Fig. 2. The evaporation process before reaching the location A leads to significant diameter differences between the cases with different droplet diameters in the V-flame configuration. Therefore, the mean droplet sizes in the zones corresponding to $0 \leq c < 0.1$, $0.1 < c \leq 0.3$ and $0.3 < c \leq 0.5$ consist of a wide spread of droplet diameter at location A due to high (low) evaporation rate of small (large) droplets. It would not be appropriate to compare the mean droplet diameter at location A, B

and C in the V-flames with spherically expanding flames. However, it is worth noting that the mean droplet sizes in the zones corresponding to $0 \leq c < 0.1$, $0.1 < c \leq 0.3$ and $0.3 < c \leq 0.5$ in the spherically expanding flame with $\phi_{ov} = 1.0$ by the present authors (Ozel-Erol et al., 2018) show the the same qualitative trend to the V-flame configuration, especially for the large droplet case.

The Damköhler and Karlovitz numbers for the stoichiometric gaseous mixture based on the inlet values of $u'/S_{b,st}$ and l_t/δ_{st} are 1.25 and 1.79 (i.e. $Da_{(\phi_g=1)} = l_t S_{b,st}/u' \delta_{st} = 1.25$ and $Ka_{(\phi_g=1)} = (u'/S_{b,st})^{1.5} (l_t/\delta_{st})^{-0.5} = 1.79$), respectively. The predominant likelihood of fuel-lean combustion in these droplet V-flame cases is expected to increase the Karlovitz number and decrease the Damköhler number of the underlying combustion process in comparison to $Da_{(\phi_g=1)}$ and $Ka_{(\phi_g=1)}$, respectively. The local Damköhler number can alternatively be estimated by $Da_L = L_{turb} S_{b,\xi}^2 / u_{rms} \alpha_{T_0}$ with $L_{turb} = \tilde{k}^{1.5} / \tilde{\epsilon}$ and $u_{rms} = \sqrt{2\tilde{k}/3}$ being local turbulent length scale and root-mean-square velocity with $\tilde{k}$ and $\tilde{\epsilon}$ being the Favre-averaged turbulent kinetic energy and its dissipation rate, respectively. Here $S_{b,\xi}$ is the laminar burning velocity corresponding to $\phi_R = \tilde{\xi}(1 - \xi_{st})/[\xi_{st}(1 - \tilde{\xi})]$. The local values of the Damköhler number are exemplarily provided at the location corresponding to $\tilde{c} = 0.5$, which for $a_d/\delta_{st} = 0.04$ are 0.79, 0.92 and 1.09, for $a_d/\delta_{st} = 0.05$ are 0.49, 0.71 and 1.00, for $a_d/\delta_{st} = 0.06$ are 0.27, 0.40 and 0.62, for the premixed case are 3.66, 3.93, 3.99 at locations A, B and C, respectively. Similarly, the corresponding values of the local Karlovitz number ($Ka_L = (u_{rms}/S_{b,\xi})^{1.5} (L_{turb} S_{b,\xi} / \alpha_{T_0})^{-0.5}$) based on $\tilde{k}$, $\tilde{\epsilon}$ and $S_{b,\xi}$ values at the location corresponding to $\tilde{c} = 0.5$ for $a_d/\delta_{st} = 0.04$ are 1.79, 1.74 and 1.79, for $a_d/\delta_{st} = 0.05$ are 2.60, 2.18 and 1.87, for $a_d/\delta_{st} = 0.06$ are 4.12, 3.33 and 2.75, for the premixed case

are 3.77, 3.39, 2.91 at locations A, B and C, respectively. According to these estimated values of Da_L and Ka_L , combustion takes places in the thin reaction zones regime (Peters, 2000). The expression "thin reaction zones regime" refers to a condition where the reaction zone thickness remains smaller than the Kolmogorov length scale and thus the reaction processes remain quasi-laminar. In this sense, the reaction occurs in a thin region in comparison to the dissipative length scale of turbulence. The differences in Da_L and Ka_L values between gaseous premixed and droplet flames arise due to the differences in respective $S_{b,\tilde{\xi}}, \tilde{k}$ and $\tilde{\epsilon}$ values originating from mixture composition and also due to difference in turbulence evolution within the flame front. This behaviour can be further illustrated by the PDFs of reaction progress variable c on the isosurfaces of the Favre-averaged reaction progress variable $\tilde{c} = 0.1, 0.5$ and 0.9 at locations A, B and C, which are shown in Fig. 4, whereas the contours of $\tilde{c} = 0.1, 0.5$ and 0.9 for the cases considered here are shown in Fig. 5a. In this paper, the Favre averaging is carried out by averaging in time (i.e. over flow through time t_{flow}) and space (i.e. spanwise z -direction). For high values of Damköhler number (i.e. $Da_{(\phi_g)} \gg 1$), the PDFs of c are expected to be bimodal with impulses at $c = 0.0$ and $c = 1.0$ (Bray et al., 1980) but Fig. 4 shows that the PDFs of c do not remain bimodal (in fact the PDFs are nearly monomodal in some instances for the cases considered here) and the probability of finding reacting mixture (i.e. $0.0 < c < 1.0$) remains significant for all locations irrespective of the value of $\tilde{c}$. The departure of the PDFs of c from the bimodal distribution with impulses at $c = 0.0$ and $c = 1.0$ provides the signature of low Damköhler number combustion (i.e. $Da_{(\phi_g)} < 1$) for the cases considered here. This suggests that combustion in these V-shaped flames takes place in the thickened flame regime and this behaviour is prominent for the case with initial $a_d/\delta_{st} = 0.06$, where local occurrences of flame thickening can be discerned from Fig. 2. Moreover, the appearance of the morphology of these V-flame surfaces has been found to be qualitatively similar to the

experimental visualisations of premixed V-flames in the thickened flame regime (Kheirkhah and Gulder, 2014). The turbulent Reynolds number remains moderate for all cases considered here. Moreover, turbulence decays within the flame and kinematic viscosity increases with increasing c as a result of temperature rise. This clearly suggests that the flame is weakly turbulent, and the effects of intermittency are expected to be prevalent in these flames. As a consequence, the internal flame structure remains quasi-laminar in nature but the combination of $Da < 1$ and weak turbulence suggests that the local occurrences of flame-front thickening takes place due to penetration of occasional turbulent eddies within the preheat zone and thus the preheat zone is perturbed, but the reaction zone remains quasi-laminar. This is consistent with the aforementioned Karlovitz number values suggesting the thin reaction zones regime combustion (Peters, 2000) in the cases considered here.

Figure 4. PDFs of c conditional on $\tilde{c} = 0.1, 0.5, 0.9$ at different locations A, B and C (top to bottom) for initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

It can be seen from Fig. 5 that the distance between $\tilde{c} = 0.1$ and 0.9 isosurfaces (i.e. $\delta_{T(0.1-0.9)}$) at a given x –location increases in the downstream direction from the flame holder, which is consistent with turbulent diffusion theory (Langevin, 1908; Taylor, 1922; Peters, 2000; Pope, 2000). This behaviour is qualitatively similar to turbulent premixed V-flame simulations (Kheirkhah and Gulder, 2014; Dunstan et al., 2011, 2012). The flame brush thickness $\delta_{T,\tilde{c}}$ at a given location can be quantified as:

$$\delta_{T,\tilde{c}} = 1/\max |\nabla \tilde{c}| \quad (14)$$

Alternatively, a flame brush thickness $\delta_{T,\bar{c}}$ can be defined as:

$$\delta_{T,\bar{c}} = 1/\max |\nabla \bar{c}| \quad (15)$$

Table 4. Flame brush thickness at locations A, B and C

Case	Gaseous premixed flame	$\frac{a_d}{\delta_{st}} = 0.04$	$\frac{a_d}{\delta_{st}} = 0.05$	$\frac{a_d}{\delta_{st}} = 0.06$
$\delta_{T(0.1-0.9)}/\delta_{st}$ at A	3.14	3.45	3.38	3.23
$\delta_{T(0.1-0.9)}/\delta_{st}$ at B	3.34	4.13	4.00	3.75
$\delta_{T(0.1-0.9)}/\delta_{st}$ at C	3.70	4.50	4.40	4.06
$\delta_{T,\tilde{c}}/\delta_{st}$ at A	3.04	3.50	3.33	3.18
$\delta_{T,\tilde{c}}/\delta_{st}$ at B	3.12	4.27	4.12	3.83
$\delta_{T,\tilde{c}}/\delta_{st}$ at C	3.35	4.79	4.97	4.35
$\delta_{T,\bar{c}}/\delta_{st}$ at A	2.47	2.82	2.69	2.72
$\delta_{T,\bar{c}}/\delta_{st}$ at B	2.34	3.28	3.12	3.09
$\delta_{T,\bar{c}}/\delta_{st}$ at C	2.37	3.84	3.62	3.45

The values of $\delta_{T(0.1-0.9)}/\delta_{st}$, $\delta_{T,\tilde{c}}/\delta_{st}$ and $\delta_{T,\bar{c}}/\delta_{st}$ are reported in Table 4 for locations A, B and C. It can be seen from Table 4 that the values of $\delta_{T,\tilde{c}}/\delta_{st}$ and $\delta_{T(0.1-0.9)}/\delta_{st}$ for the droplet cases remain close to each other but the value of $\delta_{T,\tilde{c}}/\delta_{st}$ remains smaller than $\delta_{T,\bar{c}}/\delta_{st}$ and $\delta_{T(0.1-0.9)}/\delta_{st}$. A comparison with the corresponding gaseous premixed flame indicates that the flame brush is thicker in droplet cases than in the premixed gaseous case. It has been shown

in Fig. 3 that spray flames experience considerable amount of fuel-lean (i.e. $\phi_g < 1.0$) mixture, and the flamelet thickness ($\sim \alpha_{T0}/S_b(\phi_g)$) is expected to be greater, whereas laminar burning velocity $S_b(\phi_g)$ is smaller than the corresponding values for the stoichiometric premixed flame. Thus, the spray flames experience higher values of turbulence intensity $u'/S_b(\phi_g)$ and are expected to show greater values of flamelet thickness and a combination of these gives rise to greater values of flame brush thickness in the spray flames than in the stoichiometric premixed flames, which can be substantiated from Table 4. It is worth noting that the evolution of turbulence (i.e. rms turbulent velocity and length scale) within the spray flames for different droplet sizes are likely to be different, which plays a role in determining the flame brush thickness (Meneveau and Poinso, 1991). For example, the decay of turbulence across the flame is likely to be less rapid for large droplets in comparison to small droplets because the effects of heat release are likely to be weaker due to burning of leaner mixtures. Therefore, the flame brush thickness for spray flames is not dictated only by the droplet diameter but also by the length scale and turbulence intensity within the flame brush, which is beyond the scope of this analysis. It is also worth noting that a premixed flame is not the limiting case of the small droplet diameter so it should not be expected that the premixed flame is going to follow the trend shown by the spray flames.

The change in the flame brush thickness in the flow direction indicates that the angles made by the tangent on the $\tilde{c} = 0.1, 0.5$ and 0.9 contours with the mean flow direction (i.e. x -direction) are expected to be different, which can also be verified from Table 5 where the angles $\theta_{\tilde{c}=0.1}$, $\theta_{\tilde{c}=0.5}$ and $\theta_{\tilde{c}=0.9}$ for $\tilde{c} = 0.1, 0.5$ and 0.9 isosurfaces are also listed for locations A, B and C. The angles $\theta_{\tilde{c}=0.1}$, $\theta_{\tilde{c}=0.5}$ and $\theta_{\tilde{c}=0.9}$ are evaluated by using the slope of the tangents at locations A, B and C on the contour lines of $\tilde{c} = 0.1, 0.5$ and 0.9 , as shown in Fig. 5b.

Figure 5. (a) Contours of $\tilde{c} = 0.1$ (solid line), 0.5 (dashed line) and 0.9 (dotted line) contours for gaseous premixed (—) case and droplet cases with initial droplet diameter $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—). The dashed purple lines show the sampling locations (A, B, C from left to right), and the dotted black line shows the flame centre, (b) Distributions of $\tilde{c}$ at the bottom half of the domain for initial $a_d/\delta_{st} = 0.04$ (1st row), 0.05 (2nd row) and 0.06 (3rd row). Black lines show the contour lines of $\tilde{c} = 0.1, 0.5$, and 0.9 from outer to the inner periphery and red lines are tangents to contour lines at locations A, B and C (left to right).

Table 5. Flame angle θ for $\tilde{c}$ isosurfaces

Case	Gaseous Premixed Flame	$\frac{a_d}{\delta_{st}} = 0.04$	$\frac{a_d}{\delta_{st}} = 0.05$	$\frac{a_d}{\delta_{st}} = 0.06$
Flame angle $\theta_{\tilde{c}=0.1}$ for $\tilde{c} = 0.1$ at A	16.06 °	20.47°	20.42°	18.88 °
Flame angle $\theta_{\tilde{c}=0.1}$ for $\tilde{c} = 0.1$ at B	13.56 °	15.76°	16.12°	14.80 °
Flame angle $\theta_{\tilde{c}=0.1}$ for $\tilde{c} = 0.1$ at C	17.12 °	15.46 °	16.58°	17.00 °
Flame angle $\theta_{\tilde{c}=0.5}$ for $\tilde{c} = 0.5$ at A	14.66 °	14.66°	14.49°	11.72°
Flame angle $\theta_{\tilde{c}=0.5}$ for $\tilde{c} = 0.5$ at B	7.21 °	12.07°	12.06°	15.44°
Flame angle $\theta_{\tilde{c}=0.5}$ for $\tilde{c} = 0.5$ at C	10.95 °	13.04°	14.37°	14.99 °
Flame angle $\theta_{\tilde{c}=0.9}$ for $\tilde{c} = 0.9$ at A	13.46 °	9.82°	11.20°	11.62°
Flame angle $\theta_{\tilde{c}=0.9}$ for $\tilde{c} = 0.9$ at B	10.57 °	9.31°	9.96°	9.49°
Flame angle $\theta_{\tilde{c}=0.9}$ for $\tilde{c} = 0.9$ at C	10.54 °	9.62°	10.22°	12.18°

It can be seen from Fig. 5 that the contours of $\tilde{c}$ are mildly curved for the cases considered here. However, this trend weakens with increasing $\tilde{c}$ value, which can be substantiated from $\theta_{\tilde{c}=0.1}$, $\theta_{\tilde{c}=0.5}$, $\theta_{\tilde{c}=0.9}$ values listed in Table 5. The flame angle $\theta_{\tilde{c}=0.9}$ for droplet cases is found to be smaller than that for the gaseous premixed case, whereas the flame angle $\theta_{\tilde{c}=0.1}$ for droplet cases remains larger than that for the gaseous premixed case at most locations. These differences originate as a result of the differences in flame brush thicknesses reported in Table 4, which in turn originate due to the differences between the composition of the gaseous mixture within the flame and the evolution characteristics of turbulence within the flame brush. It can be seen from Table 5 that $\theta_{\tilde{c}=0.1}$ changes appreciably with the axial distance and a similar qualitative trend is observed for $\theta_{\tilde{c}=0.5}$ but the variation of $\theta_{\tilde{c}=0.5}$ in the axial distance is much weaker than $\theta_{\tilde{c}=0.1}$. Moreover, $\theta_{\tilde{c}=0.9}$ does not change much in the axial direction for the cases considered here. In order to explain this behaviour, the PDFs of ϕ_g on $\tilde{c} = 0.1, 0.5$ and 0.9 isosurfaces at different axial locations are shown in Fig. 6. It is evident from Fig. 6 that the PDFs of ϕ_g are considerably different for different droplet diameters with higher probabilities of finding fuel-lean mixture for bigger droplet diameters. However, Fig. 6 shows that the mean value of ϕ_g increases in the downstream direction but the difference in the PDFs of ϕ_g

decreases with increasing $\tilde{c}$, and with the axial distance because of the increased extents of droplet evaporation. Thus, the increase in the mean value of ϕ_g in the downstream direction is most prominent for $\tilde{c} = 0.1$, which gives rise to its curved contours and relatively significant variations of $\theta_{\tilde{c}=0.1}$ in the axial direction. Figure 6 reveals that the mean ϕ_g values for $\tilde{c} = 0.9$ contours do not change appreciably in the downstream direction and therefore the contours of $\tilde{c} = 0.9$ remain straight for the cases considered here. Moreover, the gaseous equivalence ratio ϕ_g values remain comparable for $\tilde{c} = 0.5$ and 0.9 for different droplet diameters and therefore these contours almost coincide with each other for different values of a_d/δ_{st} . It is worth noting that the variation of the PDFs shown in Fig. 6 in the flow direction remains weaker than that in Fig. 3. In Fig. 6, the PDFs of ϕ_g are shown for a given $\tilde{c} = \bar{\rho}^{-1} \int_0^{1.0} \rho c P(c) dc$ isosurfaces where $P(c)$ is the PDF of c and $\bar{\rho}$ is the mean density. Thus ϕ_g from different c values contribute to this and the gaseous phase equivalence ratio ϕ_g values for small values of c are expected to be small. Consequently, the PDFs of ϕ_g from locations A to C in Fig. 6 do not change as much as the PDFs in Fig. 3 change from the location A to location C.

The flame angles and flame brush thicknesses are dependent on the reacting mixture composition in the gaseous phase, flame wrinkling and flame propagation rates. Thus, it is worthwhile to examine the statistical behaviours of gaseous equivalence ratio ϕ_g , flame curvature κ_m , mode of combustion and local consumption and density-weighted displacement speeds (i.e. S_c and S_d^*).

Figure 6. PDFs of ϕ_g conditional on $\tilde{c} = 0.1, 0.5, 0.9$ isosurfaces at different locations A, B and C (top to bottom) for initial $\alpha_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

The presence of droplets significantly affects the flame morphology and induces flame wrinkling due to flame-droplet interaction (Lawes and Saat, 2011). In order to understand the flame-droplet interaction, the instantaneous views of $c = 0.5$ isosurfaces, coloured by local values of flame curvature $\kappa_m \times \delta_{st}$ for all cases considered here are shown in Fig. 7. The local curvature κ_m is defined as $\kappa_m = \nabla \cdot \vec{N}/2$ where $\vec{N} = -\nabla c/|\nabla c|$ is the local flame normal vector. According to these definitions, an element of the flame surface, which is convex (concave) to the reactants, has a positive (negative) curvature and the flame normal vector points towards the reactants. It can be seen from Fig. 7 that the flame surface remains smooth for the gaseous premixed flame case, and also for the droplet case with small droplets, which evaporate rapidly ahead of the flame and do not significantly interact with the flame surface. By contrast, the flame surfaces are significantly affected by large droplets and exhibit dimples

in addition to the flame wrinkles induced by the turbulent flow field. The occurrences of flame-droplet interaction events increase in the downstream direction for larger droplets because they can survive longer in the domain due to their lower evaporation rate and bigger size.

Figure 7. Instantaneous views of $c = 0.5$ isosurface coloured with $\kappa_m \times \delta_{st}$ values for gaseous premixed and spray flames with initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ at $t = 2.0t_{flow}$.

Figure 8. PDFs of $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface at locations A, B and C (top to bottom) for gaseous premixed (—) and V-shaped spray flames with initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

The PDFs of local normalised flame curvature $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface at different planes (i.e. A, B and C) for all droplet cases and the gaseous premixed flame case considered in this study are shown in Fig. 8. The $c = 0.8$ isosurface has been chosen because the reaction rate of progress variable attains its maximum value close to this value of c for the present thermo-chemistry (Ozel-Erol et al., 2018) and thus this isosurface will henceforth be considered

to be the flame surface in this analysis. However, the PDFs of local normalised flame curvature $\kappa_m \times \delta_{st}$ for other reaction progress variable isosurfaces remain qualitatively similar to the $c = 0.8$ isosurface. The PDFs of $\kappa_m \times \delta_{st}$ peak at around zero value and show similar widths for all droplet cases at locations A, B and C. However, the width on the PDF of $\kappa_m \times \delta_{st}$ marginally increases with increasing a_d/δ_{st} , which bears the signature of droplet-induced flame wrinkling for larger droplets. This behaviour is consistent with previous computational findings for spherically expanding spray flames (Ozel-Erol et al., 2018) for weak turbulence intensities. Furthermore, a comparison between gaseous premixed and droplet cases reveals that PDFs of $\kappa_m \times \delta_{st}$ for spray flames have a wider distribution at planes A and B where droplet-flame interactions mainly occur. However, the difference in the distributions of $\kappa_m \times \delta_{st}$ between spray and gaseous premixed flame cases decreases in the flow direction because droplets increasingly evaporate in the axial direction and flame-droplet interaction becomes less frequent. The differences in the widths of $\kappa_m \times \delta_{st}$ PDFs are consistent with the differences in flame brush thicknesses for different droplets.

The mode of combustion in these flames can be characterised by the flame index $FI = (\nabla Y_F \cdot \nabla Y_O) / (|\nabla Y_F| |\nabla Y_O|)$ (Yamashita et al., 1996) so that a positive value of FI indicates a premixed mode of combustion, whereas a negative flame index FI indicates a non-premixed mode of combustion. The percentages of heat release rate arising from premixed and non-premixed modes of combustion are demonstrated in Fig. 9 for all droplet cases considered here at locations A, B and C. Figure 9 indicates that for all cases heat release mostly takes place under premixed mode at all locations. Thus, the gaseous phase combustion in these cases takes place mostly in stratified mixtures. However, it can be discerned from Fig. 9 that the percentage of overall heat release due to non-premixed combustion is greater in extent in the case with initial $a_d/\delta_{st}=0.06$ than the corresponding cases with initial $a_d/\delta_{st} = 0.04$ and 0.05 . A careful

examination of Fig. 3 reveals that there is a small peak at $\phi_g = 1.0$ in the PDFs of ϕ_g for the initial $a_d/\delta_{st}=0.06$ case, which originates due to non-premixed mode of combustion. Due to slow evaporation rate of large droplets the initial $a_d/\delta_{st}=0.06$ case gives rise to higher likelihood of obtaining local islands of high and low fuel concentration than the other corresponding cases with smaller droplets, and this gives rise to the strengthening of non-premixed mode of combustion in the case of large droplets (e.g. cases with initial $a_d/\delta_{st}=0.06$). A small number of droplets in the case of large droplet diameter (e.g. cases with initial $a_d/\delta_{st}=0.06$). escape through the flame due to turbulent motion and complete the evaporation in the high temperature zone in the region with $c = 1.0$. Some of these unburned fuel-pockets eventually diffuse into the flame and mix with the air diffusing from the unburned gas side to give rise to local diffusion mode of burning.

Figure 9. Percentage of heat release arising from premixed (for initial $a_d/\delta_{st}=0.04$ (■), 0.05 (■), 0.06 (■)) and non-premixed (for initial $a_d/\delta_{st}=0.04$ (■), 0.05 (■), 0.06 (■)) modes of combustion at locations A, B and C (left to right).

As the heat release takes place predominantly under the premixed mode, it is necessary to analyse the flame propagation statistics for the flames considered here. For this reason, it is worthwhile to analyse the terms on the right-hand side of the transport equation of the reaction

progress variable c (see Eq. 7), as they govern the statistical behaviours of density-weighted displacement speed S_d^* . The mean values of the terms $\dot{w}_c$, $\dot{S}_{liq,c}$, $\dot{A}_c$ and $\nabla \cdot (\rho D \nabla c)$ conditional on c for locations A, B and C are shown in Fig. 10. The terms contributing the flame displacement speed S_d are ensemble averaged for a given value of c for 30 equally spaced bins of c between 0.01 and 0.99, and these values are subsequently time-averaged before presenting in Fig. 10. The same approach was adopted in several previous analyses (Boger et al., 1998; Chakraborty, 2007; Chakraborty and Cant, 2004,2005; Neophytou et al., 2010; 2012; Wacks et al., 2016).

Figure 10 suggests that the mean molecular diffusion term $\nabla \cdot (\rho D \nabla c)$ takes positive values in the preheat zone (i.e. $c < 0.5$), whereas it assumes negative values and remains in approximate balance with the positive mean value of $\dot{w}_c$ in the reaction zone (i.e. $0.5 \leq c \leq 0.9$) for both gaseous premixed and spray V-shaped flames. It is evident from Fig. 10 that the mean values of $\dot{w}_c$ for droplets cases are smaller than the gaseous premixed case. This trend originates due to slower burning of stratified mixtures with $\phi_g < 1.0$ and $\phi_g > 1.0$ in the droplet cases than in the stoichiometric (i.e. $\phi_g = 1.0$) premixed flame. The mean values of $\dot{w}_c$ decreases with increasing droplet diameter due to the increased propensity of fuel-lean burning in the gaseous phase. Furthermore, the mean values for all terms show similar trends at locations A, B, C for all droplet diameters. The mean values of the terms arising due to droplet evaporation $\dot{S}_{liq,c}$ and mixture inhomogeneity $\dot{A}_c$ remain much smaller in magnitude in comparison to the magnitudes of the mean values of $\dot{w}_c$ and $\nabla \cdot (\rho D \nabla c)$ throughout the flame, which is consistent with previous findings for statistically planar (Wacks et al., 2016) and spherically expanding (Ozel-Erol et al., 2019) flames. It can further be seen from Fig. 10 that the mean value of $\rho S_d |\nabla c| = [\nabla \cdot (\rho D \nabla c) + \dot{w}_c + \dot{S}_{liq,c} + \dot{A}_c]$ remains smaller than the mean value of $\rho_0 S_{b,st} |\nabla c|$ for all

cases considered here in spite of having an overall equivalence ratio of unity (i.e. $\phi_{ov} = 1.0$) in the unburned gas. This suggests that the surface-weighted value of density-weighted displacement speed (i.e. ratio of averaged/filtered values of $S_d^*|\nabla c|$ and $|\nabla c|$) (Trouvé and Poinso, 1994; Boger et al., 1998) in all cases remains smaller than $S_{b,st}$ due to the predominance of the fuel-lean mixture within the flame in spite of having $\phi_{ov} = 1.0$ in the unburned gas. Figure 10 also reveals that the mean value of $\rho_0 S_{b,st}|\nabla c|$ decreases with increasing droplet diameter. The inverse of the maximum mean value of $|\nabla c|$ provides a measure of the flamelet thickness (i.e. $\delta \sim 1/\max|\nabla c|$) at a given location. The smaller peak mean value of $\rho_0 S_{b,st}|\nabla c|$ for larger droplets indicates a thicker flame because $\rho_0 S_{b,st}$ remains the same for all cases. As the probability of finding fuel-lean mixture increases for larger droplets, the small values of $S_{b(\phi_g)}$ are more likely for larger droplets and accordingly flamelet thickness (which scales as $\delta \sim \alpha_{T0}/S_{b(\phi_g)}$) increases with increasing droplet diameter. Thus, the occurrences of local flame thickening for large values of a_d/δ_{st} in Fig. 2 is consistent with the observations regarding local flame thickening for large droplets.

Figure 10. Variations of mean values of w_c (solid line), $\nabla \cdot (\rho D \nabla c)$ (line with star marker), $\bar{A}_c$ (dotted line), $\dot{S}_{liq,c}$ (triangle marker), $\rho S_d |\nabla c|$ (dashed line) and $\rho_0 S_{b,st} |\nabla c|$ (circle) conditional on c for premixed gaseous (—) and droplet cases with initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—) at locations A, B, C (top to bottom). All terms are normalised by $\delta_{st}/\rho_0 S_{b,st}$.

The aforementioned behaviours of $\nabla \cdot (\rho D \nabla c)$, w_c , $\dot{S}_{liq,c}$, $\bar{A}_c$ affect the statistical behaviours of

S_d^* , whereas $\dot{w}_c$ and the flame thickness determine the behaviour of consumption speed S_c . The normalised mean values of consumption speed $S_c/S_{b,st}$ and $S_c/S_{b(\langle\phi_g\rangle)}$ and density-weighted displacement speed, $S_d^*/S_{b,st}$ and $S_d^*/S_{b(\langle\phi_g\rangle)}$ evaluated on the $c = 0.8$ isosurface at locations A, B and C are shown in Fig. 11 where $\langle\phi_g\rangle$ is the averaged equivalence ratio on the $c = 0.8$ isosurface at this location and $S_{b(\langle\phi_g\rangle)}$ is the laminar burning velocity corresponding to $\langle\phi_g\rangle$. As the consumption speed S_c is directly dependent on $\dot{w}_c$, the mean values of $S_c/S_{b,st}$ show a qualitatively similar trend as the mean values of $\dot{w}_c$. Therefore, the mean values of consumption speed for the gaseous premixed V-shaped flame case assume considerably greater values than those for droplet cases. However, the mean values of $S_d^*/S_{b,st}$ remain different from the mean values of $S_c/S_{b,st}$ due to the combined influences of $\dot{S}_{liq,c}$, $\dot{A}_c$, $\nabla \cdot (\rho D \nabla c)$ and $\dot{w}_c$ (but predominantly due to $\nabla \cdot (\rho D \nabla c)$ and $\dot{w}_c$). The mean values of $S_d^*/S_{b,st}$ for a given value of a_d/δ_{st} remain comparable at locations A, B and C but slight variations can be discerned between the mean values corresponding to these locations. The mean values of $S_d^*/S_{b,st}$ remain close to unity for the gaseous premixed case. Moreover, the mean values of $S_c/S_{b,st}$ show decreasing trends with increasing a_d/δ_{st} because of the greater likelihood of obtaining fuel-lean mixtures for larger droplets (see Figs. 3 and 6).

Another alternative way to present the mean values of consumption and density-weighted displacement speeds is to normalise them with respect to the laminar burning velocity $S_{b(\langle\phi_g\rangle)}$ for the mean equivalence ratio $\langle\phi_g\rangle$ within the flame. However, the value of $S_{b(\langle\phi_g\rangle)}$ changes from one location to another and therefore, the relative magnitudes of S_c and S_d^* cannot be assessed from the values of $S_c/S_{b(\langle\phi_g\rangle)}$ and $S_d^*/S_{b(\langle\phi_g\rangle)}$. The values of $S_{b(\langle\phi_g\rangle)}$ remain smaller than $S_{b,st}$ for all the droplet cases considered here and this tendency is most prominent for large droplet diameters (e.g. initial droplet size of $a_d/\delta_{st} = 0.06$). This can be seen from the wider

PDFs of ϕ_g with increasing a_d/δ_{st} in Figs. 3 and 6, and therefore the probability of obtaining burning more reactive $\phi_g(\approx 1.0) > \langle \phi_g \rangle$ mixture increases with increasing droplet size in the droplet cases. This leads to increasing trends of $S_c/S_{b(\langle \phi_g \rangle)}$ and $S_d^*/S_{b(\langle \phi_g \rangle)}$ with increasing a_d/δ_{st} in contrast to the variations of $S_c/S_{b,st}$ and $S_d^*/S_{b,st}$, and this behaviour is more prominent at location A than in locations B and C since the leaner combustion yields small laminar burning velocities at location A.

Table 6. Time averaged normalised values of $A_s = \int_V |\nabla c| dV$, $A_{p,\tilde{c}}, \Omega_f = \int_V |\dot{w}_F| dV / \rho_0 \delta_{st}^2 S_{b,st}$, $S = \int_V \dot{w}_c dV / [\rho_0 S_{b,st} \int_V |\nabla c| dV]$ and $S' = \int_V \dot{w}_c dV / [\rho_0 S_{b(\phi_f)} \int_V |\nabla c| dV]$.

a_d/δ_{st}	Gaseous Premixed Flame	0.04	0.05	0.06
A_s/δ_{st}^2	1797	1722	1684	1708
$A_{p,\tilde{c}=0.1}/\delta_{st}^2$	1600	1494	1499	1498
$A_{p,\tilde{c}=0.5}/\delta_{st}^2$	1495	1404	1408	1413
$A_{p,\tilde{c}=0.9}/\delta_{st}^2$	1432	1350	1354	1358
Ω_f	118	75	68	58
S	1.06	0.77	0.71	0.60
S'	1.00	1.00	1.11	1.41

The time-averaged values of flame surface area A_s , the normalised volume integrated fuel reaction rate magnitude Ω_f (the volume integrated reaction progress variable reaction rate $\Omega_c = \int_V \dot{w}_c dV / \rho_0 \delta_{st}^2 S_{b,st}$ shows the same qualitative trend and thus is not shown here) and the normalised ratio of volume-integrated product formation rate to the flame surface area $S = \int_V \dot{w}_c dV / [\rho_0 S_{b,st} \int_V |\nabla c| dV]$ are listed in Table 6, which shows that A_s remains comparable for all cases with different initial droplet diameter. The probability of finding smaller values of $|\nabla c|$ is greater in the case with initial $a_d/\delta_{st} = 0.05$ than in the case with initial $a_d/\delta_{st} = 0.04$, which contributes to the smaller flame surface area A_s for the initial $a_d/\delta_{st} = 0.05$ case than

that in the $a_d/\delta_{st} = 0.04$ case. Although the probability of finding smaller values of $|\nabla c|$ is greater in the case with initial $a_d/\delta_{st} = 0.06$ than in the case with initial $a_d/\delta_{st} = 0.05$ but the larger droplets in the initial $a_d/\delta_{st} = 0.06$ case lead to more flame-wrinkling and increase the total flame volume to yield a flame area which is greater than that in the initial $a_d/\delta_{st} = 0.05$ case but still smaller than in the initial $a_d/\delta_{st} = 0.04$ case considered here. Furthermore, the time-averaged flame surface area of gaseous premixed V-shaped flame remains slightly larger than those for droplet cases.

Figure 11. The mean values of $S_c/S_{b,st}$, $S_d^*/S_{b,st}$, $S_c/S_{b((\phi_g))}$ and $S_d^*/S_{b((\phi_g))}$ on the $c = 0.8$ isosurface at locations A-C.

The time-averaged value of Ω_f decreases with increasing a_d/δ_{st} as the probability of fuel-lean

combustion increases with increasing droplet size, which is consistent with the decreasing trend of the mean values of $\dot{w}_c$ with increasing a_d (see Fig. 10). The integral $\int_V \dot{w}_c dV$ can be expressed as: $\int_V \dot{w}_c dV \approx \rho_0 S_c A_s$ and therefore $S_c < S_{b,st}$ from Fig. 11 implies that $S = \int_V \dot{w}_c dV / [\rho_0 S_{b,st} \int_V |\nabla c| dV]$ is expected to be smaller than unity for the cases considered here. The reduction of $\int_V \dot{w}_c dV$ dominates over the increase in flame surface area A_s for large droplets and ultimately gives rise to a decreasing trend of S with increasing a_d , which is also consistent with the decreasing trends of $S_c/S_{b,st}$ with increasing a_d/δ_{st} . It can be seen from Table 6 that the ratio S stays close to unity for the gaseous premixed V-shaped flame, since the mean values of $\dot{w}_c + \nabla \cdot (\rho D \nabla c)$ and $\rho_0 S_{b,st} |\nabla c|$ remain close to each other (see Fig. 10).

It has been demonstrated in Fig. 9 that most of the heat release in these flames takes place due to the premixed mode of combustion. These flames were previously referred to as premixed sprays by Mizutani and Nishimoto (1972) and Silverman et al. (1993). It has been demonstrated in several previous analyses that the equality between the enhancements of burning rate and flame surface area in turbulent premixed flames with respect to their laminar counterparts (which is commonly referred to as Damköhler's first hypothesis) remains valid for statistically planar turbulent premixed flames even for the thickened flame regimes (i.e. for small (large) values of Damköhler (Karlovitz) number) (Aspden et al., 2011; Nivarti and Cant, 2017; Ahmed et al., 2019) even though Damköhler's first hypothesis (Damköhler, 1941) was originally proposed for large values of Damköhler number (i.e. $Da \gg 1$). As the combustion in these spray flames takes place in the thickened flame regime, it is worthwhile to assess if Damköhler's first hypothesis remains valid for these flames.

Figure 10 implies that the mean value of $[\dot{S}_{liq,c} + \dot{A}_c]$ remains much smaller than the mean

value of $\rho_0 S_d^* |\nabla c|$. As $\int_V \nabla \cdot (\rho D \nabla c) dV = 0$, the integral $\int_V \dot{w}_c dV$ can be approximated as:

$$\int_V \dot{w}_c dV \approx \sum \langle \rho S_d |\nabla c| | c = c^* \rangle V_{c=c^*} \quad (18)$$

where $\langle Q | c = c^* \rangle$ is the mean value of a general quantity Q conditional upon $c = c^*$ and $V_{c=c^*}$ is the volume of the samples corresponding to $c = c^*$. It can be seen from Fig. 10 that the mean value of $\rho S_d |\nabla c|$ remains smaller than $\rho_0 S_{b,st} |\nabla c|$ which leads to $S < 1.0$ for all cases. According to Damköhler's first hypothesis (Damköhler, 1940), the enhancements of burning rate and flame surface under turbulence are proportional to each other, which implies a unity value of S (i.e. $S = 1.0$) (Chakraborty *et al.*, 2019). Thus, the non-unity values of S indicate a departure from Damköhler's first hypothesis and suggest that Damköhler's first hypothesis in its original form is not valid for turbulent spray flames. It can further be seen from Table 6 that S remains smaller than unity for all the droplet cases but $S' = \int_V \dot{w}_c dV / [\rho_0 S_{b(\phi_f)} \int_V |\nabla c| dV]$ (where ϕ_f is the volume-averaged gaseous phase equivalence ratio in the region corresponding to $0.01 \leq c \leq 0.99$) values are closer to unity and greater than the value of $S = \int_V \dot{w}_c dV / [\rho_0 S_{b,st} \int_V |\nabla c| dV]$ because $S_{b(\phi_f)} / S_{b,st}$ remains smaller than unity. However, Table 6 suggests that the departure of S' from 1.0 can also be significant for the large droplets (e.g. initial droplet size of $a_d / \delta_{st} = 0.06$), and thus the conclusions regarding Damköhler's first hypothesis in its original form do not change if S' is used.

It is possible to define a turbulent burning velocity S_T as: $S_T = \int_V \dot{w}_c dV / (\rho_0 A_{p,\tilde{c}}) = S(A_s / A_{p,\tilde{c}}) S_{b,st}$ where $A_{p,\tilde{c}}$ is the flame area of the $\tilde{c}$ isosurface with respect to which S_T is evaluated. The values of $A_{p,\tilde{c}=0.1}$, $A_{p,\tilde{c}=0.5}$ and $A_{p,\tilde{c}=0.9}$ for the cases considered here are listed in Table 6. It is evident from Table 6 that A_s and $A_{p,\tilde{c}}$ assume comparable values for different values of a_d and thus a decreasing trend of S with increasing droplet diameter gives rise to a

reduction in turbulent burning velocity S_T with an increase in droplet diameter. This can be substantiated from Table 7 where $S_T/S_{b,st}$ for the $\tilde{c} = 0.1$ and 0.5 isosurfaces are presented. It is also worth noting that $S_T/S_{b,st}$ remains smaller than unity (i.e. $S_T/S_{b,st} < 1.0$) for the droplet cases considered here but it should be considered that the normalised laminar burning velocity $S_{b(\langle\phi_g\rangle)}/S_{b,st}$ for the mean gaseous phase equivalence ratio ranges between 0.78-0.83, 0.67-0.76, 0.47-0.57 between locations A to C (with higher value at location C) for initial values of $a_d/\delta_{st} = 0.04, 0.05$ and 0.06, respectively. This suggests that $S_T/S_{b(\langle\phi_g\rangle)}$ remains greater than unity for all cases as given in Table 7 and thus the overall burning rate gets enhanced under turbulence and this augmentation is the most prominent for the case with the largest droplets as this case experiences the largest value of $S_T/S_{b(\langle\phi_g\rangle)}$ among the flames considered here. It can be seen from Table 7 that turbulent burning velocity S_T for the gaseous stoichiometric turbulent premixed flame assumes values greater than the corresponding laminar burning velocity (i.e. $S_T/S_{b,st} > 1.0$). This further suggests that the values of $S_T/S_{b,st}$ for spray V-flames are smaller than the corresponding turbulent premixed gaseous flame and $S_T/S_{b,st}$ decreases with increasing droplet diameter.

Table 7. Turbulent burning velocity S_T based on the surface area for $\tilde{c} = 0.1$ and 0.5 isosurfaces

a_d/δ_{st}	Gaseous Premixed Flame	0.04	0.05	0.06
$S_{T,\tilde{c}=0.1}/S_{b,st}$	1.19	0.88	0.80	0.69
$S_{T,\tilde{c}=0.1}/S_{b,\langle\phi_g\rangle,A}$	-	1.13	1.19	1.47
$S_{T,\tilde{c}=0.1}/S_{b,\langle\phi_g\rangle,B}$	-	1.10	1.13	1.30
$S_{T,\tilde{c}=0.1}/S_{b,\langle\phi_g\rangle,C}$	-	1.06	1.05	1.21
$S_{T,\tilde{c}=0.5}/S_{b,st}$	1.27	0.94	0.85	0.73
$S_{T,\tilde{c}=0.5}/S_{b,\langle\phi_g\rangle,A}$	-	1.21	1.27	1.55
$S_{T,\tilde{c}=0.5}/S_{b,\langle\phi_g\rangle,B}$	-	1.18	1.20	1.38
$S_{T,\tilde{c}=0.5}/S_{b,\langle\phi_g\rangle,C}$	-	1.13	1.12	1.28

5. CONCLUSIONS

The mode of combustion, droplet-induced flame wrinkling, mean behaviours of different terms of the reaction progress variable transport equation, and flame propagation statistics for V-shaped flames in a droplet-laden mixture of an overall (i.e. liquid+gaseous) equivalence ratio of unity have been investigated for different droplet diameters using three-dimensional DNS data. The flame behaviour has been compared with a turbulent gaseous stoichiometric premixed V-shaped flame under same flow conditions. It has been found that the flame brush thickness is affected by both droplet diameter and the axial distance from the flame holder and it increases with decreasing droplet diameter and with increasing axial distance. Furthermore, the flame brush has been found to be thicker in droplet cases than in the corresponding gaseous premixed flame case. The predominance of finding fuel-lean mixture within the flame decreases in the downstream direction due to evaporation of droplets and this effect is particularly strong for large droplets. The interaction of droplets with the flame surface gives rise to dimples on the reaction progress variable isosurfaces. However, droplet-induced flame wrinkling contributes to the widening of flame curvature PDFs, and also acts to increase the total flame surface area for large droplets. The mean values of the reaction rate of progress variable decrease with increasing droplet diameter. Furthermore, the mean value of the reaction rate of progress variable for a given droplet diameter shows similar magnitudes at different axial locations for all droplet cases. A similar qualitative trend has been observed for the axial distance dependences of the mean values of consumption speed and density-weighted displacement speed for a given value of droplet diameter. The mean values of consumption speed are found to decrease with increasing droplet diameter because of the greater likelihood of fuel-lean combustion in large droplet cases. By contrast, the mean density-weighted displacement speed remains comparable for all the droplet sizes considered here. Recent DNS analyses in statistically planar flames (Wacks et al., 2016) and spherically expanding flames (Ozel-Erol et

al., 2018,2019) under both laminar and weakly turbulent conditions revealed significant differences in flame curvature, density-weighted displacement speed and consumption speed in response to droplet diameter, whereas the effects of droplet diameter are relatively weaker in V-flames than in statistically planar and spherically expanding flames. For the cases with globally stoichiometric equivalence ratio (Ozel-Erol et al., 2019), the mean values of density-weighted displacement speed were found to exhibit a mild increase with the increasing droplet diameter whereas the mean values of consumption speed showed a decreasing trend with the increasing droplet diameter. The statistically planar and spherically expanding flames interact with droplets at all stages of their propagation into the unburned gas (Wacks et al., 2016; Ozel-Erol et al., 2018,2019) but in turbulent V-spray flames, the droplets evaporate in the mean flow direction. Therefore, the frequency of flame-droplet interaction decreases and the mean value of ϕ_g increases in the downstream direction.

It has been demonstrated that in turbulent droplet-laden V-shaped flames, the enhancement of burning rate under turbulence cannot be equated to the enhancement of the flame surface area with respect to the corresponding quantities under laminar conditions. Moreover, the turbulent burning velocity has been found to decrease with increasing droplet diameter due to the reduction in the volume-integrated reaction rate of reaction progress variable as a result of the greater likelihood of finding fuel-lean gaseous mixture for larger droplets. Although several previous analyses revealed that the flame speed statistics for turbulent premixed flames obtained from simple chemistry (Chakraborty and Cant, 2004, 2005; Chakraborty, 2007) remain in good agreement with the corresponding results obtained from a detailed chemical mechanism (Peters et al., 1998; Echekki and Chen, 1999), further analyses in the presence of a detailed chemical mechanism will be necessary for confirming the current findings and obtaining more comprehensive physical understanding regarding the roles played by the

intermediate species. The distance of the flame holder from the inlet can also potentially have an influence on the results, but the gaseous phase equivalence ratio remains small for the x -locations before the flame holder and thus it can reasonably be expected that the qualitative nature of the results are unlikely to change with the variation of the distance of the flame holder from the inlet. However, further study in this respect will be necessary. The aforementioned challenges will form the basis of future investigations.

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FIGURE CAPTIONS

Figure 1. Variations of the (a) normalised laminar burning velocity $S_b(\phi_g)/\{S_b(\phi_g)\}_{max}$ and (b) normalised adiabatic flame temperature $T_b(\phi_g) = (T_{ad}(\phi_g) - T_0)/(T_{ad}(\phi_{g=1}) - T_0)$ with equivalence ratio ϕ_g for n-heptane obtained from modified single step chemistry (Tarrazo et al., 2006), detailed chemical mechanism (Chaos et al., 2007) and experimental (Kumar et al., 2007) data.

Figure 2. Instantaneous distributions of (a). reaction progress variable, c and (b). gaseous equivalence ratio, ϕ_g on the central x-y midplane for initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ at $t = 2.0t_{flow}$. Blue lines show $c = 0.1, 0.5$ and 0.9 contours from outer to the inner periphery and grey dots show the droplets residing on the plane (not to the scale).

Figure 3. PDFs of ϕ_g in the region corresponding to $0.01 \leq c \leq 0.99$ at different locations A, B and C (top to bottom) for initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

Figure 4. PDFs of c conditional on $\tilde{c} = 0.1, 0.5, 0.9$ at different locations A, B and C (top to bottom) for initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

Figure 5. (a) Contours of $\tilde{c} = 0.1$ (solid line), 0.5 (dashed line) and 0.9 (dotted line) contours for gaseous premixed (—) case and droplet cases with initial droplet diameter $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—). The dashed purple lines show the sampling locations (A, B, C from left to right), and the dotted black line shows the flame centre, (b) Distributions of $\tilde{c}$ at the bottom half of the domain for initial $a_d/\delta_{st} = 0.04$ (1st row), 0.05 (2nd row) and 0.06 (3rd row). Black lines show the contour lines of $\tilde{c} = 0.1, 0.5$, and 0.9 from outer to the inner periphery and red lines are tangents to contour lines at locations A, B and C (left to right).

Figure 6. PDFs of ϕ_g conditional on $\tilde{c} = 0.1, 0.5, 0.9$ isosurfaces at different locations A, B and C (top to bottom) for initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

Figure 7. Instantaneous views of $c = 0.5$ isosurface coloured with $\kappa_m \times \delta_{st}$ values for gaseous

premixed and spray flames with initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ at $t = 2.0t_{flow}$.

Figure 8. PDFs of $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface at locations A, B and C (top to bottom) for gaseous premixed (—) and spray V-shaped spray flames with initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—).

Figure 9. Percentage of heat release arising from premixed (for initial $a_d/\delta_{st}=0.04$ (■), 0.05 (■), 0.06 (■)) and non-premixed (for initial $a_d/\delta_{st}=0.04$ (■), 0.05 (■), 0.06 (■)) modes of combustion at locations A, B and C (left to right).

Figure 10. Variations of mean values of $\dot{w}_c$ (solid line), $\nabla \cdot (\rho D \nabla c)$ (line with star marker), $\dot{A}_c$ (dotted line), $\dot{S}_{liq,c}$ (triangle marker), $\rho S_d |\nabla c|$ (dashed line) and $\rho_0 S_{b,st} |\nabla c|$ (circle) conditional on c for premixed gaseous (—) and droplet cases with initial $a_d/\delta_{st} = 0.04$ (—), 0.05 (—) and 0.06 (—) at locations A,B, C (top to bottom). All terms are normalised by $\delta_{st}/\rho_0 S_{b,st}$.

Figure 11. The mean values of $S_c/S_{b,st}$, $S_d^*/S_{b,st}$, $S_c/S_{b(\langle \phi_g \rangle)}$ and $S_d^*/S_{b(\langle \phi_g \rangle)}$ on the $c = 0.8$ isosurface at locations A-C.