A numerical investigation of the minimum ignition energy requirement for forced ignition of turbulent droplet-laden mixtures

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ABSTRACT
The effects of droplet diameter, overall (i.e. liquid and gaseous phases) equivalence ratio, and turbulence intensity on the variation of the Minimum Ignition Energy (MIE) for localised forced ignition of uniformly dispersed mono-sized n-heptane droplet-laden mixtures under homogeneous isotropic decaying turbulence have been analysed based on Direct Numerical Simulation (DNS) data. The MIE was evaluated just for (i) obtaining thermal runway irrespective of the fate of the resulting flame kernel, and (ii) also for successful self-sustained flame propagation without the assistance of an external energy source following the energy deposition by the ignitor. It has been found that the MIE requirement increases with increasing turbulence intensity and this trend for the MIE increase is especially significant for large values of turbulence intensity. The MIE requirement increases with increasing initial droplet diameter and with decreasing overall equivalence ratio. The MIE requirements for droplet-laden mixtures have been found to be greater than the corresponding value for homogeneous mixture with same nominal values of initial turbulence intensity and equivalence ratio. This behaviour arises due to the deposited energy being partially utilised to supply the latent heat of evaporation and also due to the predominantly fuel-lean composition of the gaseous flammable mixture. This tendency of obtaining fuel-lean mixture strengthens with increasing (decreasing) initial droplet diameter (overall equivalence ratio). It has also been demonstrated that combustion takes place predominantly in the fuel-lean premixed mode although there is a finite probability of having non-premixed combustion in all cases. Moreover, there is a small probability of fuel-rich combustion occurring for small droplets, especially under fuel-rich overall equivalence ratios. The stochastic nature of the ignition event has been demonstrated by considering different realisations of statistically similar turbulent flow fields. The conditions giving rise to a successful thermal runaway/self-sustained flame propagation have been identified by a detailed analysis of the energy budget.

Keywords: Minimum ignition energy, turbulence intensity, droplet diameter, overall equivalence ratio, Direct Numerical Simulations
1. INTRODUCTION

The phenomenon by which the initiation and subsequent combustion of a flammable mixture occurs due to externally imposed means (i.e. electrical or laser-induced spark, plasma jet or heated surface) is known as forced ignition. Forced ignition is of fundamental interest in turbulent reacting flows, but also due to its practical importance for industrial applications (e.g. Direct Ignition engines, industrial gas turbines, high altitude relight etc.), and it has been studied extensively across a wide range of configurations. Significant efforts have been directed towards the investigation of forced ignition of droplet-laden mixtures, both experimentally (Ballal and Lefebvre, 1978,1979, Danis et al., 1988; Singh and Polymeropoulos, 1988; Dietrich et al., 1991; El-Rabii et al., 2005; Moesl et al., 2009; Marchione et al., 2009; Letty et al., 2012; Kariuki and Mastorakos, 2017; de Oliveira et al., 2019) and computationally (Wandel et al., 2009; Wandel, 2013,2014), and key findings from the existing literature have been summarised in a review paper by Mastorakos (2017). However, in comparison to the vast body of literature on the minimum ignition energy (MIE, the threshold amount of energy required to ignite a flammable mixture) for turbulent gaseous homogeneous mixtures (Ballal and Lefebvre, 1977a; Huang et al., 2007; Shy et al., 2010,2017; Cardin et al., 2013a,b; Jiang et al., 2018; Turquand d’Auzay et al., 2019), relatively limited effort has been directed towards the characterisation of the MIE for turbulent droplet-laden mixtures (Ballal and Lefebvre, 1978,1979, Danis et al., 1988). The MIE in turbulent homogeneous mixtures is principally affected by turbulence intensity and it increases with increasing root-mean-square (rms) turbulent velocity fluctuation. A transition in the increase of MIE with increasing turbulence intensity was found beyond a critical value of rms turbulent velocity fluctuation, such that the MIE requirements for turbulence intensities greater than the critical turbulence intensity are significantly higher than the MIE requirements for turbulence intensities smaller than the critical value. This has been demonstrated based on experiments
involving spark ignition of methane-air homogeneous mixtures with different equivalence ratios under homogeneous isotropic forced turbulence (Huang et al., 2007; Shy et al., 2010, 2017; Jiang et al., 2018). A similar qualitative behaviour has been reported by Cardin et al. (2013a, b) for lean methane-air mixtures under homogeneous decaying isotropic turbulence using laser ignition. These experimental results indicated that the transition of the MIE occurs irrespective of the ignition system (spark or laser) and mixture composition considered. A DNS based investigation by the present authors (Turquand d’Auzay et al., 2019) successfully captured the transition in the MIE demand with increasing turbulence intensity for stoichiometric methane-air mixtures under homogeneous decaying isotropic turbulence and offered physical explanations for this behaviour based on energy budgets and scaling arguments. However, in turbulent droplet-laden mixtures, the droplet size and the overall equivalence ratio in addition to the turbulence intensity are also expected to affect the MIE requirements. It has been experimentally reported by Danis et al. (1988) that the MIE requirements for n-heptane droplet-laden mixtures are dependent on droplet size and overall equivalence ratio. It has been found that the MIE decreases with decreasing droplet diameter and increasing equivalence ratio (Danis et al., 1988). Direct Numerical Simulations (DNS) based investigations by Wandel et al. (2009) showed that an increase in droplet diameter has a detrimental influence on successful forced ignition. Furthermore, Wandel (2014) demonstrated that the micro-mixing characteristics of the gaseous mixture arising from droplet evaporation can also play a crucial role in determining the possibilities of thermal runaway and subsequent self-sustained combustion. Recently Stempka et al. (2018, 2019) analysed spark ignition of droplet-laden mixtures in shear flows using Large Eddy Simulations (LES), and reported that the flow field influence on the early stages of flame kernel growth was weak for small turbulence intensities.
To the best of the authors' knowledge, there have been no DNS analyses, which concentrated on the MIE variations of turbulent droplet-laden mixtures for different values of turbulence intensity, droplet diameter and overall equivalence ratio. To address this gap in the existing literature, the present study aims to analyse the effects of turbulence intensities, droplet diameters and overall equivalence ratios (alternatively can be interpreted as the number density of droplets) on the MIE of mono-disperse droplet-laden mixtures using three-dimensional DNS of localised forced ignition for n-heptane droplets under decaying homogeneous isotropic turbulence. It is important to note that the MIE is usually estimated in experimental analyses as the minimum amount of energy which results in a 50% ignition probability (Danis et al., 1988; Huang et al., 2007; Shy et al., 2010, 2017; Jiang et al., 2018). However, it becomes prohibitively expensive to follow the experimental procedure to estimate the MIE using DNS. In this analysis, the minimum energy required to (i) obtain just a thermal runaway and to (ii) obtain a self-sustained combustion once the ignitor has been switched off following a successful thermal runaway, have been estimated, as done in a previous DNS analysis (Turquand d'Auzay et al., 2019). It is worth noting that the identification of transition of the MIE requirements with increasing turbulence intensity is not the focus of the current analysis and this aspect has not been addressed here due to the large computational demand associated with it. In this respect, the main objectives of this paper are:

(a) to analyse the effects of droplet diameter, overall equivalence ratio and turbulence on the MIE for obtaining (i) just a thermal runaway and (ii) a self-sustained combustion once the ignitor has been switched off following a successful thermal runaway.

(b) to explain the observed MIE dependences of droplet diameter, overall equivalence ratio and turbulence intensity based on physical principles.

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1 Around 250 DNS cases have been used for this analysis which amounted to approximately $5.28 \times 10^5$ core hours.
(c) to demonstrate the stochastic aspects of the forced ignition process and explain the observations by analysing the energy budget.

The rest of the paper will take the following form. The information related to the mathematical background and numerical implementation will be provided in the next two sections. The results will be presented in the subsequent section along with the relevant discussion. The final section of this paper will consolidate the main findings of the present study and the conclusions will be drawn.

2. MATHEMATICAL BACKGROUND

A modified single-step Arrhenius type irreversible chemical reaction is chosen for the current analysis, to keep the computational cost of the study within reasonable limits. Three-dimensional DNS with detailed chemistry would be exorbitantly expensive for the current parametric analysis, consisting of three different turbulence intensities, droplet diameters and overall equivalence ratios. The following single-step irreversible reaction has thus been considered:

\[ \text{Fuel} + s \cdot \text{Oxidiser} \rightarrow (1 + s) \text{Products} \]  

where \( s \) is the mass of oxygen consumed per unit mass of fuel consumption. The chemical mechanism was implemented following Tarrazo et al. (2006), where the activation energy, \( E_{ac} \), and the heat of combustion have been taken to be functions of the gaseous equivalence ratio, \( \phi_g \), which provides a realistic equivalence ratio dependence for the unstrained laminar burning velocity \( S_L(\phi_g=1) \) in hydrocarbon-air flames. A similar methodology has been implemented by Haruki et al. (2018) for a two-step mechanism in a DNS study of spray flames. For further information on this thermo-chemistry, the interested readers are directed to Tarrazo et al. (2006) and Malkeson and Chakraborty (2010). The equivalence ratio dependences of the
normalised laminar burning velocity $S_{L(\phi_g)}/\left\{S_{L(\phi_g)}\right\}_{max}$ and the adiabatic flame temperature $T_{ad(\phi_g)}$ with 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 (Chaos et al., 2007). To date, 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, 2013,2014; Wacks et al., 2016; Haruki et al., 2018; Pillai and Kurose, 2018, 2019). The localised ignition of n-heptane droplet-laden mixtures and the resulting flame structure have been analysed by Neophytou et al. (2010, 2012) using detailed chemistry DNS and the findings have been found to be in qualitative agreement with single step chemistry results (Wandel et al., 2009; Wandel, 2013,2014; Papapostolou et al., 2019). In this respect, it is worth noting that the same DNS code used by Neophytou et al. (2010, 2012) is used in this analysis.

The Lewis number ($Le_i = \alpha_i/D_i$ where $\alpha_i$ is the thermal diffusivity and $D_i$ is the species diffusivity of the $i^{th}$ species) of all species was taken to be unity, while all species in the gaseous phase are considered to be perfect gases. Standard values were taken 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 volume, respectively) and Prandtl number ($Pr = \mu C_p^g/\lambda = 0.7$, where $\mu$ is the dynamic viscosity and $\lambda$ is the thermal conductivity of the gaseous phase). Each individual droplet is tracked in a Lagrangian sense, whilst the compressible Navier-Stokes equations are solved in the Eulerian frame for the carrier gaseous phase. The evolution of the droplet related quantities such as the position, $\vec{x}_d$, velocity, $\vec{u}_d$, diameter $a_d$ and temperature $T_d$ are expressed
following Lagrangian tracking used by Reveillon and Vervisch (2005). The transport equations of the position, $\vec{x}_d$, velocity, $\vec{u}_d$, diameter, $a_d$ and temperature, $T_d$, of the droplets are given by (Reveillon and Vervisch, 2005; Wang and Rutland, 2005; Wandel et al., 2009; Neophytou et al., 2010,2012; Wandel, 2013,2014):

$$\frac{d \vec{x}_d}{dt} = \vec{u}_d$$  \hspace{1cm} (2)

$$\frac{d \vec{u}_d}{dt} = \frac{\vec{u}(\vec{x}_d, t) - \vec{u}_d}{\tau^v_d}$$  \hspace{1cm} (3)

$$\frac{d a_d^2}{dt} = -\frac{a_d^2}{\tau^p_d}$$  \hspace{1cm} (4)

$$\frac{d T_d}{dt} = \frac{\tilde{T}(\vec{x}_d, t) - T_d - B_d L_v / C_p^g}{\tau^T_d}$$  \hspace{1cm} (5)

where $\tilde{T}$ is the instantaneous dimensional temperature of the gaseous phase, $L_v$ is the latent heat of vaporisation, and $\tau^v_d$, $\tau^p_d$ and $\tau^T_d$ are relaxation timescales for velocity, droplet diameter and temperature, respectively. These timescales are defined as (Reveillon and Vervisch, 2005; Wang and Rutland, 2005; Wandel et al., 2009; Neophytou et al., 2010,2012; Wandel, 2013,2014):

$$\tau^v_d = \frac{\rho_d a_d^2}{18 C_u}$$  \hspace{1cm} (6)

$$\tau^p_d = \frac{\rho_d a_d^2 Sc}{4 \mu S h_c ln (1 + B_d)}$$  \hspace{1cm} (7)

$$\tau^T_d = \frac{\rho_d a_d^2 Pr B_d C^L_p}{6 \mu N u_c ln (1 + B_d) C^g_p}$$  \hspace{1cm} (8)

Here, $\rho_d$ is the droplet density, $Sc$ is the Schmidt number which is taken to be 0.7 (i.e. $Sc = 0.7$), $C^L_p$ is the specific heat for the liquid phase, $C_u = 1 + Re^{2/3}/6$ is the correction for the drag coefficient with $Re_d$ being the droplet Reynolds number, $B_d$ is the Spalding number, $S h_c$ is the corrected Sherwood number and $N u_c$ is the corrected Nusselt number, which are defined
as (Reveillon and Vervisch, 2005; Wang and Rutland, 2005; Wandel et al., 2009; Neophytou et al., 2010, 2012; Wandel, 2013, 2014):

$$ Re_d = \frac{\rho |\vec{u}(\hat{x}_d, t) - \bar{u}_d| a_d}{\mu} \quad (9) $$

$$ B_d = \frac{Y^s_f - Y_f(\hat{x}_d, t)}{1 - Y^s_f} \quad (10) $$

$$ Sh_c = Nu_c = 2 + \frac{0.555Re_dSc}{(1.232 + Re_dSc^{4/3})^{1/2}} \quad (11) $$

where $Y^s_f$ denotes the value of $Y_f$ at the surface of the droplet and the partial pressure of the fuel vapour at the droplet surface $p^s_f$ are expressed by (Reveillon and Vervisch, 2005; Wang and Rutland, 2005; Wandel et al., 2009; Neophytou et al., 2010, 2012; Wandel, 2013, 2014):

$$ p^s_f = p_{ref} \exp \left( L_v \left[ \frac{1}{RT^s_{ref}} - \frac{1}{RT^s_d} \right] \right); \quad Y^s_f = \left( 1 + \frac{W_g}{W_F} \frac{p(\hat{x}_d, t)}{p^s_f} - 1 \right)^{-1} \quad (12) $$

In Eq. 12, $T^s_{ref}$ denotes the boiling point of the fuel at pressure $p_{ref}$, $R$ is the gas constant and $T^s_d$ is assumed to be $T_d$, and $W_g$ and $W_F$ are the molecular weights of the gaseous mixture and fuel vapour, respectively. The coupling between Lagrangian and Eulerian phases is obtained from the additional source terms in the gaseous phase transport equations in the following manner (Wandel et al., 2009; Neophytou et al., 2010, 2012; Wandel, 2013, 2014):

$$ \frac{\partial \rho \psi}{\partial t} + \frac{\partial \rho u_j \psi}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_\psi \frac{\partial \psi_1}{\partial x_j} \right) + \dot{w}_\psi + \dot{S}_g + \dot{S}_\psi \quad (13) $$

where $\psi = \{1, u_i, e, Y_F, Y_O\}$ and $\psi_1 = \{1, u_i, \hat{T}, Y_F, Y_O\}$ for the conservation equations of mass, momentum, specific stagnation internal energy, and fuel and oxidiser mass fraction, respectively. For $\psi = \{1, u_i, Y_F, Y_O\}$, the diffusion coefficient is given by $\Gamma_\psi = \rho v/\sigma_\psi$, where $v$ represents the kinematic viscosity with $\sigma_\psi$ being an appropriate Schmidt number corresponding to $\psi$, and $u_i$ represents the velocity in the $i^{th}$ direction. The $\dot{w}_\psi$ term arises due to the chemical reaction rate, $\dot{S}_g$ is an appropriate source/sink term in the gaseous phase, $\dot{S}_\psi$ is
the appropriate source term due to two-way coupling between Lagrangian and Eulerian phases, which is tri-linearly interpolated from the droplets sub-grid position, $\mathbf{x}_d$, to the eight surrounding nodes. The source term associated with two-way coupling for any variable $\psi$ is expressed as:

$$S_\psi = -\left(1/V\right)\sum_d d(m_d\psi_d)/dt$$

(14)

where, $V$ is the cell volume, $m_d = \rho_d(1/6)\pi a_d^3$ is the droplet mass. The energy conservation equation for $\psi = e = \int_{T_{ref}}^{T} C_v^\beta d\hat{T}' + u_k u_k/2$ is given as:

$$\frac{\partial}{\partial t} \rho e + \frac{\partial}{\partial x_i} \rho u_i e - C_1$$

$$= -\frac{\partial}{\partial x_i} u_i p + \frac{\partial}{\partial x_i} \tau_{ij} u_j + \dot{\omega}_T + \frac{\partial}{\partial x_k} \left[ \lambda \frac{\partial \hat{T}}{\partial x_k} \right] - \frac{\partial}{\partial x_i} \rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i}$$

$$+ q'''' + S_e$$

where $p$ is the pressure, $\tau_{ij}$ is the component of the viscous stress tensor, $\dot{\omega}_T$ is the heat release rate, $h_{s,k}$ is the sensitive enthalpy of the $k^{th}$ species, and $V_{k,i}$ is the diffusion velocity in the $i^{th}$ direction for the $k^{th}$ species. The term $D_3$ is equal to zero in the cases considered here and this arises due to the assumption that the species are considered to be perfect gases, with constant specific heats at constant pressure and volume ($C_p^\beta$ and $C_v^\beta$). The aforementioned assumptions subsequently lead to $\rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i} = C_p^\beta (T - T_0) \sum_{k=1}^{N} Y_k V_{k,i} = 0$. An additional source term, $(q'''' = A_{sp} \exp(-r^2/2R_{sp}^2)$ with $r$ being the distance from the ignitor centre and $R_{sp}$ representing the characteristic width of energy deposition) is added to the energy conservation equation to account for energy addition by the ignitor for the purpose of forced ignition. The source term follows a Gaussian distribution in the radial direction from the ignition centre, as used in several previous studies (Chakraborty et al., 2007; Espi and Liñán, 2001,2002; Wandel...
et al., 2009; Neophytou et al., 2010, 2012; Papapostolou et al., 2019; Wandel, 2013, 2014) to model the thermal aspects of localised forced ignition. The constant $A_{sp}$ is determined by a volume integration which leads to the total ignition power $\dot{Q}$ given by:

$$\dot{Q} = \int_{V} q'' dV = a_{sp} \rho_{0} C_{p} \tau T_{0} \left(\frac{4}{3} \pi \delta_{z}^{3}\right) \frac{[\mathcal{H}(t) - \mathcal{H}(t - t_{sp})]}{t_{sp}}$$

(16)

where $a_{sp}$ is a parameter determining the total energy deposited by the ignitor, $\tau = \left( T_{ad(\phi_{g}=1)} - T_{0} \right) / T_{0}$ is the heat release parameter (where $T_{ad(\phi_{g}=1)}$ and $T_{0}$ are the adiabatic flame temperature of the stoichiometric mixture and unburned gas temperature, respectively). The Zel’dovich flame thickness of the gaseous stoichiometric (i.e. $\phi_{g} = 1.0$) mixture $\delta_{z}$ is defined as $\delta_{z} = D_{0} / S_{L(\phi_{g}=1)}$, where $D_{0}$ is the thermal diffusivity of the unburned gas and $S_{L(\phi_{g}=1)}$ is the unstrained laminar burning velocity of the stoichiometric mixture. The Heaviside functions $\mathcal{H}(t)$, and $\mathcal{H}(t - t_{sp})$ in eq. 16 ensure that the ignitor is only active during $0 \leq t \leq t_{sp}$. The energy deposition duration $t_{sp}$, is expressed as $t_{sp} = b_{sp} t_{f}$, where $t_{f} = \delta_{z} / S_{L(\phi_{g}=1)}$ is a characteristic timescale and the energy deposition parameter $b_{sp}$ is taken to be $b_{sp} = 0.2$ in the present study, which falls within its optimal range as outlined by Ballal and Lefebvre (1977b). In the present study, the energy deposition duration $t_{sp}$ and the width of energy deposition $R_{sp}$ are kept unaltered (i.e. $t_{sp} = 0.2 t_{f}$ and $R_{sp} = 2.45 \delta_{z}$), whilst $a_{sp}$ is modified until the MIE is found for both successful thermal runaway irrespective of the fate of the resulting flame kernel, and self-sustained flame propagation following thermal runaway. It is vital to distinguish between the two, as a successful thermal runaway does not ensure subsequent self-sustained flame propagation (Turquand d’Auzay et al., 2019). The thermal runaway takes place due to the increase of temperature as a result of external energy addition and a misfire occurs in the absence of a thermal runaway. A successful self-sustained propagation is obtained when the flame kernel burns without the aid of the ignitor after a
successful ignition event. The outcome in terms of self-sustained flame propagation is assessed by evaluating the temporal evolution of the burned gas volume, and if its temporal derivative is positive and the maximum temperature has settled to the adiabatic flame temperature of the stoichiometric mixture at $t = 10t_{sp}$, a successful self-sustained propagation is assumed to have been obtained.

It is important to note that the methodology used in this analysis to identify the MIE is different from the experimental methodology (Huang et al., 2007; Shy et al., 2010,2017; Cardin et al., 2013a,b; de Oliveira et al., 2019). A success rate of 50% across numerous turbulent realisations (at least 30 as reported by Shy et al., 2010) is required to ascertain the MIE value for a certain case in experimental investigations, which is unfeasible to adopt for a DNS based analysis due to the high computational cost associated with it. Therefore the MIE input is evaluated for a given turbulence realisation and a few additional simulations have been used for this energy input under different realisations of statistically identical conditions (i.e. $u'/S_{L(\phi_g=1)}$ and $l_t$) of the initial turbulent flow field to analyse the stochastic aspects of thermal runaway and self-sustained flame propagation following thermal runaway.

3. NUMERICAL IMPLEMENTATION

The simulations have been carried out using a well-known three-dimensional compressible DNS code SENGA+ (Wandel et al., 2009; Neophytou et al., 2010,2012; Wandel, 2013,2014) in a domain of size $51\delta_z \times 51\delta_z \times 51\delta_z$ or $9.6l_t \times 9.6l_t \times 9.6l_t$, where $l_t$ is the longitudinal integral length scale. The centre of the ignitor is taken to be at the geometrical centre of the domain. The simulation domain is discretised by a Cartesian grid of $264 \times 264 \times 264$ cells of uniform grid size $\Delta x$, which ensures 10 grid points across the thermal flame thickness of the stoichiometric mixture $\delta_{st} = [T_{ad(\phi_g=1)} - T_0] / max (\|\nabla T\|_L)$. It also ensures $\eta_k > \Delta x$, where
\( \eta_k \) is the Kolmogorov length scale. All the boundaries of the domain are taken to be partially non-reflecting. A 10\(^{th}\) order central difference scheme is used for the internal grid points, but the order of accuracy drops gradually to a one-sided 2\(^{nd}\) order scheme at the non-periodic boundaries. A third-order explicit Runge-Kutta scheme is used for explicit time advancement.

The flame-turbulence interaction takes place under decaying isotropic homogeneous turbulence. A well-known pseudo-spectral method (Rogallo, 1981) is used to initialise the turbulent velocity fluctuation by an incompressible, homogeneous isotropic field with prescribed values of root-mean-square (rms) velocity \( u' \) and integral length scale \( l_t \). Mono-sized n-heptane droplets are taken to be uniformly dispersed in air and the overall equivalence ratio \( \phi_{ov} \) is determined by the number of droplets initially present in the domain. Three different droplet diameters \( a_d \) have been investigated (\( a_d/\delta_{st} = 0.03,0.04,0.05 \)), across three different global equivalence ratios \( \phi_{ov} = 0.8,1.0,1.2 \). For ease of reference and brevity, each case will be referred to in the following manner: U00, U04, U08 refer to \( u'/S_{L(\phi_g=1)} = 0,4,0,8,0 \) respectively; D03, D04, D05 refer to initial normalised droplet sizes \( a_d/\delta_{st} = 0.03,0.04,0.05 \) respectively, and F08, F10, F12 refer to \( \phi_{ov} = 0.8,1.0,1.2 \) respectively. The simulation parameters along with the characteristic radius of the ignitor and energy deposition time are summarised in Table 1.

<table>
<thead>
<tr>
<th>( u'/S_{L(\phi_g=1)} )</th>
<th>( l_t/\delta_z )</th>
<th>( a_d/\delta_{st} )</th>
<th>( \phi_{ov} )</th>
<th>Energy deposition characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 (U00)</td>
<td>-</td>
<td>0.03 (D03)</td>
<td>0.8 (F08)</td>
<td>( t_{sp} = 0.2t_f )</td>
</tr>
<tr>
<td>4.0 (U04)</td>
<td>5.31</td>
<td>0.04 (D04)</td>
<td>1.0 (F10)</td>
<td>( R_{sp} = 2.45\delta_z )</td>
</tr>
<tr>
<td>8.0 (U08)</td>
<td>5.31</td>
<td>0.05 (D05)</td>
<td>1.2 (F12)</td>
<td></td>
</tr>
</tbody>
</table>
The initial values of turbulent Reynolds number $Re_L = \rho_0 u'L_{turb}/\mu_0$ (where $\rho_0$ and $\mu_0$ are unburned gas density and viscosity, respectively) for initial values of $u'/S_{L(\phi_{ov}=1)} = 4.0$ and 8.0 are 71.0 and 142, respectively. The temporal evolutions of rms turbulent velocity fluctuation $u'$ and integral length scale $L_{turb} = k^{1.5}/\epsilon$ (where $k$ and $\epsilon$ are the turbulent kinetic energy and its dissipation rate evaluated over the whole domain) and turbulent Reynolds number $Re_L = \rho_0 u'L_{turb}/\mu$ normalised by their initial values for initial values of $u'/S_{L(\phi_{ov}=1)} = 4.0$ and 8.0 for $\phi_{ov} = 1.0$ are shown in the Appendix for different values of $a_d/\delta_{st}$ along with the corresponding temporal decays of purely gaseous turbulence without the chemical reaction. The trends are the same for other values of $\phi_{ov}$ and thus are not shown in the Appendix.

The normalised initial droplet number densities $\rho_N$ for these cases are given by $1.25 \leq (\rho_N)^{1/3} \delta_{st} \leq 2.39$ in the unburned gas and the percentage of liquid volume ranges from 0.009% to 0.013% for the change of $\phi_{ov}$ from 0.8 to 1.2. The corresponding mass loading can be obtained from the overall equivalence ratio, as the fuel is supplied in the form of liquid droplets. All three droplet diameters and global equivalence ratios have been investigated for different initial turbulence intensities ($u'/S_{L(\phi_{ov}=1)} = 4.0$ and 8.0). For all turbulent cases, the initial value of the ratio of integral length scale to Zel’dovich flame thickness is taken to be $l_t/\delta_z = 5.31$, which ensures about 10 large scale eddies on each side of the domain. In addition to turbulent cases, simulations have been conducted for laminar quiescent condition (i.e. $u'/S_{L(\phi_{ov}=1)} = 0.0$) for each of the values of $a_d$ and $\phi_{ov}$. The unburned gas temperature and initial droplet temperature $T_0$ are taken to be 300K, which yields a heat release parameter of $\tau = (T_{ad(\phi_{ov}=1)} - T_0)/T_0 = 6.54$ and combustion in all cases takes place under atmospheric pressure. Care has been taken to ensure that the droplet diameter remains smaller
than the Kolmogorov length scale for all cases investigated, and the ratio of initial droplet
diameter to the Kolmogorov length scales is $a_d/\eta_k = 0.22, 0.29, 0.36$ for $a_d/\delta_{st} =
0.03, 0.04, 0.05$, respectively, for the highest initial turbulence intensity, investigated. The ratios
$a_d/\eta_k$ and $a_d/\Delta x$ in this analysis remain comparable to several previous analyses by other
authors (Fujita et al., 2013; Neophytou et al., 2010, 2012; Reveillon and Vervisch, 2000;
The Stokes number, defined as $St = \tau_d^u \sqrt{k}/l_t = \rho_d a_d^2 \sqrt{k}/(18C_u \mu l_t)$ (where $\tau_d^u = \rho_d a_d^2 / 18C_u \mu$ is the particle time scale and $l_t/\sqrt{k}$ is the turbulent time scale with $k$ being the
turbulent kinetic energy evaluated over the whole volume), remains smaller than 0.56 for the
largest droplet for the highest turbulence intensity case. An alternative Stokes number $St' =
\tau_d^u S_{b(\phi_g=1)}/\delta_z = \rho_d a_d^2 S_{b(\phi_g=1)}/(18C_u \mu \delta_z)$ based on the chemical time scale $t_f = \delta_z/
S_{b(\phi_g=1)}$ remains smaller than 0.32 for the largest droplets considered in this analysis. The
mean normalised inter-droplet distance $s_d/\eta_k$ varies between 2.0 and 6.43 for the turbulent
cases considered here. Due to the high volatility of n-heptane, the size of droplets decreases
significantly ($\geq 50\%$) by the time they reach the reaction zone. Thus, the droplets, which
interact with the flame, are much smaller in reality than the initial size of the droplets. Thus,
the assumption of sub-grid evaporation is not expected to significantly affect the ignition
phenomenon and subsequent flame-droplet interaction in this analysis.

Chiu and Liu (1977) employed a group number, $G = 3(1 +
0.276Re_d^{1/2}Sc^{1/3})Le N^{2/3} (a_d/s_d)$ (where $N$ is the number of droplets in a specified volume
and $s_d$ is the mean inter-droplet distance) in order to distinguish between individually burning
droplets ($G \ll 1.0$) and external sheath combustion ($G \gg 1.0$). It has been demonstrated in
Reveillon and Vervisch (2000) that droplet-laden combustion can be simulated using DNS for
external group/sheath combustion using the point-source assumption. For the cases considered here \( N \) ranges from \( 3 \times 10^4 \) to \( 22 \times 10^4 \) depending on the value of \( \phi_{ov} \) and \( a_d/\delta_{st} \). The separation \( S = s_d/a_d \) ranges from 13.0 to 15.0 depending on the value of \( \phi_{ov} \) and \( a_d/\delta_{st} \). From the formula provided by Chiu and Liu (1977) the group number \( G \) ranges from 204.0 to 900.0 and thus all droplet cases considered here come under the category of external sheath combustion (i.e. have values of \( G \) much greater than unity).

The simulations used to evaluate whether successful propagation has been continued till at least \( t = 10t_{sp} \), which amounts to be \( 2.0t_f \) which is greater than \( 2.0t_c/\sqrt{k} \) and \( 4.0t_c/\sqrt{k} \) for the initial \( u'/S_{l(\phi_g=1)} = 4.0 \) and \( u'/S_{l(\phi_g=1)} = 8.0 \) cases, respectively. By that time, \( u' \) had decayed by 30% and 40% in comparison to its value at \( t = 0 \) for the initial \( u'/S_{l(\phi_g=1)} = 4.0 \) and \( u'/S_{l(\phi_g=1)} = 8.0 \) cases (see Appendix). This simulation time remains comparable to several previous DNS analyses on localised forced ignition of droplet-laden mixtures (Neophytou et al., 2010, 2012; Wandel et al., 2009; Wandel, 2013, 2014).

4. RESULTS AND DISCUSSION

For each case considered in this analysis, the deposited energy by the ignitor corresponds to its respective normalised MIE, \( \Gamma^{i/p}_{MIE} \) where the quantity \( \Gamma \) is defined as \( \Gamma = IE/MIE^\phi_g=1.0 \), with IE being the energy deposited by the ignitor and \( MIE^\phi_g=1.0 \) is the MIE for self-sustained flame propagation of a quiescent laminar n-heptane premixed stoichiometric mixture. In the present analysis, the MIE for self-sustained flame propagation following a thermal runaway for a laminar n-heptane premixed stoichiometric mixture is given by \( MIE^\phi_g=1.0 = 4.8[p_0C_p^g\tau T_0(4/3 \pi \delta_z^3)] \). This confirms that the MIE for a laminar quiescent premixed mixture
scales with the energy required to increase a spherical volume of unburned mixture with a radius (~1.66δz) of the order of the laminar flame thickness δz, which is consistent with pioneering analysis by Spalding (1979). The superscripts i and p are used to refer to the minimum ignition energy required just to lead to thermal runaway, and self-sustained flame propagation following thermal runaway, respectively. It is worth noting that the term thermal runaway in this paper is indicative of the kernel generation phase indicated by Mastorakos (2017), whilst the term self-sustained flame propagation in this study is equivalent to the flame growth phase (Mastorakos, 2017).

The three-dimensional views of the non-dimensional temperature \( T = (\hat{T} - T_0) / \left( T_{ad(\phi_g=1)} - T_0 \right) = 0.7 \) isosurfaces at the time instances \( t = 2.0t_{sp}, 5.0t_{sp} \) and \( 8.0t_{sp} \) for the cases with initial \( u'/S_{L(\phi_g=1)} = 4.0 \) and with initial \( a_d/\delta_s = 0.04 \), are shown in Fig. 1.

For the cases shown in Fig. 1, the flame kernels remain almost spherical at \( t = 2.0t_{sp} \) because the evolution of the hot gas region is primarily driven by the thermal diffusion of the energy deposited by the ignitor and the heat release rate within the flame kernel at that stage. However, droplets induce dimples on the \( T = 0.7 \) isosurfaces, which are consistent with previous experimental (Hayashi et al., 1977; Lawes and Saat, 2011; d’Oliviera et al., 2019) and computational (Ozel-Erol et al., 2018, 2019; Papapostolou et al., 2019) findings. However, these effects were more magnified in Lawes and Saat (2011) and Hayashi et al., (1977) due to the presence of thermo-diffusive and hydro-dynamic instabilities. The aforementioned effects are not present in this analysis because of the small separation between the integral length scale and flame thickness and also due to the unity Lewis number assumption.
Figure 1: Instantaneous views of $T = 0.7$ isosurface coloured by local values of normalised fuel reaction rate magnitude $|\dot{\omega}_f| \times \delta_z / \rho_0 S_{L(\phi_g=1)}$ at $t = 2.0t_{sp}, 5.0t_{sp}$ and $8.0t_{sp}$ (from left to right) for cases U04D04F08, U04D04F10, U04D04F12 (from top to bottom) for the respective MIE for self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}^p$) for each case. The inset shows the magnified surface of the kernel, without the droplets present.

The mixture inhomogeneity in the gaseous phase arising from droplet evaporation gives rise to the variations of fuel reaction rate magnitude on the isosurfaces of $T = 0.7$ in Fig. 1. For all the turbulent cases investigated in the present study, the kernel becomes increasingly wrinkled and deformed as time advances, as illustrated by Fig. 1, in conjunction with the aforementioned dimples induced by flame-droplet interaction. However, the effects of turbulence dominate over the droplet-induced wrinkling as reported in previous studies (Hayashi et al., 1977; Lawes and Saat, 2011; Ozel-Erol et al., 2018, 2019; Papapostolou et al., 2019). As initial $\phi_{op}$ increases
so too does the number of droplets present within the domain, which has a significant impact on $\Gamma_{\text{MIE}}^p$. The amount of combustible mixture present in the domain increases with an increase of $\phi_{ov}$, which makes self-sustained propagation easier. This is reflected by the increasing volume of the flame kernels with increasing $\phi_{ov}$ (top to bottom) at $t = 5.0t_{sp}$ and $8.0t_{sp}$ where the only difference is the value of $\phi_{ov}$.

The effects of initial droplet size and turbulence intensity on the hot gas kernel evolution for the MIE for self-sustained flame propagation are illustrated in Fig. 2 where the isosurfaces of $T = 0.7$ at $t = 2.0t_{sp}$, $5.0t_{sp}$ and $8.0t_{sp}$ for all the cases with initial $\phi_{ov} = 1.0$ are exemplarily shown superimposed on each other, along with the volume of the energy deposition by the ignitor. It can be seen from Fig. 2 that the hot gas kernels in the laminar quiescent case (top row) maintain their approximate spherical shape as a result of the molecular diffusion of the deposited energy in the absence of turbulent fluid motion. However, the isosurfaces are not perfectly spherical as would be the case for a successful self-sustained flame propagation for a premixed homogeneous mixture under a laminar condition. The behaviour observed in the present study arises from the presence of mixture inhomogeneity in the gaseous phase arising from droplet evaporation, and this behaviour was reported previously by Ozel-Erol et al. (2018,2019). Under turbulent conditions, the flame kernels deform considerably due to flame-turbulence interaction and no longer retain their spherical shape. Moreover, for large values of $u'/S_{L(\phi_g = 1)}$, the centre of the mass of the hot gas kernel may move away from the ignitor centre, which suggests that fluid turbulence away from the ignitor volume plays a significant role in determining the possibility of self-sustained flame propagation. Of particular interest, is the differences in volumes of the hot gas kernels with the variations of $u'/S_{L(\phi_g = 1)}$ and $a_d/\delta_{st}$. It can be seen from Fig. 2 that the size of the hot gas kernels at $t = 2.0t_{sp}$ in the case of the MIE input for self-sustained flame propagation increases with increasing turbulence
intensity $u'/S_{L(\phi_g=1)}$ (top to bottom). A larger volume of the hot gas kernel at this early stage after thermal runaway (e.g. $t = 2.0t_{sp}$) is a reflection of the greater amount of energy input in order to obtain a successful thermal runaway and subsequent self-sustained propagation at higher turbulence intensities. At later times (e.g. $t = 5.0t_{sp}$ and $8.0t_{sp}$) the volume of the kernels is indicative of their burning rate, and an increase of droplet diameter (left to right) leads to a decrease of the volume of the hot gas kernel, indicating that as initial droplet diameter increases, so too does the energy required to obtain a successful thermal runaway and subsequent self-sustained propagation.

The non-dimensional temperature isosurfaces presented in Figs. 1 and 2 indicate that the energy contents of these hot kernels are different, which suggests that the values of $\Gamma_{MIE}^{i/p}$ are expected to be affected by turbulence intensity, droplet diameter and overall equivalence ratio. This can be substantiated from Fig. 3 where the effects of $u'/S_{L(\phi_g=1)}$, $a_d/\delta_{st}$ and $\phi_{ov}$ on $\Gamma_{MIE}^{i}$ and $\Gamma_{MIE}^{p}$ are shown for all cases considered here. It can be seen from Fig. 3 that both $\Gamma_{MIE}^{i}$ and $\Gamma_{MIE}^{p}$ increase with increasing turbulence intensity $u'/S_{L(\phi_g=1)}$ for a given set of values of $a_d/\delta_{st}$ and $\phi_{ov}$, which is consistent with previous experimental findings (Ballal and Lefebvre, 1978, 1979, Danis et al., 1988) for droplet-laden mixtures. A qualitatively similar trend was previously observed for the MIE variation of gaseous homogeneous mixtures in the past (Ballal and Lefebvre, 1977a; Huang et al., 2007; Shy et al., 2010, 2017; Cardin et al., 2013a,b; Patel et al., 2014, 2016; Jiang et al., 2018; Turquand d’Auzay et al., 2019). Figure 3 further shows that $\Gamma_{MIE}^{p}$ slowly increases with increasing turbulence intensity for moderate values of $u'/S_{L(\phi_g=1)}$ but a more rapid increase in $\Gamma_{MIE}^{p}$ is observed for large values of $u'/S_{L(\phi_g=1)}$ (e.g. initial $u'/S_{L(\phi_g=1)} = 8.0$ cases). For example, the increase in $\Gamma_{MIE}^{p}$ between $u'/S_{L(\phi_g=1)} = 4.0$ and $8.0$ cases is much higher than the increase of $\Gamma_{MIE}^{p}$ between $u'/S_{L(\phi_g=1)} = 0.0$ and $4.0$. This is
indicative of the transition of $\Gamma_{MIE}^P$ increases with increasing $u'/S_{\Gamma}(\phi_g=1)$, which was reported earlier for the MIE behaviour for turbulent gaseous homogeneous mixtures (Huang et al., 2007; Shy et al., 2010,2017; Cardin et al., 2013a,b; Jiang et al., 2018; Turquand d’Auzay et al., 2019). The heat release rate within the hot gas kernel needs to overcome the rate of heat transfer from the hot gas kernel to the surrounding cold gas in order to obtain a successful self-sustained flame propagation. An increase in $u'$ for a given value of $l_t$ increases the turbulent diffusivity $D_t \sim u'l_t$ which acts to increase the heat transfer rate from the hot gas kernel and therefore the demand for the MIE increases with increasing turbulence intensity $u'/S_{\Gamma}(\phi_g=1)$. The turbulence-induced flame wrinkling acts to generate an increase of the flame surface area, which acts to increase the burning rate. However, the increase in $D_t$ with an increase in $u'/S_{\Gamma}(\phi_g=1)$ takes place more rapidly than the increase in flame surface due to flame wrinkling and therefore MIE demand increases with increasing $u'/S_{\Gamma}(\phi_g=1)$ and eventually a transition in $\Gamma_{MIE}^P$ requirement can be observed above a threshold value of turbulence intensity (Turquand d’Auzay et al., 2019). Identification of the transition of $\Gamma_{MIE}^P$ with increasing $u'/S_{\Gamma}(\phi_g=1)$ is not the focus of the current analysis but the considerably increase in $\Gamma_{MIE}^P$ between initial $u'/S_{\Gamma}(\phi_g=1) = 4.0$ and 8.0 cases in comparison to that between laminar quiescent and initial $u'/S_{\Gamma}(\phi_g=1) = 4.0$ cases is indicative of the transition of MIE for forced ignition of droplet-laden mixtures.
Figure 2: Isosurfaces of $T = 0.7$ at $t = 2.0 t_{sp}$ (blue), $5.0 t_{sp}$ (green) and $8.0 t_{sp}$ (magenta), with the energy deposition region indicated by the red sphere, obtained for $\Gamma = \Gamma_{MIE}^p$ for $\phi_{ov} = 1.0$ cases with laminar, initial $u'/S_{L(\phi_{g}=1)} = 4.0$ and initial $u'/S_{L(\phi_{g}=1)} = 8.0$ (from top to bottom) for initial $a_d/\delta_{st} = 0.03, 0.04$ and $0.05$ (from left to right). The vertical black line indicates the centre of the domain.

Figure 3 reveals that in addition to turbulence intensity, both droplet diameter and overall equivalence ratio affect both $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$. It can be seen from Fig. 3 that both $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$ decrease with increasing $\phi_{ov}$. An increase in $\phi_{ov}$ increases the number density of droplets and thus the availability of fuel vapour in the gaseous phase increases with an increase in overall equivalence ratio. This leads to a decrease in $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$ with increasing $\phi_{ov}$ irrespective of the values of turbulence intensity and droplet diameter, but this can most clearly be seen for the quiescent laminar cases with initial $a_d/\delta_{st} = 0.03$. Figure 3 also indicates that droplet diameter has a strong influence on the variation of $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$ and these values increase with increasing $a_d/\delta_{st}$. The evaporation rate decreases with increasing droplet size and thus
large droplets do not readily release enough fuel vapour to ensure thermal runaway, and to support self-sustained flame propagation without a sufficiently large external energy input. These $\phi_{ov}$ and $a_d/\delta_{st}$ dependences of $\Gamma_{MIE}^t$ and $\Gamma_{MIE}^p$ are consistent with previous experimental findings of Danis et al. (1988). The computational analysis by Wandel et al. (2009) also revealed that it is relatively more difficult to ignite large droplets.

**Figure 3:** Normalised MIE variations only for successful thermal runaway $\Gamma_{MIE}^t$ (left), and for successful self-sustained propagation, $\Gamma_{MIE}^p$ (right) for different initial values of $u'/S_L(\phi_{ov}=1)$, $a_d/\delta_{st}$ and $\phi_{ov}$. 
Figure 4: Temporal evolution of maximum non-dimensional temperature, $T_{\text{max}}$ for the minimum ignition energy inputs for self-sustained flame propagation (i.e. $\Gamma = \Gamma_{\text{MIE}}^p$) in the case of different turbulence intensities for initial $a_d/\delta_{st} = 0.05$ and $\phi_{\text{VP}} = 1.2$.

It can be seen from Fig. 3 that $\Gamma_{\text{MIE}}^p$ values are consistently higher than $\Gamma_{\text{MIE}}^i$. This is also consistent with previous findings for localised forced ignition of homogeneous mixtures (Turquand d’Auzay et al., 2019). This suggests that the energy input which is sufficient for thermal runaway may not be sufficient for ensuring self-sustained combustion without any external energy addition once the ignitor is switched off. It can be seen from Figs. 1 and 2 that the hot gas kernel created by external energy addition gets significantly deformed for large values of $u'/S(L(\phi_{y=1})$, and the hot gas kernel might get convected from the centre of the ignitor for large values of $u'/S(L(\phi_{y=1})$. This suggests that the turbulent flow conditions not only at the ignitor location but also in the vicinity determine the chance of obtaining successful self-
sustained combustion, once the ignitor is switched off. This necessitates that more energy input is needed for successful self-sustained flame propagation than for just obtaining a thermal runaway, as the flame may quench following a thermal runaway if the rate of heat transfer supersedes the heat release rate when the ignitor is switched off. In order to obtain further insights into the increase in $\Gamma_{MIE}^P$ with increasing initial $u'/S_L(\phi_g=1)$, the temporal evolutions of the maximum non-dimensional temperature $T_{max}$ for different turbulence intensities are exemplarily shown in Fig. 4 for initial $a_d/\delta_{st} = 0.05$ and $\phi_{av} = 1.2$. It can be seen from Fig. 4 that $T_{max}$ increases with time during the energy deposition duration (i.e. $t \leq t_{sp}$). Figure 4 further shows that for the normalised MIE for successful self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}^P$), the maximum non-dimensional temperature $T_{max}$ at the end of the energy deposition period, remains too small to give rise to thermal runaway for laminar conditions and small/moderate turbulence intensities (i.e. $u'/S_L(\phi_g=1) = 4.0$) and the maximum value of $T_{max}$ in these cases occurs at around $t = 1.5t_{sp}$ as a result of autoignition of the evaporated fuel vapour. By contrast, for high turbulence intensities (e.g. $u'/S_L(\phi_g=1) = 8.0$), the thermal runaway takes place during the energy deposition duration, and the maximum temperature $T_{max}$ attains a value much larger than the adiabatic flame temperature of the stoichiometric mixture (i.e. $T_{max} > 1.0$) for the MIE for ensuring successful self-sustained flame propagation. This high value of $T_{max}$ resulting from thermal runaway decreases with time and eventually settles to a value close to the adiabatic flame temperature of the stoichiometric mixture (i.e. $T_{max} = 1.0$) long after the energy deposition duration (i.e. $t >> t_{sp}$) if the long mode of ignition failure described by Mastorakos (2017) does not happen. These qualitative differences in the temporal evolution of $T_{max}$ clearly indicate that the MIE value for high turbulence intensity (e.g. $u'/S_L(\phi_g=1) = 8.0$) is expected to be significantly greater than those for laminar and moderate turbulence intensities (e.g. $u'/S_L(\phi_g=1) = 4.0$). The energy requirements to
obtain a successful propagation for the highly turbulent cases (e.g. $u'/S_{L(\phi_g=1)} = 8.0$) are significantly higher than in case of small turbulence intensities because one needs more energy to raise the temperature such that enough droplets are evaporated to produce a flammable mixture, and produce a critical burned gas volume with $T_{max} \geq 1.0$ within $t_{sp}$. The observed differences in the nature of thermal runaway for the MIE input in response to the changes in $u'/S_{L(\phi_g=1)}$ is qualitatively similar to the previous findings by Turquand d’Auzay et al. (2019) for turbulent gaseous homogeneous mixtures.

![Figure 5](image)

**Figure 5**: Temporal evolution of the volume of the burned gas region with $c \geq 0.9$ (i.e. $V_{c \geq 0.9}$) normalised by the spark volume (i.e. $V_{sp} = (4\pi/3)R_{sp}^3$) in the case of MIE input for successful self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}$): (a/left) for different initial droplet diameters for initial $u'/S_{L(\phi_g=1)} = 4.0$ and $\phi_{ov} = 0.8$, (b/centre) for cases with initial $u'/S_{L(\phi_g=1)} = 4.0$ and $a_d/\delta_{st} = 0.05$, (c/right) for cases with initial $a_d/\delta_{st} = 0.05$ and $\phi_{ov} = 0.8$.

It is worth noting that the initial values of $a_d/\delta_{st}$ and $\phi_{ov}$ do not have significant influences on the temporal evolution of $T_{max}$ and thus are not shown here. However, the influences of $a_d/\delta_{st}$ and $\phi_{ov}$ on the MIE can be illustrated by examining the temporal evolutions of the volume of the burned gases. In order to characterise the burned gas volume, it is useful to quantify the extent of completion of combustion from the unburned gas to the fully burned gas in terms of reaction progress variable $c$, which increases monotonically from 0 in the unburned
gas to 1.0 in the fully burned gas. The reaction progress variable $c$ in this analysis is defined here in terms of oxidiser mass fraction in the following manner (Wandel et al., 2009; Neophytou et al., 2010, 2012; Wandel, 2013, 2014; Ozel-Erol et al., 2018, 2019):

$$c = \frac{[(1 - \xi)Y_{O\infty} - Y_0]}{[(1 - \xi)Y_{O\infty} - \max(0, (\xi_{st} - \xi)/\xi_{st})Y_{O\infty}]}$$  \hspace{1cm} (16)$$

where $\xi = (Y_F - Y_0/s + Y_{O\infty}/s)/(Y_{F\infty} + Y_{O\infty}/s)$ is the mixture fraction (Bilger, 1988), $Y_{O\infty} = 0.233$ is the oxygen mass fraction in air, and $Y_{F\infty} = 1.0$ is the fuel mass fraction in the pure gaseous fuel stream. For n-heptane ($C_7H_{16}$) combustion, $s = 3.52$ leads to a stoichiometric mixture fraction value of $\xi_{st} = Y_{O\infty}/(sY_{F\infty} + Y_{O\infty}) = 0.0621$. The temporal evolutions of the volume of the burned gas region with $c \geq 0.9$ (i.e. $V_{c \geq 0.9}$) normalised by the spark volume (i.e. $V_{sp} = (4\pi/3)R_{sp}^3$) for different initial droplet diameters for initial $u'/S_{L(\phi_g=1)} = 4.0$ and $\phi_{ov} = 0.8$ (e.g. U04D03F08, U04D04F08 and U04D05F08) are exemplarily shown in Fig. 5a for their corresponding MIE inputs for self-sustained flame propagation. It can be seen from Fig. 5a that $V_{c \geq 0.9}/V_{sp}$ shows a decreasing trend with increasing $a_d/\delta_{st}$. This suggests that the critical volume of the burned gas for self-sustained combustion (i.e. $V_{crit} \approx (4\pi/3)(2.45\delta_{st})^3 \approx (4\pi R_{sp}^3/3) = V_{sp}$ according to Turns (2000)) is more readily obtained for smaller values of droplet diameter, which is indicative of a decreasing trend in $P_{MIE}^p$ with decreasing droplet diameter. In order to illustrate the influences of $\phi_{ov}$ on the burnt gas volume, the temporal evolutions of $V_{c \geq 0.9}/V_{sp}$ for cases with initial $u'/S_{L(\phi_g=1)} = 4.0$ and $a_d/\delta_{st} = 0.05$ (e.g. U04D05F08, U04D05F10, and U04D05F12) are exemplarily shown in Fig. 5b for their corresponding MIE inputs for self-sustained flame propagation. Figure 5b shows that $V_{c \geq 0.9}/V_{sp}$ increases with increasing $\phi_{ov}$ for a given set of values of $u'/S_{L(\phi_g=1)}$ and $a_d/\delta_{st}$, which suggests that the critical volume of the burned gas for self-sustained combustion is more readily obtained for higher values of $\phi_{ov}$, suggesting a
decreasing trend in $\Gamma_{MIE}^p$ with increasing overall equivalence ratio. Finally, the temporal evolutions of $V_{c>0.9}/V_{sp}$ for cases with initial $a_d/\delta_{st} = 0.05$ and $\phi_{ov} = 0.8$ (e.g. U00D05F08, U04D05F08, and U08D05F08) are exemplarily shown in Fig. 5c to illustrate the effects of $u'/S_L(\phi_g=1)$ on $\Gamma_{MIE}^p$, which reveals an increasing trend of $V_{c>0.9}/V_{sp}$ with decreasing $u'/S_L(\phi_g=1)$, indicating a decrease in energy requirement for obtaining the critical burned gas volume for self-sustained combustion, which leads to a decrease in $\Gamma_{MIE}^p$ with decreasing $u'/S_L(\phi_g=1)$.

**Table 2:** The MIE values of the droplet-laden mixtures normalised by the corresponding MIE values for homogeneous mixtures for the identical values of $u'/S_L(\phi_g=1)$ and $\phi_{ov}$.

<table>
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<th>Case</th>
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<th>$a_d/\delta_{st}$</th>
<th>$\phi_{ov}$</th>
<th>$\Gamma_{MIE}^g/(\Gamma_{MIE}^g)_p$</th>
<th>$\Gamma_{MIE}^p/(\Gamma_{MIE}^p)_p$</th>
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In Figs. 5a-c, an increasing trend of $V_{c20.9}/V_{sp}$ after the energy deposition period (i.e. $t \geq t_{sp}$) is indicative of self-sustained flame propagation. It is worth noting that for $\Gamma < \Gamma_{MIE}^p$ the normalised burned gas volume $V_{c20.9}/V_{sp}$ would either remain zero in the case of misfire (i.e. $\Gamma < \Gamma_{MIE}^i$) or decrease with time after thermal runaway before vanishing eventually for $\Gamma_{MIE}^i < \Gamma < \Gamma_{MIE}^p$. If a larger amount of energy than the MIE (i.e. $\Gamma > \Gamma_{MIE}^p$) was to be deposited, both a higher value of $T_{max}$ would be observed, and the $V_{c20.9}/V_{sp}$ profiles would be qualitatively similar to the ones corresponding to $\Gamma = \Gamma_{MIE}^p$ but their magnitude would be higher. Interested readers are directed to Papapostolou et al. (2019) where the amount of energy deposited was greater than the respective MIE for self-sustained flame propagation (i.e. $\Gamma > \Gamma_{MIE}^p$) for every case investigated for near-identical parameters to the present study. The behaviours illustrated in Figs. 5a-c remain valid across all the cases considered here and thus are not shown here for the sake of brevity.

It can be seen from Fig. 3 that both $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$ values for the quiescent laminar cases with $\phi_{ov} = 1.0$ remain greater than unity, which suggest that the MIEs for the quiescent laminar droplet-laden mixtures with $\phi_{ov} = 1.0$, even only for obtaining thermal runaway remain greater than the MIE value for self-sustained flame propagation for the quiescent laminar homogeneous stoichiometric n-heptane-air mixture. The MIE values of the droplet-laden mixtures normalised by the corresponding MIE values for homogeneous mixtures for the identical values of $u'/S_l(\phi_g=1)$ and $\phi_{ov}$ are listed in Table 2. It can be seen from Table 2 that $\Gamma_{MIE}^p/(\Gamma_{MIE}^p)_p$ remains greater than unity for droplet cases where $(\Gamma_{MIE}^p)_p = [IE]_{\phi_g=\phi_{ov}}/MIE_{l \phi_g=1.0}$ is the normalised MIE for self-sustained flame propagation for the corresponding turbulent homogeneous mixture with $\phi_g = \phi_{ov}$. A similar qualitative behaviour has been
observed for $\Gamma_{MIE}^i/\left(\Gamma_{MIE}^i\right)_p$. This suggests that the MIE requirements for the droplet-laden mixtures are greater than those for homogeneous gaseous mixtures. This behaviour is expected because a part of the input energy is utilised to evaporate the droplets. However, this contribution is not solely responsible for $\Gamma_{MIE}^i/\left(\Gamma_{MIE}^i\right)_p > 1$, because the value of $\Gamma_{MIE}^i$ in comparison to $\left(\Gamma_{MIE}^i\right)_p$ changes in response to the variations of initial values of $u'/S_{L(\phi_g=1)}$, $a_d/\delta_{st}$ and $\phi_{ov}$. In order to explain this behaviour, the probability density functions (PDFs) of gaseous equivalence ratio $\phi_g$ at $t = 5.0 t_{sp}$ are exemplarily shown in Fig. 6. It is evident from Fig. 6 that the gaseous phase combustion for all the droplet cases takes place under fuel-lean conditions in comparison to the overall equivalence ratio (i.e. $\phi_g < \phi_{ov}$) and the probability of obtaining $\phi_g \geq \phi_{ov}$ decreases with increasing (decreasing) normalised droplet diameter $a_d/\delta_{st}$ (overall equivalence ratio $\phi_{ov}$). This behaviour originates due to the smaller evaporation rate of larger droplets, and the predominance of $\phi_g < \phi_{ov}$ in the gaseous phase for combustion of droplet-laden mixtures is consistent with several previous analyses (Neophytou and Mastorakos, 2009; Wacks et al., 2016; Ozel-Erol et al., 2018; Papapostolou et al., 2019).

The lean and rich flammability limits are shown in Fig. 6, which reveal that the probability of finding flammable gaseous mixtures decreases with increasing droplet diameter. Across all cases, the probability of finding gaseous mixtures within the flammability limits is significantly higher for initial $a_d/\delta_{st} = 0.03$ cases than that for the corresponding initial $a_d/\delta_{st} = 0.04$ and 0.05 cases, and in the initial $a_d/\delta_{st} = 0.04$ and 0.05 cases the PDFs of $\phi_g$ peak at, or below the lean flammability limit. It is well-known that the MIE values increase with decreasing $\phi_g$ for the fuel-lean gaseous mixtures and therefore the predominance of $\phi_g < 1.0$
in the droplet cases yields \( \Gamma_{MIE}^i / (\Gamma_{MIE}^i)_p > 1.0 \) and \( \Gamma_{MIE}^p / (\Gamma_{MIE}^p)_p > 1.0 \) for all droplet cases considered here (see Table 2).

It can further be seen from Fig. 6 the PDFs of \( \phi_g \) for the initial \( a_d/\delta_{st} = 0.04 \) and 0.05 cases exhibit similar behaviour (peaking outside the lean flammability limit), but the PDFs of the initial \( a_d/\delta_{st} = 0.03 \) cases indicate a significantly higher likelihood of encountering flammable mixtures than for other droplet sizes considered here. Accordingly, both \( \Gamma_{MIE}^i \) and

---

**Figure 6:** PDFs of equivalence ratio in the gaseous phase \( \phi_g \) in the region given by \( 0.1 \leq c \leq 0.9 \) for all cases at \( t = 5.0t_{sp} \) for \( \Gamma = \Gamma_{MIE}^p \) in the case of initial normalised droplet size \( a_d/\delta_{st} = 0.03, 0.04 \) and 0.05 (from left to right) and initial turbulence intensity \( u'/S_{\phi=1} = 0.0, 4.0 \) and 8.0 (from top to bottom) in the case of \( \phi_{av} = 0.8 \) (black), 1.0 (blue) and 1.2 (red). The vertical dashed black lines indicate flammability limits, whilst the vertical bold dotted lines indicate initial \( \phi_{av} \) and are colour coded respectively.

---
\( \Gamma_{MIE}^p \) requirements drastically increase from D03 to D04 cases, but minimally increase from D04 to D05 cases, as can be seen from Fig. 3, and it must also be mentioned that \( \phi_{ov} \) also has a smaller but a significant influence on the MIE values.

As \( \phi_{ov} \) increases so does the probability of finding \( \phi_g \) close to unity, thus allowing for easier thermal runaway and subsequent self-sustained flame propagation, which in turn corresponds to smaller \( \Gamma_{MIE}^i \) and \( \Gamma_{MIE}^p \) requirements, as observed in Fig. 3. The effects of \( \phi_{ov} \) are consistent for all cases, but these effects weaken with increasing \( a_d/\delta_{st} \) and \( u'/S_L(\phi_g=1) \), as illustrated by the cases with initial \( a_d/\delta_{st} = 0.05 \), where the variations in \( \phi_{ov} \), marginally affect the profiles and peak values of the PDFs of \( \phi_g \). Figure 6 indicates that the peaks of the PDFs of \( \phi_g \) slightly shift towards leaner conditions for higher values of \( u'/S_L(\phi_g=1) \), but these effects are marginal when compared to the effects induced by the change in initial droplet diameter and \( \phi_{ov} \). For large values of \( u'/S_L(\phi_g=1) \) the evaporated fuel is dispersed more readily from the evaporation sites due to enhanced turbulence mixing, which increases the likelihood of obtaining leaner mixtures with increasing turbulence intensity. A similar qualitative behaviour was observed in previous analyses (Ozel-Erol et al., 2018; Papapostolou et al., 2019). In addition to the increased eddy thermal diffusivity and heat transfer rate from the hot gas kernel, the increased likelihood of obtaining leaner gaseous phase mixture acts to increase \( \Gamma_{MIE}^i \) and \( \Gamma_{MIE}^p \) with increasing turbulence intensity for droplet-laden mixtures.

The composition of the fuel-air mixture in the gaseous phase resulting from droplet evaporation affects the subsequent combustion behaviour. This can be illustrated by analysing the behaviour of the flame index \( \phi \) within the flame (i.e. \( 0.1 \leq c \leq 0.9 \)). The flame index \( \phi \) can be defined as (Briones et al., 2006):
\[
\psi = \frac{1}{2} \frac{\xi - \xi_{st}}{|\xi - \xi_{st}|} \left(1 + \frac{\nabla Y_F \cdot \nabla Y_O}{|\nabla Y_F| \cdot |\nabla Y_O|}\right)
\]  

(17)

According to the definition, \( \psi = -1.0 \) and \( \psi = 1.0 \) indicate fuel-lean and fuel-rich premixed combustion respectively, whereas \( \psi = 0 \) is indicative of non-premixed (diffusion mode) combustion. The PDFs of the flame index \( \psi \) in the region corresponding to \( 0.1 \leq c \leq 0.9 \) at \( t = 5.0 t_{sp} \) are exemplarily shown in Fig. 7 but a similar qualitative behaviour has been observed for other time instants. It is evident from Fig. 7 that the combustion process predominantly takes place under fuel-lean premixed and non-premixed modes. The diffusion flame is stabilised at the stoichiometric mixture (i.e. \( \phi_g = 1.0 \)) and thus the non-dimensional maximum temperature \( T_{max} \) settles to unity long after the energy deposition duration (i.e. \( t \gg t_{sp} \)) in the case of self-sustained flame propagation irrespective of the values of turbulence intensity, droplet diameter and droplet number density. It can be seen from Fig. 7 that the probability of obtaining \( \psi = 0 \) (i.e. non-premixed combustion) increases with increasing \( u'/S_{L(\phi_g=1)} \). This behaviour originates due to the strengthening of diffusion of fuel vapour from the droplet sites with the surrounding air under high turbulence intensities. The aforementioned trend is observed for the \( \phi_{ov} = 0.8 \) cases irrespective of droplet diameters investigated in the present study. This observation can be attributed to the increased level of mixing of the fuel from the evaporated droplets, which is driven by turbulence. It can also be seen from Fig. 7 that the probability of finding \( \psi = 0 \) increases with increasing \( \alpha_d/\delta_{st} \) due to the slower evaporation rate for larger droplets, which gives rise to increased mixture inhomogeneity, and in turn increases the extent of the non-premixed mode of burning. As shown in Fig. 7, fuel-lean premixed mode of burning is predominantly obtained for \( \phi_{ov} = 0.8 \) and 1.0, and the occurrence of fuel-rich premixed flames becomes more likely when \( \phi_{ov} = 1.2 \). This is consistent with the predominance of \( \phi_g < \phi_{ov} \) in the \( \phi_{ov} = 0.8 \) and 1.0 cases, as demonstrated in Fig. 6. In the case of \( \phi_{ov} = 1.0 \) and 1.2, the probability of finding fuel-rich
premixed combustion mode (i.e. $\psi = 1.0$) is predominantly obtained for initial $a_d/\delta_{st} = 0.03$ and 0.04 cases due to the relatively high probability of finding $\phi_g > 1.0$ as a result of rapid evaporation of small droplets (see Fig. 7).

Figure 7: PDFs of flame index $\psi$ in the region given by $0.1 \leq c \leq 0.9$ for $\Gamma = \Gamma_{MIE}^P$ at $t = 5.0t_{sp}$ for initial $a_d/\delta_{st} = 0.03, 0.04$ and 0.05 (from left to right) and overall equivalence ratios $\phi_{ov} = 0.8, 1.0$ and 1.2 (from top to bottom), in the case of laminar (black), initial $u'/S_{L\phi_g=1} = 4.0$ (blue) and initial $u'/S_{L\phi_g=1} = 8.0$ (red) conditions.

Figure 7 further demonstrates that the likelihood of fuel-lean burning (i.e. $\psi = -1$) increases with increasing turbulence intensity and droplet diameter but with decreasing overall equivalence ratio. This is reflected in the decreasing trends of $V_{c=0.9}/V_{sp}$ with increasing initial
values of $u'/S_{L(\phi_g=1)}$ and $a_d/\delta_{st}$ and with decreasing $\phi_{ov}$ as a result of the weak burning rate of fuel-lean mixtures.

It is worth noting that successful thermal runaway as a result of external energy addition and subsequent flame propagation for the minimum ignition energy input are stochastic events and therefore sensitive to the realisations of turbulent flow conditions. In experimental investigations, a success rate of 50% across numerous turbulent realisations (at least 30 as reported by Shy et al., 2010) is required to ascertain the MIE value for a certain case, which is impossible to adopt for a DNS-based analysis due to the high computational cost associated with it. Therefore, to investigate the stochastic nature of thermal runaway and subsequent flame propagation for the MIE input, two additional simulations have been carried out for the energies corresponding to $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$ for each case under different realisations of statistically identical conditions (i.e. $u'/S_{L(\phi_g=1)}$ and $l_{t}$) of the initial turbulent flow field. The findings for the above analysis are summarised in terms of the number of successful thermal runaway and self-sustained propagation events in Fig. 8. It is worth noting that the MIE requirements are evaluated based on only one turbulent realisation (i.e. realisation S01) due to the computational cost arising from needing multiple simulations to ascertain the MIE for a certain set of parameters. This inherently means that successful thermal runaway and self-sustained flame propagation are always obtained for one of the turbulent realisations (mentioned as the realisation S01 in Fig. 8) for $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$, respectively. It can be seen from Fig. 8 that across all three turbulent realisations investigated for both $\Gamma_{MIE}^i$ and $\Gamma_{MIE}^p$, successful events were observed for at least 2 out of the three turbulent realisations.

Figure 8 shows that misfire is observed for only two cases with initial $u'/S_{L(\phi_g=1)} = 4.0$ (U04D03F10 and U04D03F12) for the realisation S02, out of all the cases investigated. As
demonstrated in Fig. 4, thermal runaway for the cases with initial \( u'/S_{L(\phi_g=1)} = 4.0 \) takes place as a result of autoignition. The possibility of autoignition depends on the statistical behaviour and the magnitude of scalar dissipation rate (SDR) of mixture fraction \( D \nabla \xi \cdot \nabla \xi \) values at the location of energy deposition (Mastorakos et al., 1997, 2017). Therefore, a misfire takes place for the realisation S02 in the U04D03F10 and U04D03F12 cases if the gaseous phase mixture is either too fuel-lean or SDR values are too high to allow thermal runaway. However, for the cases with initial \( u'/S_{L(\phi_g=1)} = 8.0 \), the maximum value of \( T_{max} \) is obtained within the energy deposition period for the MIE (see Fig. 4), which ensures that the temperature to result in a thermal runaway is created while energy is being externally deposited and this reduces the uncertainty in terms of obtaining thermal runaway. Thus, the turbulent realisation is not expected to play a significant role on the success of thermal runaway. However, obtaining successful self-sustained propagation after a thermal runaway is highly dependent on the turbulent conditions at times long after the energy deposition period (i.e. \( t \gg t_{sp} \)) and thus the realisation of the turbulent flow field plays an important role in determining whether self-sustained propagation is obtained. It can be seen from Fig. 8 that a failed propagation is obtained for realisation S02 is in the cases U04D03F10 and U04D03F12, which is in line with misfire for these cases for this particular turbulent flow realisation, although successful thermal runaway is achieved for the MIE for self-sustained flame propagation because \( \Gamma_{MIE}^p \) is greater than \( \Gamma_{MIE} \). Failed self-sustained flame propagation for realisation S03 is observed for the initial \( u'/S_{L(\phi_g=1)} = 4.0 \) cases with initial \( a_d/\delta_{st} = 0.05 \) for \( \phi_{ov} = 0.8 \) and 1.0. The evaporation rate for large droplets (e.g. \( a_d/\delta_{st} = 0.05 \)) is small and therefore the probability of finding flammable mixtures is relatively small in the cases with the small/moderate values of droplet number density (see Fig. 6). Thus, the resulting flame eventually extinguishes for \( t \gg t_{sp} \) due to the long mode of quenching (Mastorakos, 2007) if the flame kernel does not encounter a sufficient amount of flammable mixture during its evolution, and the heat transfer rate from
the hot gas kernel overcomes heat release rate. For initial $u'/S_{L(\phi_g=1)} = 8.0$ cases successful self-sustained combustion has been obtained for all cases for realisations S01 and S03 for the energy input corresponding to $\Gamma_{MIE}^p$ but successful self-sustained flame propagation is observed for the U08D03F08 and U08D03F10 cases for realisation S02. The evaporation rate is high for small droplets and thus a flammable mixture is more readily obtained for initial $a_d/\delta_{st} = 0.03$ cases amongst all the droplet sizes considered here. Thus, self-sustained combustion is more readily obtained for different turbulent flow realisations for an external energy input corresponding to $\Gamma = \Gamma_{MIE}^p$ for $\phi_{ov} = 0.8$ and 1.0 cases. Although the evaporation rate is high for droplets with initial $a_d/\delta_{st} = 0.03$, the number of evaporation sites are greater in the $\phi_{ov} = 1.2$ case than in the $\phi_{ov} = 0.8$ and 1.0 cases. This gives rise to larger SDR $D \nabla \xi \cdot \nabla \xi$ in the $\phi_{ov} = 1.2$ case, which makes successful self-sustained combustion comparatively less likely than in the $\phi_{ov} = 0.8$ and 1.0 cases, which is reflected in the failure to obtain successful self-sustained flame propagation in the case of initial $u'/S_{L(\phi_g=1)} = 8.0$ and $a_d/\delta_{st} = 0.03$ for realisation S02.

Although the majority of realisations lead to successful thermal runaway or/and self-sustained flame propagation for the MIE input evaluated for realisation S01, it is worth emphasising that compared to a typical MIE from experiments, i.e. the energy leading to a probability of self-sustained flame establishment of 50%, a more statistically representative sample would be required to ascertain the precise MIE values. However, this becomes extremely expensive to obtain a more statistically representative sample using DNS and therefore only 3 realisations have been considered here. Therefore, any comparison between the MIE values from DNS and experiments should be conducted with the acknowledgement of the differences in the evaluation methodology and the level of statistical convergence.
Figure 8: Number of successful events out of three different turbulent realisations (S01, S02, S03) across all turbulent cases investigated for only successful thermal runaway (i.e. $\Gamma = \Gamma^{i}_{MIE}$ (top row) and for successful self-sustained flame propagation (i.e. $\Gamma = \Gamma^{p}_{MIE}$ bottom row).

To understand the physical mechanisms that govern the stochastic nature of thermal runaway and self-sustained flame propagation after a successful thermal runaway, the budget of the terms in the energy conservation equation (Eq. 15) for the selected cases has been extracted at specified time instants for different turbulent realisations. Care has been taken to select the characteristic cases for which a misfire/failed self-sustained propagation was observed for a specific turbulent realisation, and the energy budget for the unsuccessful realisation was then compared with the energy budget arising from a successful realisation. As outlined previously in the discussion regarding Fig. 8, the only difference between the cases investigated here is
the turbulent realisation as everything else is kept the same \((a_{sp}, \text{initial } u'/S_{L(\phi_{\text{st}}=1)}, a_d/\delta_{st}, \phi_{\text{ov}} \text{ and droplet distribution})\), and thus a successful or failed thermal runaway/self-sustained arises solely due to the nature of a particular turbulent flow realisation. For this reason, two characteristic cases, which illustrate the stochasticity in terms of thermal runaway and self-sustained propagation, respectively are exemplarily shown in Fig. 9.

As the energy budget in Fig. 9 is shown at \(t > t_{sp}\), the term \(q'''\) (see Eq. 15 for all terms) is identically zero because the energy deposition has already been completed, and thus is not shown to preserve clarity. The viscous term \(D_1\), which is also not shown here to preserve clarity, is not a leading order contributor and does not play any significant role in thermal runaway and subsequent flame propagation dynamics, as found in a previous analysis (Turquand d’Auzay et al., 2019). The convective \(C_1\) and the pressure work \(P_1\) terms follow similar trends, being predominantly negative, as they are affected by dilatation rate induced by thermal expansion. The mean values of \(C_1\) and \(P_1\) conditional on \(T\) exhibit negative values as the reactants are pushed outwards, which is consistent with previous findings (Turquand d’Auzay et al., 2019). The mean value of the heat release term \(\dot{\omega}_T\) conditional upon \(T\) remains deterministically positive, whereas the mean value of the molecular diffusion term \(D_2\) assumes positive values on the unburned gas side before exhibiting negative values towards the burned gas side of the flame. The mean value of the evaporation contribution \(\dot{S}_e\) assumes non-negligible magnitudes at the leading edge of the flame front but its magnitude in comparison to that of \(\dot{\omega}_T\) and \(D_2\) remains negligible for the majority of the flame.
To investigate the effects that different realisations of turbulence have on the thermal runaway, the energy budgets for the cases U04D03F10S02 and U04D03F10S03 at $t = 2.0t_{sp}$ (when the energy input by the ignitor is equal to zero) are presented in Fig. 9a. It has already been demonstrated in Fig. 4 that thermal runaway in cases with initial $u'/S_{L(\phi = 1)} = 4.0$ occurs as a result of autoignition at around $t = 1.5t_{sp}$. As outlined in Fig. 8, a misfire is obtained for S02 realisation and this is also reflected by the energy budget, where the terms in the energy transport equation including the heat release term $\dot{\omega}_T$ are of significantly smaller magnitude than those observed for a thermal runaway as is the case for S03 realisation. The maximum value of $T_{max}$ is obtained at approximately $2.0t_{sp}$ if a successful autoignition is to be observed, and this occurs for S03 and is reflected by the corresponding energy budget. However, $T_{max}$
decreases rapidly after the energy deposition period in the absence of thermal runaway for S02 realisation, and thus the magnitudes of the terms of the energy conservation equation remain small.

Moving onto the energy budgets in Fig. 9b for the turbulent realisations S01 and S02 for the case U08D04F12 extracted at \( t = 5.0t_{sp} \) for \( \Gamma = \Gamma_{MIE}^{P} \), a successful self-sustained propagation is expected for S01 realisation, but a failed propagation is to be observed for S02 realisation according to the observations made from Fig. 8. The behaviour of all the terms are similar for realisations S01 and S02 but there are some subtle differences. Regarding the thermal diffusion rate term \( D_2 \) for S01 realisation, its mean value remains positive for higher values of \( T \) than that observed for S02 realisation. Additionally, there are significant differences in the magnitude of the mean value of the heat release term \( \dot{\omega}_T \), which as expected is positive for both realisations, but for the realisation (i.e. S01) which leads to successful self-sustained flame propagation \( \dot{\omega}_T \) has a higher magnitude than in the realisation (i.e. S02) where a failed propagation is obtained. The mean contributions of the convective and pressure terms in these cases play a minor role, due to their small magnitudes and exhibit the same qualitative and quantitative behaviour between these different turbulent flow realisations.

It is worth noting that the inertial effects can potentially play an important role (Lawes and Saat, 2011) in droplet-laden mixtures, especially for large values of \( u'/S_{\phi} \) and \( a_d/\delta_{st} \) (i.e. Stokes number is high under these conditions). The initial droplet distribution (i.e. at \( t = 0 \)) was identical for all turbulent flow realisations but the number of droplets the kernel interacts with changes from one realisation to another as time advances. The variability of the number of droplets in the vicinity of the ignitor, and thus also the kernel at early times (\( t < 2.0t_{sp} \)), can play a role in deciding the likelihood of obtaining successful thermal runaway and
subsequent self-sustained flame propagation, especially for large values of $u'/S_{t(\phi_o=1)}$ and $a_d/\delta_{st}$. In order to demonstrate this, a sphere with $r = 3R_{sp}$ has been taken as a control volume ($V_{cv}$), as it encompasses the growing kernel across all cases within its volume for up to $t = 2.0t_{sp}$. The initial droplet number density is the same for a given set of $a_d/\delta_{st}$ and $\phi_{ov}$ values for all realisations, and thus the number density of droplets normalised by its initial value (i.e. $t = 0$) within $V_{cv}$ (i.e.$V_{cv} = 4/3\pi(3R_{sp})^3$ at the centre of the domain) at $t = t_{sp}$ and $t = 2.0t_{sp}$ for S01, S02 and S03 realisations in Fig. 8 are listed in Table 3 for $\Gamma = \Gamma_{MIE}^i$.

Table 3: The number density of droplets normalised by its initial value (i.e. $t = 0$) within $V_{cv}$ (i.e.$V_{cv} = 4/3\pi(3R_{sp})^3$ at the centre of the domain) for S01, S02 and S03 realisations at $t = t_{sp}$ and $t = 2.0t_{sp}$ for $\Gamma = \Gamma_{MIE}^i$. in all turbulent cases shown in Fig. 8.

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</table>

Although the normalised droplet number densities within $V_{cv}$ are shown in Table 3 for $\Gamma = \Gamma_{MIE}^i$, the qualitative behaviour remains unchanged for $\Gamma = \Gamma_{MIE}^P$. The number density of the
droplets decreases with time for the cases where thermal runaway is observed. This decrease in number density may occur due to evaporation, which acts to produce flammable mixture in the vicinity of the energy deposition location. However, the chosen control volume is not impermeable, and thus the number of droplets found within the control volume can also increase and decrease as turbulence interacts with droplets and moves them. Thus, the change of normalised droplet number density within the control volume, as time advances is not conclusive on its own in indicating whether a misfire, or a thermal runaway would occur for $\Gamma = \Gamma_{MIE}^i$ (alternatively if thermal runaway and subsequent self-sustained propagation can be obtained for $\Gamma = \Gamma_{MIE}^p$). Simultaneous occurrences of a reduction in droplet number density and an increase in the gaseous phase equivalence ratio within $V_{cv}$ with time are indicative of the availability of gaseous fuel vapour as a result of droplet evaporation. To investigate this further, it is worthwhile to analyse the histograms of the number $N$ of samples with $\phi_g$ normalised by the total number of samples available within $V_{cv}$ (i.e. $N_{cv}$, which is identical for all cases) at $t = t_{sp}$ and $2t_{sp}$ for the cases presented in Table 3. For brevity, the histograms are shown in Fig. 10a for all the cases with initial $u'/S_{L(\phi_g=1)} = 4.0$ and $a_d/\delta_{st} = 0.03$, for $\Gamma = \Gamma_{MIE}^i$ at $t = t_{sp}$ and $t = 2t_{sp}$ across all turbulent realisations. The trends observed in Fig. 10 hold across all turbulent cases shown in Fig. 8.
Figure 10: (a) Histograms of number of samples $N$ corresponding to a particular gaseous equivalence ratio $\phi_g$ normalised by the total number of samples within the control volume $N_{cv}$ for different ranges of the gaseous phase equivalence ratio $\phi_g$ within $V_{cv}$ at $t = 1.0t_{sp}$ (blue bars) and $t = 2.0t_{sp}$ (red bars) for $\Gamma = \Gamma_{Blank}$ in the case of initial normalised droplet size $a_d/\delta_{st} = 0.03$ and initial turbulence intensity $u'/S_L(\phi_g=1) = 4.0$ for $\phi_{ov} = 0.8$, 1.0 and 1.2 (from top to bottom) across all realisations S01, S02 and S03 (from left to right). The vertical dashed lines indicate $\phi_{g_{mean}}$ at the respective time instants. The black dotted vertical lines at $\phi_g = 0.6$ and 1.5 show the lean and rich flammability limit; (b) Same as (a) but the magnified views of histograms are shown within the lean and rich flammability limits.
Figure 10a shows that the histograms are similar at \( t = t_{sp} \), and thus not much insight can be gleaned from them. An increase in \( \phi_{ov} \) (top to bottom) leads to an increased number of samples with gaseous equivalence ratio above the lean flammability limit, which can be substantiated from Fig. 10b where the histograms of samples within \( V_{cv} \) for different values of \( \phi_g \) within the lean and rich flammability limits are shown. The mean value of the gaseous equivalence ratio \( \phi_g \) within the control volume (i.e. \( \left( \phi_g^{mean} \right)_{cv} \)) increases with time due to the increased availability of gaseous fuel vapour as a result of evaporation of droplets. It is worth noting that the profiles of the histograms, and \( \left( \phi_g^{mean} \right)_{cv} \) are near identical at \( t = t_{sp} \) across the different turbulent realisations (left to right). This is also reflected in the number density of droplets within \( V_{cv} \), which does not differ significantly between realisations at \( t = t_{sp} \) (see Table 3). However, at \( t = 2.0t_{sp} \) the distributions of the histograms are different for different turbulent realisations. Referring to Fig. 8, misfires are observed for realisation S02 for cases U04D03F10 and U04D03F12. The S02 realisation in cases U04D03F10 and U04D03F12 exhibits smaller mean values of \( \phi_g \) (i.e. \( \left( \phi_g^{mean} \right)_{cv} \)) than that found for the S03 realisation for \( \phi_{ov}=1.0 \) and 1.2. This is consistent with higher number density of droplets within \( V_{cv} \) for the S02 realisation than in the S03 realisation. The higher value of \( \left( \phi_g^{mean} \right)_{cv} \) in the S03 realisation acts to increase the possibility of successful thermal runaway occurring in comparison to the S02 realisation for cases U04D03F10 and U04D03F12. However, \( \left( \phi_g^{mean} \right)_{cv} \) between S01 and S02 realisations is very similar for cases U04D03F10 and U04D03F12, but Fig. 10b reveals that both S01 and S03 realisations show more samples within the flammable range than in the case of S01 realisation. Thus, the differences in droplet number density and the distribution of gaseous phase equivalence ratio (i.e. availability of flammable mixture and SDR of mixture
fraction) in the vicinity of the energy deposition location affect the statistical behaviours of $\dot{\omega}_T$ and $D_2$ in the energy conservation equation for localised ignition of droplet-laden mixtures.

The above discussion indicates that the variation of the turbulent realisation has a significant influence on the energy budget terms, which in turn govern whether successful thermal runaway or self-sustained flame propagation is observed for a particular turbulent realisation. This is principally governed by the competition between the leading order contributions of the heat release and thermal diffusion rate terms (i.e. $\dot{\omega}_T + D_2$). Effectively, a net positive mean value of $(\dot{\omega}_T + D_2)$ (i.e. $(\dot{\omega}_T + D_2) > 0$) is indicative of the iso-surface propagating into the unburnt mixture, whilst a net negative mean value (i.e. $(\dot{\omega}_T + D_2) < 0$) suggests that the hot gas kernel shrinks, as the positive heat release rate is overcome by the negative contribution of the heat transfer from the hot gas kernel as a result of thermal diffusion. Indeed, the mean value of $(\dot{\omega}_T + D_2)$ remains positive (i.e. $(\dot{\omega}_T + D_2) > 0$) throughout the flame for all the turbulent realisations where a successful self-sustained propagation is observed, whilst failed propagation (and also valid for failed thermal runaway) is observed where the mean value of $(\dot{\omega}_T + D_2)$ becomes negative (i.e. $\dot{\omega}_T + D_2) < 0$). This behaviour is also found to be qualitatively similar to the energy budget for localised forced ignition of turbulent homogeneous mixtures by Turquand d’Auzay et al. (2019).

5. CONCLUSIONS

The minimum ignition energy (MIE) for uniformly dispersed mono-sized n-heptane droplet-laden mixtures under homogeneous isotropic decaying turbulence has been numerically evaluated for a range of different initial turbulence intensities, droplet diameters and overall equivalence ratios. It has been demonstrated that a decrease in droplet diameter reduces the MIE requirement due to the faster evaporation of smaller droplets, thus leading to more readily
available flammable fuel-air mixture in the gaseous phase. These findings have been found to be in good qualitative agreement with experimental results of Danis et al. (1987). The availability of gaseous flammable mixture also increases with increasing overall equivalence ratio (or number density of droplets) and this leads to a reduction in the MIE requirement with increasing overall equivalence ratio. The MIE has been found to increase with increasing turbulence intensity and this increase in the MIE demand increases significantly for large turbulence intensities, which is consistent with previous findings in the case of turbulent homogeneous mixtures (Cardin et al., 2013a,b; Huang et al., 2007; Shy et al., 2010,2017; Jiang et al., 2018; Turquand d’Auzay et al., 2019). Additionally, it has been demonstrated that the MIE required for droplet laden mixtures remains greater than the MIE required for a corresponding homogeneous gaseous mixture. This behaviour arises from the fact that a part of the externally added energy is used to evaporate the droplets and also due to the predominantly fuel-lean mode of gaseous phase combustion. The tendency for fuel-lean combustion increases with increasing droplet size due to the slower evaporation of the larger droplets, and this tendency is also observed with decreasing overall equivalence ratio due to the reduced availability of the fuel vapour in the gaseous phase. It has also been found that finite probabilities of the occurrences of non-premixed combustion have also been observed in all cases in spite of predominant fuel-lean premixed combustion, and a small probability of fuel-rich premixed combustion has been observed for the smallest droplet diameter especially for fuel-rich overall equivalence ratios. It was found that a successful self-sustained propagation after the energy deposition period (i.e. \( t \gg t_{sp} \)) has been found to be critically dependent on the balance between the heat release rate and thermal diffusion rate terms in the energy conservation equation, exhibiting similarity to the previous findings for ignition of turbulent homogeneous gaseous mixtures (Turquand d-Auzay et al., 2019). It must be mentioned that the current analysis, excludes the effects of complex transport, low-temperature
kinetics, gas ionisation effects on the ignition process and their influences on the MIE for
turbulent droplet-laden mixtures. Although the qualitative nature of the results are not expected
to be affected by the choice of chemical mechanism, further investigation with detailed
chemistry and transport will form the basis of future investigations.

APPENDIX

The temporal evolutions of rms turbulent velocity fluctuation $u$, integral length scale $L_{turb} = k^{1.5}/\varepsilon$
(where $k$ and $\varepsilon$ are turbulent kinetic energy and its dissipation rate evaluated over the whole
domain) and turbulent Reynolds number $Re_L = \rho_0 u' L_{turb} / \mu$ normalised by their initial values
for initial values of $u'/S_{L(\phi_d=1)} = 4.0$ and $8.0$ for $\phi_{ov} = 1.0$ are shown in Fig. 11 for different
values of $a_d/\delta_{st}$ along with the corresponding temporal decays of purely gaseous turbulence
with no chemical reactions. The trend is the same for other values of $\phi_{ov}$ and thus they are not
shown here.

It can be seen from Fig. 11 that the decay rates of $u'$, $L_{turb}$ and $Re_L$ for droplet-laden reacting
cases is not hugely different from the non-reacting purely gaseous turbulent cases, with the
non-reacting cases exhibiting a slightly faster rate of decay than the droplet-laden reacting
cases. At the end of the energy deposition duration both $L_{turb}$ and $u'$ decay slightly from their
initial values. As the kernel grows the exothermic chemical reaction results in thermal energy
that raises the gas temperature and lowers its density, causing the hot gas kernel to expand, thus
creating a local source of kinetic energy, resulting in the slight differences observed between
the reacting and non-reacting cases.
Figure 11: Temporal evolutions of $u'$ (top row), $L_{turb}$ (middle row) and $Re_L$ (bottom row), normalised by their respective initial values ($u'_0$, $L_{turb}^0$ and $Re_L^0$ respectively), for all turbulent cases with $\phi_{ov} = 1.0$. Blue indicates cases with initial $u'/S_L(\phi_g=1) = 4.0$, and red indicates cases with initial $u'/S_L(\phi_g=1) = 8.0$, whilst the circle markers indicate the corresponding purely gaseous turbulence with no chemical reactions. The dashed vertical black line indicates the end of the energy deposition duration.

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REFERENCES


FIGURE CAPTIONS

Figure 1: Instantaneous views of $T = 0.7$ isosurface coloured by local values of normalised fuel reaction rate magnitude $|\dot{\omega}_f| \times \delta_Z/\rho_0 S_L(\phi_g=1)$ at $t = 2.0t_{sp}$, $5.0t_{sp}$ and $8.0t_{sp}$ (from left to right) for cases U04D04F08, U04D04F10, U04D04F12 (from top to bottom) for the respective MIE for self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}^P$) for each case.

Figure 2: Isosurfaces of $T = 0.7$ at $t = 2.0t_{sp}$ (blue), $5.0t_{sp}$ (green) and $8.0t_{sp}$ (magenta), with the energy deposition region indicated by the red sphere, obtained for $\Gamma = \Gamma_{MIE}^P$ for $\phi_{ov} = 1.0$ cases with laminar, initial $u'/S_L(\phi_g=1) = 4.0$ and initial $u'/S_L(\phi_g=1) = 8.0$ (from top to bottom) for initial $a_d/\delta_{st} = 0.03, 0.04$ and $0.05$ (from left to right). The vertical black line indicates the centre of the domain.

Figure 3: Normalised MIE variations only for successful thermal runaway $\Gamma_{MIE}^I$ (left), and for successful self-sustained propagation, $\Gamma_{MIE}^P$ (right) for different initial values of $u'/S_L(\phi_g=1)$, $a_d/\delta_{st}$ and $\phi_{ov}$.

Figure 4: Temporal evolution of maximum non-dimensional temperature, $T_{max}$ for the minimum ignition energy inputs for self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}^P$) in the case of different turbulence intensities for initial $a_d/\delta_{st} = 0.05$ and $\phi_{ov} = 1.2$.

Figure 5: Temporal evolution of the volume of the burned gas region with $c \geq 0.9$ (i.e. $V_{ce0.9}$) normalised by the spark volume (i.e. $V_{sp} = (4\pi/3)r_{sp}^3$) in the case of MIE input for successful self-sustained flame propagation (i.e. $\Gamma = \Gamma_{MIE}^P$): (a/left) for different initial droplet diameters for initial $u'/S_L(\phi_g=1) = 4.0$ and $\phi_{ov} = 0.8$, (b/centre) for cases with initial $u'/S_L(\phi_g=1) = 4.0$ and $a_d/\delta_{st} = 0.05$, (c/right) for cases with initial $a_d/\delta_{st} = 0.05$ and $\phi_{ov} = 0.8$.

Figure 6: PDFs of equivalence ratio in the gaseous phase $\phi_g$ in the region given by $0.1 \leq c \leq 0.9$ for all cases at $t = 5.0t_{sp}$ for $\Gamma = \Gamma_{MIE}^P$ in the case of initial normalised droplet size $a_d/\delta_{st} = 0.03, 0.04$ and $0.05$ (from left to right) and initial turbulence intensity.
\( u' / S_L(\phi_g = 1) = 0.0, 4.0 \) and 8.0 (from top to bottom) in the case of \( \phi_{ov} = 0.8 \) (black), 1.0 (blue) and 1.2 (red). The vertical dashed black lines indicate flammability limits, whilst the vertical bold dotted lines indicate initial \( \phi_{ov} \) and are colour coded respectively.

**Figure 7:** PDFs of flame index \( \psi \) in the region given by \( 0.1 \leq c \leq 0.9 \) for \( \Gamma = \Gamma_{MIE}^p \) at \( t = 5.0t_{sp} \) for initial \( a_d / \delta_{st} = 0.03, 0.04 \) and 0.05 (from left to right) and overall equivalence ratios \( \phi_{ov} = 0.8, 1.0 \) and 1.2 (from top to bottom), in the case of laminar (black), initial \( u' / S_L(\phi_g = 1) = 4.0 \) (blue) and initial \( u' / S_L(\phi_g = 1) = 8.0 \) (red) conditions.

**Figure 8:** Number of successful events out of three different turbulent realisations (S01, S02, S03) across all turbulent cases investigated for only successful thermal runaway (i.e. \( \Gamma = \Gamma_{MIE}^i \) (top row) and for successful self-sustained flame propagation (i.e. \( \Gamma = \Gamma_{MIE}^p \) bottom row).

**Figure 9:** Budget of the mean values of the different terms (i.e. \( C_1 - solid line; \) pressure work term \( P_1 - dashed line; \) heat release \( \dot{\omega}_T - dotted line \) and thermal diffusion rate \( D_2 - dashed dotted line \) of the energy conservation equation (i.e. Eq. 14) conditional on non-dimensional temperature \( T \) for the U04D03F10 case (left), with \( \Gamma = \Gamma_{MIE}^i \) at \( t = 2.0t_{sp} \) in the case of two different turbulent realisations (S02 and S03), and for the U08D04F12 case (right), with \( \Gamma = \Gamma_{MIE}^p \) at \( t = 5.0t_{sp} \) in the case of two different turbulent realisations (S01 and S02). The line with star markers indicates the sum of the mean combined contribution of heat release and thermal diffusion rate \( (\dot{\omega}_T + D_2) \), whilst the line with circle markers indicates \( S' \). The terms for S02 in Fig. 9a are multiplied by 10 to increase readability as indicated in the legend.

**Figure 10:** (a) Histograms of number of samples \( N \) corresponding to a particular gaseous equivalence ratio \( \phi_g \) normalised by the total number of samples within the control volume \( N_{cv} \) for different ranges of the gaseous phase equivalence ratio \( \phi_g \) within \( V_{cv} \) at \( t = 1.0t_{sp} \) (blue bars) and \( t = 2.0t_{sp} \) (red bars) for \( \Gamma = \Gamma_{MIE}^i \) in the case of initial normalised droplet size \( a_d / \delta_{st} = 0.03 \) and initial turbulence intensity \( u' / S_L(\phi_g = 1) = 4.0 \) for \( \phi_{ov} = 0.8, 1.0 \) and 1.2
(from top to bottom) across all realisations S01, S02 and S03 (from left to right). The vertical dashed lines indicate \((\phi_g^{mean})_{cv}\) at the respective time instants. The black dotted vertical lines at \(\phi_g = 0.6\) and 1.5 show the lean and rich flammability limit; (b) Same as (a) but the magnified views of histograms are shown within the lean and rich flammability limits.

**Figure 11:** Temporal evolutions of \(u'\) (top row), \(L_{turb}\) (middle row) and \(Re_L\) (bottom row), normalised by their respective initial values \((u'_0, L_{turb}^0\) and \(Re_L^0\) respectively), for all turbulent cases with \(\phi_{av} = 1.0\). Blue indicates cases with initial \(u'/S_{L(\phi_g=1)} = 4.0\), and red indicates cases with initial \(u'/S_{L(\phi_g=1)} = 8.0\), whilst the circle markers indicate the corresponding purely gaseous turbulence with no chemical reactions. The dashed vertical black line indicates the end of the energy deposition duration.