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# Propagation of heterogeneous and homogeneous planar flames in fuel droplet mists



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### ABSTRACT

Propagation of one-dimensional planar flames laden with fuel droplets is theoretically investigated in this work. Localized homogeneous and heterogeneous flames are considered, characterized by different relative locations of dispersed droplets and propagating flame front. With the assumption of large activation energy for the chemical reaction, correlations describing flame propagation speed, flame temperature, evaporation onset front and completion front are derived. The influences of droplet and fuel properties on propagation of fuel-droplet-laden planar flames are studied. The results indicate that the flames are enhanced under fuel-lean conditions but weakened under fuel-rich conditions. Both effects are intensified with increased droplet mass loading. Fuel vapor and temperature gradient are observed in the post-flame evaporation zone of heterogeneous flames. Evaporation completion front location is considerably affected by the droplet diameter, but the evaporation onset front varies little with droplet properties. Flame bifurcation occurs with high droplet mass loading under fuel-rich mixture, leading to multiplicity of flame propagation speed as well as droplet evaporation onset and completion fronts. Sprayed fuels with larger latent heat of vaporization would weaken the flame enhancement effect under fuel-lean conditions, due to larger evaporation heat loss. Moreover, for homogeneous flames, evaporative heat loss only occurs in the pre-flame zone. However, for heterogeneous flames, heat loss from the post-flame evaporation zone becomes dominant for relatively large droplets. Besides, for fuel-lean mixtures laden with medium-sized fuel droplets, the propagation speed of heterogeneous flames increases with Lewis number, due to the enhanced fuel vapor diffusion in the post-flame zone.

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### 1. Introduction

Spray combustion has been widely used in different propulsion systems, e.g. internal combustion engines, gas turbines and liquid rocket engines (Lefebvre and McDonell, 2017). Liquid fuels have numerous advantages, including high energy capacity, easy accessibility and extensive supply sources. Generally, they are injected into the combustors in the form of liquid sheets, and then broken up into smaller droplets to generate fuel sprays or clouds. Efficient droplet evaporation and vapor mixing with the surrounding oxidizer are significant premises for subsequent combustion in gas phase. Due to the intrinsic complexity arising from interphase interactions and high relevance to engineering practice, numerous investigations have been conducted to understand the fundamental aspects of droplet-laden combustion.

The effects of dispersed fuel droplets on flame propagation speed are studied by many researchers. It is found that the flame

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https://doi.org/10.1016/j.ijmultiphaseflow.2020.103452 0301-9322/© 2020 Elsevier Ltd. All rights reserved. speed decreases with increasing liquid fuel loading and droplet size for overall lean and stoichiometric sprays (Ballal and Lefebvre, 1981). Then more effects (e.g. total equivalence ratio or carrier gas velocity) of droplets and oxidizer gas on flame speed are further studied with various hydrocarbon fuels by the same group (Myers and Lefebvre, 1986). Hayashi and Kumagai (1975) observed that the flame speed decreases with fuel loading for lean spray, but increases for rich spray. Nomura et al. (2007, 2000, 1998) found that the flame speed of fuel droplet-vapor-air mixtures exceeds that of premixed gaseous of the same total equivalence ratio in the fuel-lean and fuel-rich regions of the total equivalence ratio. Atzler et al. (2006) observed that the burning rates of isooctane/air aerosols are markedly affected by droplet diameter only when the equivalence ratio is high. Similar results are also measured by Bradley et al. (2014), through further analyzing equivalence ratio and droplet size effects on flame propagation speed of isooctane and ethanol aerosols.

Meanwhile, simulations of laminar flame propagation in fuel droplet mists are also available. They can provide supplemental insights about detailed flame and/or droplet dynamics, besides confirming the relations between flame speed and various properties of two phases in droplet-laden flames. For instance, droplet evaporation behind the flame front may result in reactant stratification and localized diffusion flames (Aggarwal and Sirignano, 1985; Continillo and Sirignano, 1989; Seth et al., 1980). It is also seen by Neophytou and Mastorakos (2009) that with low pressure and temperature, which correspond to the conditions of engine relight at high altitudes, the effects of pressure and temperature on droplet evaporation are competitive to the gas equivalence ratio and flame speed.

In most of the above studies, how instantaneous distributions of evaporating droplets influence laminar flame propagation is not highlighted. In reality, droplets with large diameters may travel across the flame front to the post-flame zone and continue evaporating there, while small droplets can complete evaporation in the pre-flame zone and the mixture is homogeneous at the flame front. These phenomena have been observed by numerous experimental studies (Sulaiman, 2006; Sulaiman et al., 2007; Thimothée et al., 2017a) and also highlighted by Bradley et al. (2014). However, identifications of the relation between droplet distribution and flame propagation characteristics (e.g. flame speed enhancement) in measurements or simulations are not straightforward due to the comprehensive interphase coupling.

Theoretical analysis is an alternative and attractive method, since it can simplify the problems and retain the most relevant factors in our studies, thereby demonstrating physical relevance and clarity to the large extent. Its success in analyzing two-phase flames can be confirmed by numerous previous work (Greenberg, 2007; Han and Chen, 2016, 2015; Joulin, 1981; Ju and Law, 2000; Li et al., 2020; Lin et al., 1988; Liu and Lin, 1991; Liu et al., 1993; Mitani, 1981; Nicoli et al., 2005; Zhuang and Zhang, 2020, 2019). In particular, Lin and his coworkers (1988, 1991) developed a theoretical model considering the fully and partially pre-vaporized burning sprays. More recently, Belyakov et al. (2018) considered the evaporation onset and completion of water droplets before and behind the flame front, and therefore two flame regimes are obtained with different relations between propagation speed and evaporative heat loss. Later, Zhuang and Zhang (2020) investigated multiplication of propagation speed of spherical flames with water droplets. However, how different distributions of liquid fuel droplets influence two-phase flame propagation are still not well understood.

The present work aims to conduct the theoretical analysis on laminar flame propagation in pre-mixtures laden with fuel droplets, through deriving general theoretical correlations for different flame regimes under both fuel-lean and fuel-rich conditions. The effects of different properties of liquid fuel droplets on planar flame propagation will be discussed, via changing the droplet size, mass loading and latent heat of vaporization. The critical conditions for two flame regimes, i.e. homogeneous and heterogeneous flames, will also be studied. The rest of the paper is structured as below. Mathematical model and theoretical analysis are presented in Sections 2 and 3, respectively. The results from our theoretical analysis will be discussed in Section 4. Section 5 closes the paper with the main conclusions.

### 2. Physical and mathematical model

### 2.1. Physical model

In this work, one-dimensional planar flame propagation in a premixed gas with fuel droplet mists will be studied. The schematic of the physical models is shown in Fig. 1. The current model includes four zones, i.e. zones 1-4, to describe the fuel droplet evaporation and fuel vapor combustion. These four zones are demarcated by the evaporation onset front  $x_v$ , flame front  $x_f$ 

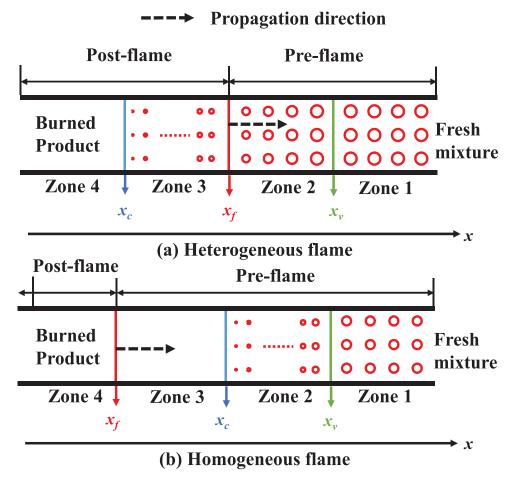
and evaporation completion front  $x_c$ . It should be noted that, for droplet characteristic locations  $x_v$  and  $x_c$ , the term "front" is loosely used here to identify where the droplets critically start and finish vaporization. Specifically,  $x_{\nu}$  corresponds to the location where the droplet starts to evaporate, and the droplets are just heated up to boiling temperature. Behind this front (i.e.  $x < x_v$ ), the droplet temperature maintains the boiling point and evaporation continues (Belyakov et al., 2018; Han and Chen, 2016, 2015; Zhuang and Zhang, 2020, 2019). The evaporation onset front  $x_v$  is always before the flame front  $x_f$ , indicating that onset of vaporization spatially precedes the gaseous combustion. Moreover,  $x_c$  corresponds to the location at which all the droplets are critically vaporized. When  $x < x_c$ , no droplets are left and hence their effects on the gaseous flame diminish. The reader is reminded that  $x_v$  and  $x_f$  are determined from our theories as the eigenvalues of the problem, instead of being specified a prior. Similar physical models with multiple zones have been successfully used for analyzing droplet-laden laminar flames in previous theoretical analyses (Belyakov et al., 2018; Lin et al., 1988; Zhuang and Zhang, 2020).

Various evaporation dynamics of sprayed fuel droplets and their interactions with gaseous flames may be presented in practical spray combustion. For example, it is observed through experimental measurements (Atzler et al., 2006b; Sulaiman, 2006; Sulaiman et al., 2007; Thimothée et al., 2017a) that droplets with small diameters would complete evaporation in the pre-flame zone or close to the flame front, but relatively large droplets can penetrate through the flame front and continue vaporizing in the postflame zone. Hence, in the latter scenario, droplets are distributed in the pre-flame zone and part of the post-flame zone.

In our work, both foregoing scenarios will be investigated. Firstly, the evaporation completion front lies after the flame front (i.e.  $x_c < x_f$ ), as shown in Fig. 1(a). In this case, the local mixture around the flame front is heterogeneous, including gas and liquid droplets. Secondly, the evaporation completion front is located before the flame front (i.e.  $x_f < x_c < x_v$ ), and the local mixture around the flame front is purely gaseous and therefore homogeneous, since there all the droplets have been converted into vapor. For brevity, hereafter, we term the first and second cases as heterogeneous and homogeneous flames, respectively. As shown in Figs. 1(a) and 1(b), for both flames, zone 1 represents the prevaporization zone before  $x_{y}$ . Zone 2 indicates pre-flame evaporation zone before  $x_f$  for heterogeneous flame and before  $x_c$  for homogeneous flame. As for zone 3, it represents post-flame evaporation zone before  $x_c$  for heterogeneous flame, and pre-flame zone without evaporation for homogeneous flame. Meanwhile, zone 4 is the post-flame zone without evaporation for both flames. In this model, introduction of multiple liquid droplet zones renders it more general, thereby better mimicking practical spray flame problems compared with previous studies (Greenberg et al., 2001; Han and Chen, 2016, 2015).

### 2.2. Governing equation

For gaseous flames, the well-known diffusive-thermal model (Joulin and Clavin, 1979) is adopted, in which the density and thermal and transport properties (e.g. thermal conductivity and heat capacity) can be assumed to be constant. Gas motion induced by combustion heat release and droplet evaporation is not considered and hence the convection flux is neglected (Han and Chen, 2015; Joulin and Clavin, 1979). This model has been used in numerous previous studies on gaseous and two-phase flame (Chen and Ju, 2007; Han and Chen, 2016, 2015; Li et al., 2020; Zhuang and Zhang, 2020, 2019). One-step chemistry is considered, i.e.  $F + O \rightarrow P$ , with *F*, *O* and *P* being fuel vapor, oxidizer and product. For completeness, both fuel-lean and fuel-rich conditions for gas composition are studied in this work. Both are relevant in practical droplet-



**Fig. 1.** Schematic of four flame and evaporation zones of laminar planar flames propagating in liquid fuel mists. (a) Heterogeneous flame: droplets complete evaporation in the post-flame zone; (b) Homogeneous flame: droplets complete evaporation in the pre-flame zone. Circles: fuel droplets.  $x_f$ : flame front;  $x_c$ : droplet evaporation completion front;  $x_v$ : droplet evaporation onset front.

laden flame systems, e.g. resulting from various extents of droplet pre-vaporization (Lefebvre and McDonell, 2017).

For liquid fuel droplets, we assume that they are monodispersed in the initial gaseous pre-mixture (Sacomano et al., 2018). The droplets are spherical and their properties (e.g. density and heat capacity) are assumed to be constant. The Eulerian description is adopted for the liquid phase, which is treated as an interpenetrating continuum. Due to the dilute droplet concentration assumption, the inter-droplet collisions are not considered and therefore the diffusion terms in the governing equations for liquid phase can be neglected. Meanwhile, the kinematic equilibrium between two phases is assumed, and droplet dispersion is not considered. The above assumptions for the liquid phase are also used in previous theoretical work on two-phase flames (Blouquin et al., 1997; Ju and Law, 2000; Lin et al., 1988; Blouquin and Joulin, 1995). Furthermore, in zone 1 (pre-vaporization) presented in Fig. 1, thermal equilibrium between droplets and fresh mixture is assumed, and hence they have the same temperature (Belyakov et al., 2018; Han and Chen, 2016, 2015; Zhuang and Zhang, 2020, 2019).

Based on the above assumptions, for the gas phase, the governing equations for temperature, oxidizer and fuel mass fractions are

$$\tilde{\rho}_{g}\tilde{C}_{p,g}\frac{\partial\tilde{T}}{\partial\tilde{t}} = \tilde{\lambda}_{g}\frac{\partial}{\partial\tilde{x}}\left(\frac{\partial\tilde{T}}{\partial\tilde{x}}\right) + \tilde{q}_{c}\tilde{\omega}_{c} - \tilde{q}_{v}\tilde{\omega}_{v},\tag{1}$$

$$\tilde{\rho}_g \frac{\partial \tilde{Y}_0}{\partial \tilde{t}} = \tilde{\rho}_g \tilde{D}_0 \frac{\partial}{\partial \tilde{x}} \left( \frac{\partial \tilde{Y}_0}{\partial \tilde{x}} \right) - \tilde{\omega}_c, \tag{2}$$

$$\tilde{\rho}_{g}\frac{\partial\tilde{Y}_{F}}{\partial\tilde{t}} = \tilde{\rho}_{g}\tilde{D}_{F}\frac{\partial}{\partial\tilde{x}}\left(\frac{\partial\tilde{Y}_{F}}{\partial\tilde{x}}\right) - \tilde{\omega}_{c} + \tilde{\omega}_{\nu},\tag{3}$$

where the upper tilde symbol ~ is used to indicate that the variables are dimensional.  $\tilde{t}$  and  $\tilde{x}$  are respectively the time and spatial coordinates,  $\tilde{T}$  is the gas temperature.  $\tilde{\rho}_g$ ,  $\tilde{C}_{p,g}$ , and  $\tilde{\lambda}_g$  are the gas density, heat capacity and thermal conductivity, respectively.  $\tilde{Y}$  and  $\tilde{D}$  are the mass fraction and molecular diffusivity of the gaseous oxidizer or fuel (subscript *O* for oxidizer, *F* for fuel), respectively.  $\tilde{q}_c$  is the reaction heat release per unit mass of the deficient reactant (oxidizer for fuel-rich case and fuel for fuel-lean case).  $\tilde{q}_v$  is the latent heat of vaporization per unit mass of the fuel droplet, and  $\tilde{\omega}_v$  is the evaporation rate of the fuel droplet.

The chemical reaction rate  $\tilde{\omega}_c$  is assumed to be Arrhenius-type and therefore takes the following form

$$\tilde{\omega}_{c} = \tilde{\rho}_{g} \tilde{A} \tilde{Y}_{F}^{\alpha} \tilde{Y}_{0}^{1-\alpha} \exp\left(-\tilde{E}/\tilde{R}^{0} \tilde{T}\right).$$

$$\tag{4}$$

Here,  $\alpha$  is an indicator for premixture composition, i.e.  $\alpha = 1$  for fuel-lean condition and  $\alpha = 0$  for fuel-rich condition. Moreover,  $\tilde{A}$  is the pre-exponential factor,  $\tilde{E}$  is the activation energy for the reaction, and  $\tilde{R}^0$  is the universal gas constant.

The Eulerian equation for droplet mass loading  $Y_d (\equiv \tilde{N}_d \tilde{m}_d / \tilde{\rho}_g)$  can be derived from single droplet mass equation for  $\tilde{m}_d$  and reads (Belyakov et al., 2018; Hayashi and Kumagai, 1975; Zhuang and Zhang, 2020, 2019)

$$\frac{\partial}{\partial \tilde{t}} \left( \frac{\tilde{N}_d \tilde{m}_d}{\tilde{\rho}_g} \right) = \frac{\partial Y_d}{\partial \tilde{t}} = -\frac{\tilde{\omega}_v}{\tilde{\rho}_g},\tag{5}$$

where  $\tilde{N}_d$  is the number density of the droplets.

We assume that the heat transferred from the surrounding gas to the droplets is completely used for phase change, which is related to the latent heat of evaporation  $\tilde{q}_{\nu}$  (Belyakov et al., 2018; Hayashi and Kumagai, 1975; Zhuang and Zhang, 2020, 2019). Therefore,  $\tilde{\omega}_{\nu}$  in Eq. (5) can be estimated from the heat transfer rate as

$$\tilde{\omega}_{\nu} = \frac{\tilde{N}_d \tilde{s}_d \tilde{h} \left( \tilde{T} - \tilde{T}_{\nu} \right) H \left( \tilde{T} - \tilde{T}_{\nu} \right)}{\tilde{q}_{\nu}},\tag{6}$$

where  $\tilde{s}_d = \pi d^2$  is the surface area of a single droplet,  $\tilde{d}$  is the diameter of the droplet, *Nu* is the Nusselt number,  $\tilde{T}_v$  is the boiling temperature of the fuel droplet.  $H(\cdot)$  is the Heaviside function, which indicates that the evaporation process of fuel droplets only exists when the droplets reach the boiling temperature (i.e. when  $\tilde{x}$  is between  $\tilde{x}_c$  and  $\tilde{x}_v$ ).  $\tilde{h}$  is the heat transfer coefficient, which can be estimated using the following correlation as (Ranz and Marshall, 1952)

$$Nu = \frac{\tilde{h}\tilde{d}_p}{\tilde{\lambda}_g} = 2.0 + 0.6 \text{Re}^{1/2} P r^{1/3},$$
(7)

where *Nu*, *Pr* and *Re* are the Nusselt number, Prandtl number and particle Reynolds number, respectively. We can neglect the effect of particle Reynolds number *Re* due to the assumption of kinematic equilibrium and therefore  $Nu \approx 2$ . Accordingly, the evaporation rate  $\tilde{\omega}_{v}$  in Eq. (5) can be written as

$$\tilde{\omega}_{\nu} = \frac{\tilde{N}_d \tilde{s}_d \tilde{\lambda}_g N u \left(\tilde{T} - \tilde{T}_{\nu}\right) H \left(\tilde{T} - \tilde{T}_{\nu}\right)}{\tilde{d} \tilde{q}_{\nu}}.$$
(8)

The above evaporation model is different from the classic models, e.g. presented in Ref. (Sazhin, 2006). Typically,  $\tilde{\omega}_{v}$  is a function of Sherwood number, Spalding mass transfer number, as well as gas and droplet properties (e.g. density and diameter). In the current study, since we assume that the kinematic equilibrium has been reached between the gaseous and droplet, it can be expected that the effect of the Sherwood number is small. Furthermore, since it is assumed that evaporation proceeds at the boiling temperature and constant atmospheric pressure, the fuel vapor at the droplet surface is relatively constant and hence the Spalding number would change slightly. The difference is that the current model is based on the assumption of energy balance between phase change and heat transfer from the gaseous mixture. In spite of these, it is still physically comprehensive since it considers various effects of the gas and liquid phase properties as mentioned above. Therefore, the current evaporation model is expected to be sufficient. This can also be confirmed by the previous theoretical work using the same model (Belyakov et al., 2018; Zhuang and Zhang, 2020, 2019), from which the physically sound critical flame phenomena have been observed.

To render the analytical analysis in general, Eqs. (1) - (3) can be normalized. As such, the following non-dimensional parameters are introduced

$$U = \frac{\tilde{u}}{\tilde{u}_b}, x = \frac{\tilde{x}}{\tilde{l}_{th}}, t = \frac{\tilde{t}}{\frac{\tilde{l}_{th}}{\tilde{u}_b}}, Y = \frac{\tilde{Y}}{\tilde{Y}_0}, T = \frac{\tilde{T} - \tilde{T}_0}{\tilde{T}_b - \tilde{T}_0}.$$
(9)

Here  $\tilde{T}_0$  and  $\tilde{Y}_0$  denote the temperature and fuel mass fraction in the fresh mixture, respectively.  $\tilde{u}_b$ ,  $\tilde{T}_b = \tilde{T}_0 + \tilde{q}_c \tilde{Y}_0 / \tilde{C}_{p,g}$  and  $\tilde{l}_{th} = \tilde{D}_{th} / \tilde{u}_b$  are the adiabatic laminar flame speed, temperature and thickness without fuel droplet addition, respectively.  $\tilde{D}_{th} = \tilde{\lambda}_g / \tilde{\rho}_g \tilde{C}_{p,g}$  is the thermal diffusivity of the gas phase.

Steady propagation (i.e.  $\partial/\partial t = 0$ ) of planar flames in liquid fuel droplet is assumed, same as Refs. (Belyakov et al., 2018; Lin et al., 1988). Meanwhile, for convenience, our ensuing analysis will be performed in the coordinate system attached to the flame front

X(t), i.e.  $\eta = x - X(t)$ . Under the above assumption and simplification, the non-dimensional equations of Eqs. (1) – (3) can be written as

$$-U\frac{dT}{d\eta} = \frac{d^2T}{d\eta^2} + \omega_c - q_\nu \omega_\nu, \tag{10}$$

$$-U\frac{d\left(Y_{F}^{\alpha}Y_{O}^{1-\alpha}\right)}{d\eta} = \frac{Le_{O}^{\alpha-1}}{Le_{F}^{\alpha}}\frac{d^{2}\left(Y_{F}^{\alpha}Y_{O}^{1-\alpha}\right)}{d\eta^{2}} - \omega_{c} + \alpha\omega_{\nu},$$
(11)

$$-U\frac{dY_d}{d\eta} = -\omega_\nu,\tag{12}$$

where U = dX/dt is the non-dimensional flame propagating speed.  $q_{\nu} = \tilde{q}_{\nu}/[\tilde{C}_{p,g}(\tilde{T}_b - \tilde{T}_0)]$  is the normalized latent heat of vaporization.  $Le_F = \tilde{D}_{th}/\tilde{D}_F$  and  $Le_O = \tilde{D}_{th}/\tilde{D}_O$  are the Lewis numbers of fuel and oxidizer, respectively. In Eq. (11), due to the assumption that the chemical reaction depends on the deficient reactant, for fuel-lean conditions ( $\alpha = 1$ ), we only need to solve the governing equation for the fuel mass fraction  $Y_F$ . While in fuel-rich condition ( $\alpha = 0$ ), the oxidizer mass fraction  $Y_O$  needs to be solved instead of  $Y_F$ . The normalized chemical reaction rate  $\omega_c$  in Eqs. (10) and (11) reads

$$\omega_c = \frac{Le_0^{\alpha-1}}{Le_F^{\alpha}} Y_F^{\alpha} Y_0^{1-\alpha} Z^2 \exp\left[\frac{Z(T-1)}{\sigma + (1-\sigma)T}\right],\tag{13}$$

where Z is the Zel'dovich number, and  $\sigma$  is the thermal expansion ratio.

The non-dimensional droplet evaporation rate  $\omega_v$  takes the following form

$$\omega_{\nu} = \frac{\Omega(T - T_{\nu})}{q_{\nu}} H(T - T_{\nu}), \qquad (14)$$

where  $T_{\nu}$  is the non-dimensional boiling temperature. The heat exchange coefficient  $\Omega$  is

$$\Omega = \pi \tilde{N}_d N u \tilde{d} \tilde{D}_{th}^2 \tilde{u}_b^{-2}.$$
(15)

### 2.3. Jump and boundary conditions

The non-dimensional boundary conditions for both gas phase (*T* and *Y*) and liquid phase (*Y*<sub>d</sub>) at the left boundary ( $\eta = -\infty$ ) in the burned zone and the right boundary ( $\eta = +\infty$ ) in the unburned zone can be given as (Belyakov et al., 2018)

$$\eta = -\infty : \frac{dT}{d\eta} = 0, \quad \frac{dY_F}{d\eta} = \frac{dY_O}{d\eta} = 0, \quad Y_d = 0, \quad (16)$$

$$\eta = +\infty$$
:  $T = 0$ ,  $Y_F = 1$ ,  $Y_0 = 1$ ,  $Y_d = \delta$ . (17)

Here  $\delta$  is the initial mass loading of the fuel droplet in the fresh mixture.

At the evaporation onset front,  $\eta = \eta_{\nu}$ , the gas temperature (*T*), the mass fractions of oxidizer and fuel (*Y<sub>F</sub>* and *Y<sub>O</sub>*), and the fuel droplet mass loading (*Y<sub>d</sub>*) satisfy the following jump conditions (Belyakov et al., 2018)

$$T = T_{\nu}, \ [T] = [Y_F] = [Y_O] = \left[\frac{dY_F}{d\eta}\right] = \left[\frac{dY_O}{d\eta}\right] = 0, \ Y_d = \delta.$$
(18)

where the square brackets, i.e.  $[T] = T(\eta^+) - T(\eta^-)$ , denote the difference between the variables at two sides in a particular location.

At the evaporation completion front,  $\eta = \eta_c$ , the jump conditions for the gas temperature (*T*), the mass fractions of oxidizer and fuel ( $Y_F$  and  $Y_O$ ), and the fuel droplet mass loading ( $Y_d$ ) take the following form (Belyakov et al., 2018)

$$\begin{bmatrix} T \end{bmatrix} = \begin{bmatrix} Y_F \end{bmatrix} = \begin{bmatrix} Y_O \end{bmatrix} = \begin{bmatrix} \frac{dY_F}{d\eta} \end{bmatrix} = \begin{bmatrix} \frac{dY_O}{d\eta} \end{bmatrix} = 0, \ Y_d = 0, \ \eta_c > 0, \ T \end{bmatrix} = 0, \ \frac{dT}{d\eta}|_+ = 0, \ [Y_d] = 0, \ \eta_c < 0$$
(19)

Here, the "+" symbol indicates the value being on the positive side of  $\eta_c$ .

Large activation energy of the gas phase reaction is assumed in this study. This assumption has been successfully used for theoretical analysis of both gaseous (Chen and Ju, 2007; He, 2000; Li et al., 2018; Zhang et al., 2013; Zhang and Chen, 2011) and particle- or droplet-laden (Blouquin et al., 1997; Greenberg, 2007; Han and Chen, 2015; Ju and Law, 2000; Li et al., 2020; Blouquin and Joulin, 1995; Zhuang and Zhang, 2019) flames. It is shown to be adequate to predict main flame dynamics, such as ignition and propagation. In the limit of large activation energy, chemical reaction is confined at an infinitesimally thin flame sheet (i.e.  $\eta = 0$ ) and the jump conditions at the flame front ( $\eta = 0$ ) are

$$T = T_f, Y_F^{\alpha} Y_0^{1-\alpha} = [Y_d] = 0,$$
(20)

$$-\left[\frac{dT}{d\eta}\right] = \frac{Le_0^{\alpha-1}}{Le_F^{\alpha}} \left[\frac{dY_F^{\alpha}Y_0^{1-\alpha}}{d\eta}\right] = \left[\sigma + (1-\sigma)T_f\right]^2$$
$$\exp\left[\frac{Z}{2}\left(\frac{T_f - 1}{\sigma + (1-\sigma)T_f}\right)\right],$$
(21)

where  $T_f$  is the flame temperature.

### 3. Analytical solution

Eqs. (10)–(12) with boundary and jump conditions (i.e. Eqs. (16)–(21)) can be solved analytically. The distributions of the gas temperature *T*, fuel mass fraction  $Y_F$  (fuel-lean condition), oxidizer mass fraction  $Y_0$  (fuel-rich condition) and droplet mass loading  $Y_d$  in four zones and the correlations for the flame speed *U*, flame temperature  $T_f$ , evaporation onset front  $\eta_v$  and evaporation completion front  $\eta_c$  are presented below.

### 3.1. Distributions of T, $Y_{\{F, O\}}$ and $Y_d$

The distributions for temperature T from zone 1 to 4 are (the number subscript for T indicates the corresponding zone, which also applies for other variables hereafter)

$$T_1(\eta) = \frac{T_v e^{-U\eta}}{e^{-U\eta_v}},\tag{22}$$

$$T_2(\eta) = T_\nu + \frac{UT_\nu}{\gamma_b - \gamma_a} \Big[ e^{\gamma_a(\eta - \eta_\nu)} - e^{\gamma_b(\eta - \eta_\nu)} \Big],$$
(23)

$$T_{3}(\eta) = \begin{cases} \frac{T_{\nu}}{\gamma_{b}-\gamma_{a}} \Big[ \gamma_{a} e^{\gamma_{a}(\eta_{c}-\eta_{\nu})} - \gamma_{b} e^{\gamma_{b}(\eta_{c}-\eta_{\nu})} \Big] \Big[ 1 - e^{-U(\eta-\eta_{c})} \Big] + T_{\nu} \\ + \frac{UT_{\nu}}{\gamma_{b}-\gamma_{a}} \Big[ e^{\gamma_{a}(\eta_{c}-\eta_{\nu})} - e^{\gamma_{b}(\eta_{c}-\eta_{\nu})} \Big], \eta_{c} > 0 \\ T_{\nu} + \frac{T_{f}-T_{\nu}}{\frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{b}} - \frac{e^{\gamma_{a}(\eta-\eta_{c})}}{\gamma_{a}}} \Big[ \frac{e^{\gamma_{b}(\eta-\eta_{c})}}{\gamma_{b}} - \frac{e^{\gamma_{a}(\eta-\eta_{c})}}{\gamma_{a}} \Big], \eta_{c} < 0 \end{cases}$$

$$(24)$$

$$T_4(\eta) = \begin{cases} T_f, \eta_c > 0\\ T_\nu + \frac{T_f - T_\nu}{\frac{e^{-\gamma_b \eta_c}}{\gamma_b} - \frac{e^{-\gamma_b \eta_c}}{\gamma_a}} \left(\frac{1}{\gamma_b} - \frac{1}{\gamma_a}\right), \eta_c < 0, \end{cases}$$
(25)

where  $\gamma_{a,b} = 0.5[-U \pm \sqrt{4\Omega + U^2}].$ 

Substituting the temperature distribution into the droplet mass loading equation, we can obtain the distribution of the droplet mass loading  $Y_d$  as

$$Y_{d,1}(\eta) = \delta, \tag{26}$$

$$Y_{d,2}(\eta) = \begin{cases} \frac{\Omega T_{\nu}}{q_{\nu}(\gamma_{b}-\gamma_{a})} \bigg[ \frac{e^{\gamma_{a}(\eta-\eta_{\nu})} - e^{\gamma_{a}(\eta_{c}-\eta_{\nu})}}{\gamma_{a}} - \frac{e^{\gamma_{b}(\eta-\eta_{\nu})} - e^{\gamma_{b}(\eta_{c}-\eta_{\nu})}}{\gamma_{b}} \bigg], \eta_{c} > 0\\ \delta + \frac{\Omega T_{\nu}}{q_{\nu}(\gamma_{b}-\gamma_{a})} \bigg[ \frac{e^{\gamma_{a}(\eta-\eta_{\nu})} - 1}{\gamma_{a}} - \frac{e^{\gamma_{b}(\eta-\eta_{\nu})} - 1}{\gamma_{b}} \bigg], \eta_{c} < 0 \end{cases}$$
(27)

$$Y_{d,3}(\eta) = \begin{cases} 0, \eta_{c} > 0\\ \frac{\Omega(T_{f} - T_{v})}{Uq_{v} \left(\frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{b}} - \frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{a}}\right)} \left[\frac{e^{\gamma_{b}(\eta - \eta_{c})} - 1}{\gamma_{b}^{2}} - \frac{e^{\gamma_{a}(\eta - \eta_{c})} - 1}{\gamma_{a}^{2}}\right], \eta_{c} < 0, \end{cases}$$
(28)  
$$Y_{d,4}(\eta) = 0.$$
(29)

The distributions of fuel mass fraction  $Y_F$  (fuel-lean condition), oxidizer mass fraction  $Y_O$  (fuel-rich condition) can be obtained by solving Eq. (11) with the temperature distributions (i.e. Eqs. (22)–(25)) in the respective zones. For the fuel-lean condition ( $\alpha = 1$ ), fuel mass fraction distributions in four zones are

$$Y_{F,1}(\eta) = \begin{cases} \begin{bmatrix} \frac{l'_{2}(\eta_{\nu})}{l'_{1}(\eta_{\nu})}(l_{1}(0) - l_{1}(\eta_{\nu})) - \frac{l'_{2}(\eta_{c})}{l'_{1}(\eta_{c})}(l_{1}(0) - l_{1}(\eta_{c})) + l_{2}(\eta_{\nu}) - l_{2}(\eta_{c}) - 1}{l_{1}(0)} \\ I_{1}(0) \\ I_{1}(0) \\ I_{1}(0) \\ \frac{l'_{2}(\eta_{\nu})}{l'_{1}(\eta_{\nu})}(l_{1}(0) - l_{1}(\eta_{\nu})) - 1 + l_{2}(\eta_{\nu}) - l_{2}(0)}{l_{1}(0)} \\ I_{1}(\eta) + 1, \ \eta_{c} < 0 \end{cases}$$

$$(30)$$

$$Y_{F,2}(\eta) = \begin{cases} 1 - \left[ \frac{1 + \frac{l'_2(\eta_v)}{l'_1(\eta_v)} I_1(\eta_v) + \frac{l'_2(\eta_c)}{l'_1(\eta_c)} (I_1(0) - I_1(\eta_c)) - I_2(\eta_v) + I_2(\eta_c)}{I_1(0)} \right] I_1(\eta) \\ + I_2(\eta) + \frac{l'_2(\eta_v)}{l'_1(\eta_v)} I_1(\eta_v) - I_2(\eta_v), \ \eta_c > 0 \\ 1 - \frac{\frac{l'_2(\eta_v)}{l'_1(\eta_v)} I_1(\eta_v) + I_2(\eta_v)}{I_1(0)} I_1(\eta) + I_2(\eta) \\ + \frac{l'_2(\eta_v)}{l'_1(\eta_v)} I_1(\eta_v) - I_2(\eta_v), \ \eta_c < 0 \end{cases}$$
(31)

$$Y_{F,3}(\eta) = \begin{cases} \left[ 1 + \frac{I'_{2}(\eta_{\nu})}{I'_{1}(\eta_{\nu})} I_{1}(\eta_{\nu}) - \frac{I'_{2}(\eta_{c})}{I'_{1}(\eta_{c})} I_{1}(\eta_{c}) - I_{2}(\eta_{\nu}) + I_{2}(\eta_{c}) \right] \\ \left[ 1 - \frac{I_{1}(\eta)}{I_{1}(0)} \right], \eta_{c} > 0 \\ \frac{I'_{3}(\eta_{c})}{I'_{1}(\eta_{c})} [I_{1}(0) - I_{1}(\eta)] + I_{3}(\eta) - I_{3}(0), \ \eta_{c} < 0 \end{cases}$$

$$(32)$$

$$Y_{F,4}(\eta) = \begin{cases} 0, \ \eta_c > 0\\ \frac{I'_3(\eta_c)}{I'_1(\eta_c)} [I_1(0) - I_1(\eta_c)] + I_3(\eta_c) - I_3(0), \ \eta_c < 0, \end{cases}$$
(33)

where  $I'_1(\eta)$ ,  $I'_2(\eta)$  and  $I'_3(\eta)$  are respectively the first order derivatives of  $I_1(\eta)$ ,  $I_2(\eta)$  and  $I_3(\eta)$ , which read

$$I_1(\eta) = \frac{e^{-Le_F U \eta}}{Le_F U},\tag{34}$$

$$I_{2}(\eta) = -\frac{Le_{F}\Omega T_{\nu}U}{q_{\nu}(\gamma_{b} - \gamma_{a})} \left[ \frac{e^{\gamma_{a}(\eta - \eta_{\nu})}}{\gamma_{a}(Le_{F}U + \gamma_{a})} - \frac{e^{\gamma_{b}(\eta - \eta_{\nu})}}{\gamma_{b}(Le_{F}U + \gamma_{b})} \right], \quad (35)$$

$$I_{3}(\eta) = -\frac{Le_{F}\Omega\left(T_{f} - T_{\nu}\right)}{q_{\nu}\left(\frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{b}} - \frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{a}}\right)} \left[\frac{e^{\gamma_{b}(\eta - \eta_{c})}}{\gamma_{b}^{2}\left(Le_{F}U + \gamma_{b}\right)} - \frac{e^{\gamma_{a}(\eta - \eta_{c})}}{\gamma_{a}^{2}\left(Le_{F}U + \gamma_{a}\right)}\right].$$
(36)

For fuel-rich condition ( $\alpha = 0$ ), oxidizer mass fraction distributions in the four zones are

$$Y_{0,12}(\eta) = 1 - e^{-Le_0 U \eta},$$
(37)

$$Y_{0,3}(\eta) = \{ \begin{cases} 1 - e^{-Le_0 U\eta}, \eta_c > 0\\ 0, \eta_c < 0 \end{cases},$$
(38)

$$Y_{0,4}(\eta) = 0. (39)$$

### 3.2. Correlations for propagating planar flame with fuel droplets

The correlations between the flame propagating speed *U*, flame temperature  $T_f$ , evaporation onset front  $\eta_v$  and evaporation completion front  $\eta_c$  can be derived based on jump conditions at the flame front, i.e. Eq. (21).

### 3.2.1. Heterogeneous flame

When the flame propagates in the locally heterogeneous mixture, the correlation  $\mathcal{F}(U, T_f, \eta_v, \eta_c) = 0$  takes the following form

$$\frac{T_{f} - T_{\nu}}{\frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{b}} - \frac{e^{-\gamma_{a}\eta_{c}}}{\gamma_{a}}} \left[ e^{-\gamma_{b}\eta_{c}} - e^{-\gamma_{a}\eta_{c}} \right] - \frac{UT_{\nu}}{\gamma_{b} - \gamma_{a}} \left[ \gamma_{a}e^{-\gamma_{a}\eta_{\nu}} - \gamma_{b}e^{-\gamma_{b}\eta_{\nu}} \right] = Q(T_{f})$$

$$(40)$$

$$\begin{cases} U(1+\delta) + \frac{\Omega(T_f - T_v)}{q_v \left(\frac{e^{-\gamma_b \eta_c}}{\gamma_b} - \frac{e^{-\gamma_b \eta_c}}{\gamma_a}\right)} H(\eta_c) = Q(T_f), \ \alpha = 1, \\ U = Q(T_f), \ \alpha = 0 \end{cases},$$
(41)

$$T_{\nu} + \frac{UT_{\nu}}{\gamma_b - \gamma_a} \Big[ e^{-\gamma_a \eta_{\nu}} - e^{-\gamma_b \eta_{\nu}} \Big] = T_f,$$
(42)

$$\frac{\Omega(T_{f} - T_{\nu})}{Uq_{\nu}\left(\frac{e^{-\gamma_{b}\eta_{c}}}{\gamma_{b}} - \frac{e^{-\gamma_{a}\eta_{c}}}{\gamma_{a}}\right)} \left[\frac{e^{-\gamma_{b}\eta_{c}} - 1}{\gamma_{b}^{2}} - \frac{e^{-\gamma_{a}\eta_{c}} - 1}{\gamma_{a}^{2}}\right]$$

$$= \delta + \frac{\Omega T_{\nu}}{q_{\nu}(\gamma_{b} - \gamma_{a})} \left[\frac{e^{-\gamma_{a}\eta_{\nu}} - 1}{\gamma_{a}} - \frac{e^{-\gamma_{b}\eta_{\nu}} - 1}{\gamma_{b}}\right],$$
(43)

where

$$Q(T_f) = \left[\sigma + (1 - \sigma)T_f\right]^2 \exp\left[\frac{Z}{2}\left(\frac{T_f - 1}{\sigma + (1 - \sigma)T_f}\right)\right], \quad (44)$$

$$H(\eta_{c}) = \frac{\gamma_{b}(1 - e^{LeU(1)} + LeU(1 - e^{-\gamma_{b}\eta_{c}}))}{\gamma_{b}^{2}(\gamma_{b} + LeU)} - \frac{\gamma_{a}(1 - e^{LeU\eta_{c}}) + LeU(1 - e^{-\gamma_{a}\eta_{c}})}{\gamma_{a}^{2}(\gamma_{a} + LeU)}.$$
(45)

### 3.2.2. Homogeneous flame

When the liquid droplets are fully vaporized ahead of the flame front, the correlation  $\mathcal{F}(U, T_f, \eta_v, \eta_c) = 0$  reads

$$-\frac{UT_{\nu}}{\gamma_{b}-\gamma_{a}}\Big[\gamma_{a}e^{\gamma_{a}(\eta_{c}-\eta_{\nu})+U\eta_{c}}-\gamma_{b}e^{\gamma_{b}(\eta_{c}-\eta_{\nu})+U\eta_{c}}\Big]=Q(T_{f}),$$
(46)

$$\begin{cases} U(1+\delta) = Q(T_f), \alpha = 1\\ U = Q(T_f), \alpha = 0 \end{cases},$$
(47)

$$\frac{T_{\nu}}{\gamma_{b} - \gamma_{a}} \left\{ (\gamma_{a} + U - \gamma_{a} e^{U\eta_{c}}) e^{\gamma_{a}(\eta_{c} - \eta_{\nu})} - (\gamma_{b} + U - \gamma_{b} e^{U\eta_{c}}) e^{\gamma_{b}(\eta_{c} - \eta_{\nu})} \right\} + T_{\nu} = T_{f},$$
(48)

$$\frac{\Omega T_{\nu}}{q_{\nu}(\gamma_b - \gamma_a)} \left[ \frac{1 - e^{\gamma_a(\eta_c - \eta_{\nu})}}{\gamma_a} - \frac{1 - e^{\gamma_b(\eta_c - \eta_{\nu})}}{\gamma_b} \right] = \delta.$$
(49)

For homogeneous flames, when  $\delta \rightarrow 0$  and  $\Omega \rightarrow 0$ , the correlations from our model can recover that for purely gaseous planar flames in Ref. (Chen and Ju, 2007), which is shown in Supplementary Material.

Through solving the above systems  $\mathcal{F}(U, T_f, \eta_v, \eta_c) = 0$ , we can analyze the relations between the droplets properties (i.e. evaporation onset and completion fronts,  $\eta_v$  and  $\eta_c$ ) and flame propagation properties (e.g. flame speed *U* and temperature  $T_f$ ), subject to various droplet parameters (e.g. droplet diameter and mass loading, latent heat of vaporization). Thus, propagation of heterogeneous and homogeneous flames with fuel droplets can be analyzed theoretically.

## 3.3. Critical condition between heterogeneous and homogeneous flames

The critical condition between heterogeneous and homogeneous flames can be derived from the current model when the evaporation completion front coincides with the flame front, i.e.  $\eta_c \rightarrow 0$ . This physically corresponds to the case in which the liquid fuel droplets are just fully vaporized at the flame front. Practically, it may occur when the droplet diameter is small or the latent heat of vaporization is low (Atzler et al., 2006; Thimothée et al., 2017b). In this case, the correlations for flame propagating speed *U*, flame temperature  $T_f$  and evaporation onset front  $\eta_v$  read

$$-\frac{UT_{\nu}}{\gamma_{b}-\gamma_{a}}\left[\gamma_{a}e^{-\gamma_{a}\eta_{\nu}}-\gamma_{b}e^{-\gamma_{b}\eta_{\nu}}\right]=Q(T_{f}),$$
(50)

$$\begin{cases} U(1+\delta) = Q(T_f), \alpha = 1\\ U = Q(T_f), \alpha = 0 \end{cases},$$
(51)

$$T_{\nu} + \frac{UT_{\nu}}{\gamma_b - \gamma_a} \Big[ e^{-\gamma_a \eta_{\nu}} - e^{-\gamma_b \eta_{\nu}} \Big] = T_f,$$
(52)

$$\delta + \frac{\Omega T_{\nu}}{q_{\nu}(\gamma_b - \gamma_a)} \left[ \frac{e^{-\gamma_a \eta_{\nu}} - 1}{\gamma_a} - \frac{e^{-\gamma_b \eta_{\nu}} - 1}{\gamma_b} \right] = 0.$$
(53)

### 4. Results and discussion

In this Section, analysis on propagation of one-dimensional planar flames laden with fuel droplets will be conducted based on the correlations derived in Section 3. Zel'dovich number *Z* and thermal expansion ratio  $\sigma$  are set to be Z = 10 and  $\sigma = 0.15$ , following the values used in previous theoretical analysis (Chen and Ju, 2007; Han and Chen, 2016, 2015; Li et al., 2020; Zhuang and Zhang, 2020, 2019). The non-dimensional boiling temperature  $T_v$  is assumed to be  $T_v = 0.15$  (Han and Chen, 2015; Lefebvre and McDonell, 2017), which can represent the boiling temperature of most liquid hydrocarbon fuels.

### 4.1. Effects of droplet diameter and mass loading

Fig. 2 shows the flame speed U and temperature  $T_f$  as functions of the initial droplet diameter  $d_0$ , under fuel-lean conditions. The normalized latent heat of vaporization  $q_v$  is assumed to be 0.4 in this Section, corresponding to typical liquid hydrocarbon fuels (e.g. ethanol) (Lefebvre and McDonell, 2017). Note that each curve corresponds to a fixed initial droplet mass loading  $\delta$ . For fuel-lean results in Fig. 2(a) and 2(b), when  $d_0$  is small (< 30 µm), the flames are kinetically enhanced, parameterized by higher propagation speed and flame temperature, compared with the dropletfree gaseous mixture (i.e. U = 1 and  $T_f = 1$ ). This is caused by the fuel vapors from droplet evaporation, which enrich the gas mixture towards stoichiometry. This kinetic enhancement dominates the thermal weakening effects through evaporative heat loss for this range of droplet sizes. Meanwhile, the net enhancement effects become more pronounced with decreased  $d_0$ , due to the faster evaporation rate of smaller droplets. This is also observed through the

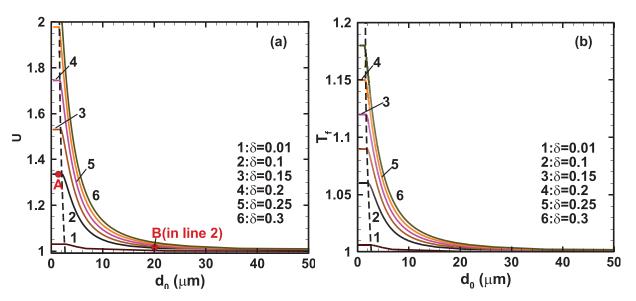


Fig. 2. Effect of droplet diameter and mass loading under fuel-lean conditions: (a) propagation speed, (b) flame temperature. Homogeneous (heterogeneous) flames: left (right) to the dashed flame regime line.

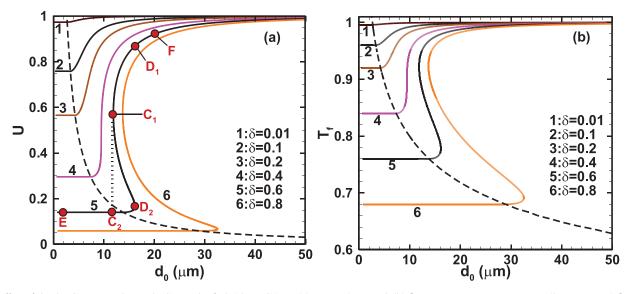


Fig. 3. Effect of droplet diameter and mass loading under fuel-rich conditions: (a) propagation speed, (b) flame temperature. Homogeneous (heterogeneous) flames: left (right) to the dashed flame regime line.

theoretical analysis (Lin et al., 1988; Lin and Sheu, 1991) and numerical simulations (Neophytou and Mastorakos, 2009) of laminar flame propagation in dilute fuel sprays. Furthermore, for a fixed  $d_0$  less than 30 µm, the higher the mass loading  $\delta$ , the higher the propagation speed *U*. This is justifiable since more fuels would be vaporized from the liquid phase. When  $d_0$  is large (> 30 µm), the effects of  $d_0$  on the propagating flames are negligible, as seen from Figs. 2(a) and 2(b), since the fuel droplet with larger  $d_0$  has slower evaporation rate.

The fuel-rich flame results are shown in Figs. 3(a) and 3(b). It should be highlighted that, different from the above fuel-lean cases, the kinetic effects from the fuel vapor would weaken the flame, through rendering the originally fuel-rich gas mixture more off-stoichiometric. As such, this kinetic weakening, together with the heat loss from droplet evaporation, is responsible for much lower flame speed and temperature than those of droplet-free cases (i.e. U = 1 and  $T_f = 1$ ). This is particularly obvious for small-sized droplets (i.e.  $d_0 \le 40 \ \mu\text{m}$ , see Figs. 3a and 3b). For large droplets (e.g.  $d_0 > 40 \ \mu\text{m}$ ), the kinetic weakening effects on flame

propagation speed and temperature become marginal, similar to the findings from large droplets in fuel-lean cases in Fig. 2(a) and 2(b). In general, the tendencies of flame speeds with droplet size and mass loading in both fuel-lean and -rich situations (see Figs. 2 and 3) are qualitatively consistent with the previously theoretical analysis (Lin et al., 1988) and experimental measurements (Ballal and Lefebvre, 1981; Hayashi et al., 1977; Hayashi and Kumagai, 1975).

Moreover, in fuel-rich cases, when the initial mass loading  $\delta$  is small or intermediate, i.e.  $\delta \leq 0.2$ ,  $U - d_0$  and  $T_f - d_0$  curves are monotonic, and smaller  $d_0$  would lead to lower flame speed and temperature, closer to the results of droplet-free flames, due to both kinetic and thermal weakening effects caused by droplet evaporation. However, when  $\delta$  is large, i.e.  $\delta \geq 0.6$  in Fig. 3,  $U - d_0$  and  $T_f - d_0$  curves become *S*-shaped, and multiplicity of the flame propagation speed and temperature is observed. Similar bifurcation is also found in theoretical analysis of premixed planar flames with water or fuel droplets (Belyakov et al., 2018; Lin et al., 1988; Zhuang and Zhang, 2020) and solid particles (Ju and Law, 2000;

 Table 1

 Conditions of selected flames in Figs. 2(a) and 3(a).

Flame	Condition	$d_0 \ (\mu m)$	$q_{v}$	δ
A	Fuel-lean	2	0.4	0.1
В	Fuel-lean	20	0.4	0.1
С	Fuel-rich	11.5	0.4	0.6
D	Fuel-rich	16.1	0.4	0.6
Е	Fuel-rich	2	0.4	0.6
F	Fuel-rich	20	0.4	0.6

Li et al., 2020). There are three branches for these cases, e.g.  $\delta = 0.6$  in Figs. 3(a) and 3(b): upper stable strong flame (branch above  $C_1$ , indicated in Fig. 3a), middle unstable flame (branch between  $C_1$  and  $D_2$ ), and lower stable weak flame (branch left to  $D_2$ ). A detailed linear stability analysis is provided in the Supplementary Material. Slight increase of  $d_0$  around the turning point  $D_2$  would make this weak flame jump to a stronger flame  $D_1$ . Likewise, sudden transition would occur from strong flame  $C_1$  to weak flame  $C_2$  when  $d_0$  is perturbed towards a reduced value. These changes between the foregoing kinetic and thermal effects caused by the dispersed liquid phase.

The results of a constant mass loading  $\delta$ , i.e. each curve in both Figs. 2 and 3, correspond to two flame regimes, i.e. heterogeneous and homogeneous flames, depending on the relative locations of the droplet distribution and flame front, as described in Section 2.1. They are demarcated by dashed lines calculated from Eqs. (50) – (53), and the homogeneous (heterogeneous) flames lie left (right) of the  $U - d_0$  or  $T_f - d_0$  plane to these lines (termed as flame regime line hereafter). In general, homogeneous flames only exist when  $d_0$  is relatively small. This is reasonable because small droplets are more prone to complete evaporation before the flame front arrives, due to comparatively fast evaporation. As such, the local mixture immediately before the flame front is purely gaseous. Meanwhile, U and  $T_f$  of homogeneous flames for a fixed mass loading remain constant, since the same amount of the fuel is vaporized into the mixture. However, for heterogeneous flames, different tendencies are observable for fuel-lean and fuel-rich conditions as presented in Figs. 2 and 3, which have been discussed above. This indicates the strong effects of the initial droplet diameter and mass loading on propagation of heterogeneous flames, which will be further discussed later. It should also be highlighted that flame bifurcations can occur within the same flame regime (from  $D_2$  to  $D_1$ in heterogeneous regime), or between the different flame regimes (from heterogeneous  $C_1$  to homogeneous  $C_2$ ).

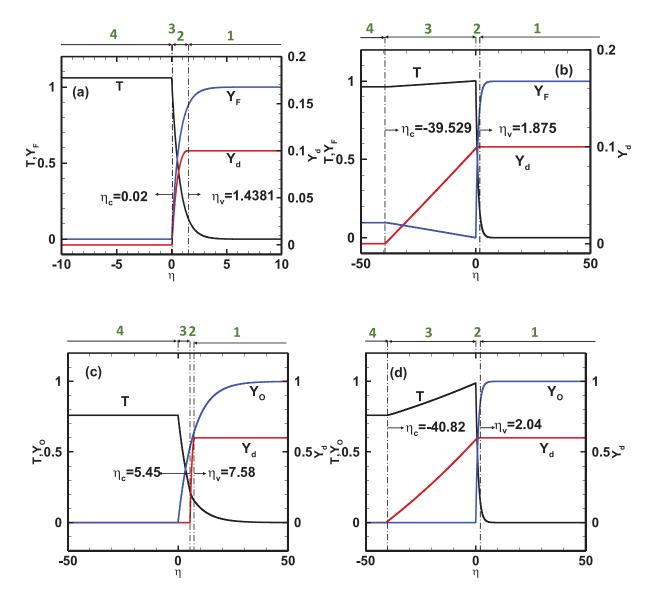
Distributions of gas temperature T, deficient species mass fraction,  $Y_F$  or  $Y_O$ , and droplet mass loading  $Y_d$  of different dropletladen flames are shown in Fig. 4. For reference, the locations of evaporation onset and completion fronts, i.e.  $\eta_v$  and  $\eta_c$ , are also shown. Four flames are considered, i.e. A, B, E, and F, which are denoted in Figs. 2(a) or 3(a). Flames A and B are under fuel-lean condition. Specifically, A is a homogeneous flame (initial droplet size  $d_0 = 2 \ \mu m$ ), while B ( $d_0 = 20 \ \mu m$ ) corresponds to a heterogeneous one. For flame A in Fig. 4(a), the droplets are fully vaporized (i.e.  $Y_d \rightarrow 0$ ) slightly before the flame front, and therefore all of them are consumed in the flame. The extra fuel vapor from droplet evaporation increases the overall fuel concentration in the gaseous mixture, leading to slightly higher temperature (i.e. T > 1) in the post-flame zone compared to the droplet-free flame. Meanwhile, due to no droplets  $(Y_d = 0)$  in the post-flame zone, the local evaporative heat loss is zero, and hence the local temperature T is uniform and no temperature gradient exists in the burned zone. Therefore, in homogeneous flames, the thermal effects discussed

in Fig. 2, i.e. heat loss from evaporation of liquid fuel droplets, are only present in the pre-flame zone.

The structure of heterogeneous flame B in Fig. 4(b) is different from that of flame A. Firstly, finite values of fuel mass fraction  $Y_F$ can be found in the post-flame zone (i.e.  $\eta < 0$ ), due to evaporation of the penetrated droplets. Part of them contribute towards the flame through the back diffusion from the post-flame zone to the flame front, which is also observed from the one-dimensional simulations of propagating flame in fuel mists (Aggarwal and Sirignano, 1985). However, there are still finite residual fuel vapors beyond the evaporation zone in the burned area, i.e.  $\eta < \eta_c$ . This is different from the results in flame A, and the kinetic effects of flame B arise from both pre- and post-flame evaporation zones. Secondly, the gas temperature in the post-flame zone gradually decreases from the flame front in the post-flame evaporation zone. Heat conduction in this zone (i.e.  $\eta_c < \eta < 0$ ) would also weaken the flame reactivity, due to the considerable temperature gradient near the flame front. This is also observed from the results of laminar premixed flame with water mists (Belyakov et al., 2018). Therefore, the thermal effects on heterogeneous flames include evaporative heat loss in the pre- and post-flame evaporation zones and also heat conduction in the post-flame evaporation zone.

For fuel-rich condition, the structures of flames E and F are shown in Figs. 4(c) and 4(d), respectively. Note that mass fraction of oxidizer  $Y_0$ , instead of  $Y_F$ , is shown here. As seen from Fig. 3(a), flame E is from the lower branch ( $d_0 = 2 \mu m$ ) and a homogeneous flame. However, flame F lies at the upper branch (initial droplet diameter  $d_0 = 20 \ \mu m$ ) and hence is a heterogeneous flame. They have the same initial droplet mass loading  $\delta = 0.6$ . Qualitatively, the distributions of gas temperature and droplet mass loading of flames E and F are respectively similar to the counterpart homogeneous and heterogeneous flames, i.e. A and B. However, different from them, the burned gas temperatures at  $\eta = -\infty$  in both cases are considerably below that of the purely gaseous flame. This is justifiable, because the addition of the fuel vapor into the mixture would render rich gaseous composition deviate more from stoichiometry. Particularly, in Flame F, the lower temperature of burned gas also results in larger temperature gradient in the postflame evaporation zone, as shown in Fig. 4(d), and therefore more heat conduction from the flame. The structures of fuel-rich flames E and F are also similar to those of water-droplet-laden planar flames by Belyakov et al. (2018).

Locations of evaporation onset and completion fronts,  $\eta_{v}$  and  $\eta_{c}$ , relative to the flame front can also be analytically determined from our theories in Section 3.2, subject to gas and droplet properties. As seen from Fig. 4, they are considerably different in homogeneous and heterogeneous flames, and differentiate the thermal and kinetic effects of the respective evaporating fuel droplets. Therefore, Fig. 5 generalizes  $\eta_v$  and  $\eta_c$  of droplet-laden flames with different initial droplet size and mass loading. For fuel-lean conditions in Fig. 5(a), the curves are reverse 7-shaped, and it is shown that initial mass loading  $\delta$  has relatively small effects on  $\eta_{v}$  and  $\eta_{c}$ . Moreover, the evaporation onset front  $\eta_{v}$  is before the flame front and varies little when  $d_0 > 10 \ \mu\text{m}$ . However, for  $d_0$  $\leq$  10 µm,  $\eta_{\nu}$  slowly decrease with smaller  $d_0$ . This is because for smaller droplets they reach the boiling temperature closer to the flame front. Meanwhile, with increased  $d_0$ , evaporation completion front  $\eta_c$  firstly precedes the flame front and then penetrates across the flame front (i.e.  $\eta = 0$ ) into the post-flame zone. The further droplet penetration is parameterized by increased magnitudes of  $\eta_c$ . Note that crossing the flame front implies the transition from homogenous flame to heterogeneous one, as also can be from Fig. 1. Besides, the length of the evaporation zone increases with  $d_0$ , which can be measured as the relative distance between  $\eta_v$  and  $\eta_c$ , i.e.  $|\eta_c - \eta_v|$ . In addition, as shown in the inset of Fig. 5(a), asymptotically, when the droplet diameter approaches



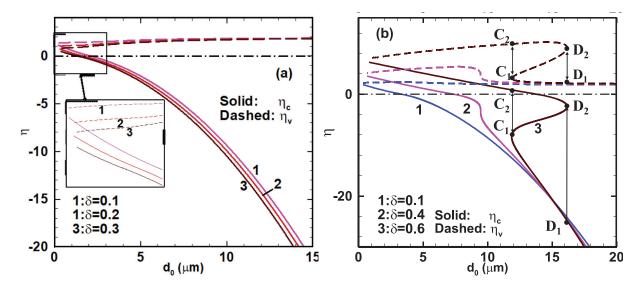
**Fig. 4.** Structures (*T*,  $Y_{(F, 0)}$ ,  $Y_d$ ) of four flames: (a) A, (b) B, (c) E and (d) F. They are marked in Figs. 2(a) or 3(a). The dash-dotted lines denote the locations of evaporation onset and completion fronts. The flame front lies at  $\eta = 0$ . A and E: homogeneous flames; B and F: heterogeneous flames. Green numbers above the upper  $\eta$ -axis indicate the flame / evaporation zones.

zero (i.e. infinitely small droplets),  $\eta_v$  and  $\eta_c$  tend to be equal, due to the infinitely fast evaporation time.

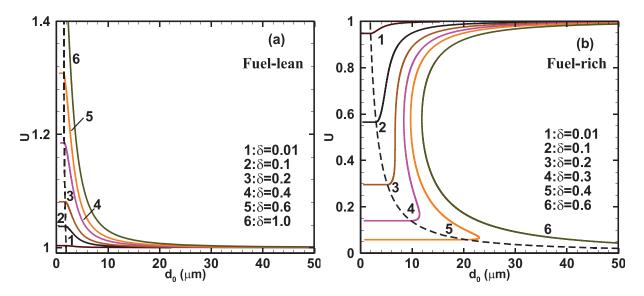
For fuel-rich flames, when the initial mass loadings are small (e.g.  $\delta = 0.1$  or 0.4) the curves of  $\eta_v$  and  $\eta_c$  versus initial droplet diameter are qualitatively similar to those from fuel-lean flames. Nevertheless, bifurcation of droplet evaporation front locations,  $\eta_{v}$ and  $\eta_c$ , can be observed from Fig. 5(b) with larger  $\delta$  (e.g. 0.6), characterized by Z-shaped curves and consistent with the concurrent bifurcations of flame propagation speed and temperature discussed in Fig. 3. Note that the upper (lower) branch of Z-shaped  $\eta_v$  curve corresponds to the upper (lower) branch of Z-shaped  $\eta_c$  curve. For ease to reference back to Fig. 3, we mark the corresponding turning points  $C_1$ ,  $C_2$ ,  $D_1$  and  $D_2$  in Fig. 5(b). For the heterogeneous  $C_1 - D_1$  branch, with increased  $d_0$ ,  $\eta_v$  is marginally affected, but the norm of  $\eta_c$  increases considerably, indicating larger burned zone with evaporating droplets. As such, the length of evaporation zone increases accordingly. For the upper  $C_2 - D_2$  branch, they are mixed with the homogeneous and heterogeneous flames, demarcated by the intersection point at  $\eta = 0$ . When  $d_0$  approaches zero,  $\eta_{\nu}$  and  $\eta_c$  are asymptotically equal, which is also seen in Fig. 5(a). As  $d_0$  increases, the evaporation zone increased, but when  $d_0$  is slightly beyond 20 µm, the heterogeneous flame bifurcates:  $\eta_{\nu}$  moves closer to the flame, and  $\eta_c$  lies well behind the flame front.

### 4.2. Effects of latent heat of vaporization

In the last section, the latent heat of vaporization  $q_v$  is fixed to be 0.4. In reality, different liquid fuels have different values of latent heat of vaporization (Lefebvre and McDonell, 2017). Therefore, Figs. 6 and 7 show the flame propagation speed as a function of the initial droplet diameter with  $q_v = 0.8$  and 1.2, respectively. These values correspond to those of liquid fuels with high latent heat, e.g. methanol. Both fuel-lean and fuel-rich flame results are presented. For  $q_v = 0.8$ , when the droplet diameter and mass loading are fixed (e.g.  $d_0 = 5 \ \mu m$  and  $\delta = 0.2$ ), the propagation speed *U* is lower and therefore closer to that of the dropletfree flame, compared to the results with  $q_v = 0.4$  in Figs. 2 and 3. This indicates that the flame enhancement under fuel-lean con-



**Fig. 5.** Evaporation onset and completion fronts versus initial droplet diameter: (a) fuel-lean (b) fuel-rich conditions. The dash-dotted lines are flame front, i.e.  $\eta = 0$ , the bi-arrow lines show the flame bifurcation in the labeled points.  $C_1$ ,  $C_2$ ,  $D_1$  and  $D_2$  are consistent with the corresponding points in Fig. 3(a).



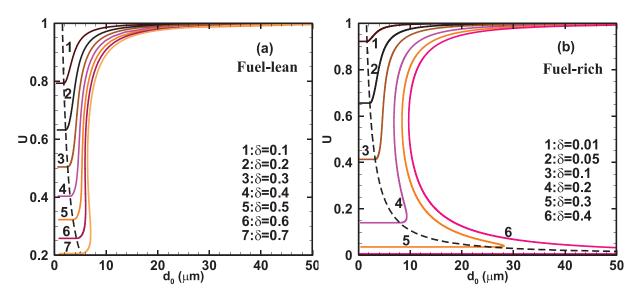
**Fig. 6.** Effect of droplet diameter and mass loading on the flame propagation speed for  $q_v = 0.8$ : (a) fuel-lean, (b) fuel-rich. Homogeneous (heterogeneous) flames: left (right) to the dashed flame regime line.

dition is weakened. This may be due to more heat absorbed from the gas phase to vaporize the fuel droplets. However, for the fuelrich case in Fig. 6(b), when the flame is locally homogeneous, the flame propagation speed is lower for the same  $d_0$  and  $\delta$  (e.g.  $d_0 = 5 \ \mu m$  and  $\delta = 0.2$ ) when  $q_v$  is 0.8, compared to the results with  $q_v = 0.4$  in Figs. 2 and 3. Meanwhile, bifurcation of *U* occurs with smaller  $\delta$  compared to the results in Fig. 3. As such, for the same droplet mass loading under which bifurcation occurs e.g.  $\delta = 0.4$  in Fig. 3(b) and Fig. 6(b), both upper and lower stable branches tend to obtain smaller flame speed for same  $d_0$  when  $q_v$ increased from 0.4 to 0.8.

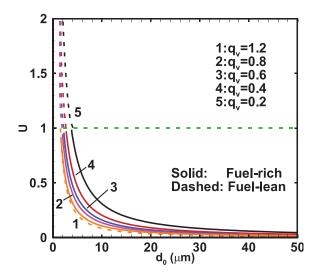
When  $q_{\nu}$  is further increased to 1.2, the flame propagation speed is below that of the gaseous flames, i.e. U = 1 for both fuellean and fuel-rich conditions as shown in Figs. 7(a) and 7(b). The results in Fig. 7(a) are different from other fuel-lean results as discussed in Figs. 2 and 7(a), due to the dominancy of evaporative heat loss over the kinetic enhancement effects.

### 4.3. Critical condition for homogeneous and heterogeneous flames

Plotted in Fig. 8 are the flame regime lines in the plane of  $U - d_0$  between the homogeneous and heterogeneous flames. Various droplet properties, including initial droplet diameter  $d_0$  and latent heat of vaporization  $q_v$ , are considered. Like the flame regime lines in Figs. 2, 3, 6 and 7, each curve in Fig. 8 is calculated using Eqs. (50) - (53) based on a fixed mass loading. In the  $U - d_0$  plane here, the left part to each regime line corresponds to homogeneous flames, whilst the right part heterogeneous ones. With decreased  $q_v$  from 0.2 to 0.8, the range of the initial droplet diameters where homogeneous flames exist is extended, for both fuellean (i.e.  $U \ge 1$ ) and fuel-rich (i.e.  $U \le 1$ ) flames. Different from the above cases, when  $q_v$  is increased to 1.2, no solutions exist beyond U = 1, and both regime lines of fuel-lean and fuel-rich conditions are below unity.

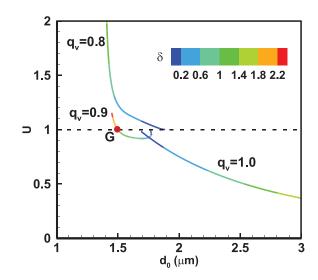


**Fig. 7.** Effect of droplet diameter and mass loading on the flame propagation speed for  $q_v = 1.2$ : (a) fuel-lean, (b) fuel-rich. Homogeneous (heterogeneous) flames: left (right) to the dashed flame regime line.



**Fig. 8.** Effect of fuel latent heat and droplet diameter on the flame regime lines (homogeneous flame: left to the line, heterogeneous flame: right to the line).

To further identify the critical latent heat of vaporization with which the regime lines critically cross the flame front, Fig. 9 further shows the critical regime curves for fuel-lean flames with latent heat of vaporization  $q_v = 0.8$ , 0.9 and 1.0. For  $q_v = 0.8$  and 1.0, their flame propagation speeds U are respectively consistently higher and lower than that of the droplet-free flame (i.e.  $\delta = 0$ seen from Fig. 9), i.e. U = 1. They respectively correspond to the fact that the flames are overall enhanced and weakened due to the liquid droplets. However, when  $q_v = 0.8$ , the regime line is firstly (with small mass loading) below the line of U = 1. When the mass loading  $\delta$  increases, the critical conditions, i.e. the solutions along the regime line, move towards smaller droplet diameter, but still below U = 1. At point G, the propagation speed of the two-phase flame is the same as that of the droplet-free flame, indicating the kinetic and thermal effects caused by the droplet evaporation counterbalance. Further increasing  $\delta$  leads to regime line in the upper part of the  $U - d_0$  plane, corresponding to flame enhancement by the fuel droplets.



**Fig. 9.** Effect of fuel latent heat and droplet diameter on flame regime line for fuellean condition (homogeneous flame: left to the line, heterogeneous flame: right to the line).

### 4.4. Evaporative heat loss

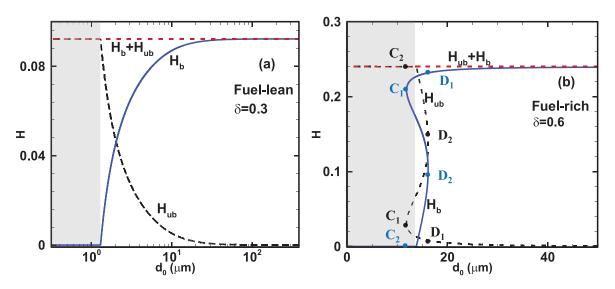
The heat loss effects of droplet evaporation on homogeneous and heterogeneous flames have been mentioned in Figs. 2, 3 and 4. In this Section, normalized evaporation heat loss, H, is calculated to quantify these effects in the pre-flame and post-flame zones respectively as

$$H_{ub,HT} = \Omega \int_{0}^{\eta_{\nu}} [T_2(\xi) - T_{\nu}] d\xi / \left( \left. \frac{dT}{d\eta} \right|_{-} - \left. \frac{dT}{d\eta} \right|_{+} \right), \tag{54}$$

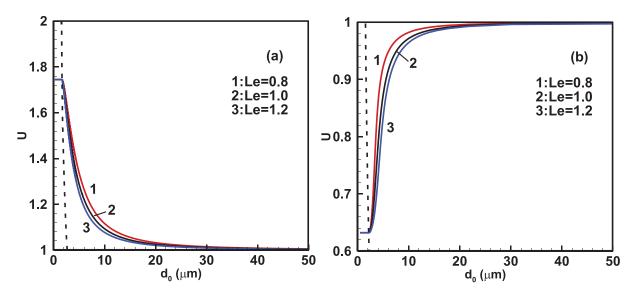
$$H_{ub,HM} = \Omega \int_{\eta_c}^{\eta_v} [T_2(\xi) - T_v] d\xi / \left( \frac{dT}{d\eta} \bigg|_{-} - \frac{dT}{d\eta} \bigg|_{+} \right), \tag{55}$$

$$H_{b,HT} = \Omega \int_{\eta_c}^{0} [T_3(\xi) - T_\nu] d\xi / \left( \frac{dT}{d\eta} \Big|_{-} - \frac{dT}{d\eta} \Big|_{+} \right), \tag{56}$$

$$H_{b,HM} = 0,$$
 (57)



**Fig. 10.** Normalized evaporation heat loss as a function of initial droplet diameter: (a)  $\delta = 0.3$ , fuel-lean; (b)  $\delta = 0.6$ , fuel-rich.  $q_{\nu} = 0.4$ . The shaded area indicates homogeneous flames, while the rest is heterogeneous flame. Points  $C_1$ ,  $C_2$ ,  $D_1$  and  $D_2$  correspond to the same points in Fig. 3(a).



**Fig. 11.** Effect of the Lewis number and droplet diameter on the flame propagation speed for fuel-lean condition with fixed  $\delta = 0.2$  when (a)  $q_v = 0.4$ , (b)  $q_v = 1.2$ . Dashed line: flame regime line. Homogeneous flame: left to the dashed line; heterogeneous flame: right to the dashed line.

where the subscripts "*ub*" and "*b*" respectively denote pre- and post-flame evaporation zones, whereas "*HM*" and "*HT*" respectively denote homogeneous and heterogeneous flames.  $\left(\frac{dT}{d\eta}\Big|_{-} - \frac{dT}{d\eta}\Big|_{+}\right)$  in the denominator of Eqs. (54) – (56) is the total heat release from the chemical reaction.  $T_2(\xi)$  and  $T_3(\xi)$  are the temperature distributions in zones 2 and 3, respectively. The integrands,  $[T_{\{2,3\}}(\xi) - T_v]$ , indicate the interphase temperature difference in the evaporation zone, where the droplets are at the boiling temperature  $T_v$ . Fig. 10 shows the normalized evaporation heat loss (i.e.  $H_{ub,HT}$ ,  $H_{b,HT}$ ,  $H_{ub,HM}$  and  $H_{b,HM}$ ) of the selected fuel-lean ( $\delta = 0.3$ ) and fuel-rich ( $\delta = 0.6$ ) flames. Their corresponding flame propagation speeds *U* as functions of initial droplet diameter  $d_0$  with these two mass loadings have been discussed in Figs. 2 and 3.

Since the initial mass loading  $\delta$  is constant in all the flame solutions in Figs. 10(a) and 10(b), the sum (i.e.  $H_{ub,HT} + H_{b,HT}$ , or  $H_{ub,HM} + H_{b,HM}$ ) of evaporative heat loss in their pre- and post-flame zones remains constant, as indicated with the dash-dotted lines. For homogeneous flames (in the shaded area), no droplets are in the burned zone and therefore  $H_{b,HM} = 0$ , i.e. Eq. (57). More-

over,  $H_{ub, HM}$  is constant with  $d_0$ , due to the fixed mass of liquid fuels. For heterogeneous flames, the evaporative heat loss in the pre- and post-flame zones,  $H_{ub,HT}$  and  $H_{b,HT}$ , monotonically decreases and increases with  $d_0$ , respectively. Based on the definitions of mass loading and evaporative heat exchange coefficient, they are correlated through  $\Omega \sim \delta/d_0^2$ . Therefore, for a constant  $\delta$ , the larger the droplet diameter  $d_0$ , the slower the evaporative rate and hence smaller heat exchange coefficient  $\Omega$ . Meanwhile, when  $d_0$  decreases, the interphase temperature difference is reduced as well. Both effects jointly result in monotonic reduction of  $H_{ub, HT}$ . For post-flame evaporation zone, the high interphase temperature difference leads to gradual increase of  $H_{b, HT}$ , although  $\Omega$  decreases, with increased  $d_0$ . When  $d_0 > 30 \,\mu$ m,  $H_{ub, HT}$  tends to be zero and the evaporative heat loss is dominantly from the post-flame zone.

Fig. 10(b) shows the normalized evaporative heat loss for selected fuel-rich flames with  $\delta = 0.6$ . Note that the turning points  $C_1$ ,  $C_2$ ,  $D_1$  and  $D_2$  correspond to the same points in Fig. 3(a). Solutions of branch  $C_1$ -  $D_1$  are strong flames with higher U and  $T_f$ , whilst those along  $C_2$ -  $D_2$  are weak ones. In the shaded area for homogeneous flames,  $H_{b,HM} = 0$ , same as those in Fig. 10(a). In the heterogeneous flames,  $H_{ub, HT}$  of branch  $C_2$ -  $D_2$  is higher than  $H_{b, HT}$ . However, for branch  $C_1$ -  $D_1$ , the tendency is opposite.

### 4.5. Lewis number effect

Up to this point, the Lewis number is assumed to be Le = 1. For fuel-rich flames, the Lewis number is affected by the oxidizer mass diffusion and therefore variations of the Lewis number do not affect the flame propagation speed (results not shown here for brevity). To examine this effect on fuel-lean planar spray flame propagation, Fig. 11 show the flame propagation speed as a function of initial droplet diameter when Le = 0.8, 1.0 and 1.2. The initial droplet loading  $\delta$  is fixed to be 0.2. It is seen that propagation speed of homogeneous flame is not dependent on Lewis number for both high and low latent heat. Since the droplet evaporation is completed before the flame front, all the fuel vapor in the pre-flame zone would be depleted by the chemical reaction at the flame front and it behaves like a purely gaseous flame.

For heterogeneous flames, droplet evaporation occurs in the post-flame zone and fuel vapor exists therein, as seen from the structure of heterogeneous flames in Fig. 4(b). In this case, the fuel vapor diffusion considerably influences the consumption at the flame front. Specifically, the smaller (larger) Lewis number indicates a higher (lower) mass diffusivity and therefore more (less) fuel vapor from the post-flame zone can contribute towards the combustion, thereby leading to an enhanced (reduced) flame propagation speed. Note that these are remarkable only for intermediate droplet diameters. For heterogeneous flames laden with relatively small ( $d_0$  slightly larger than 2 µm) or large ( $d_0 > 20$  µm) droplets, dependence of heterogeneous flame propagation speed on Lewis number is minimized. This is because for small droplets, the evaporation completion location  $\eta_c$  in the post-flame zone is close to the flame front and fuel vapor can be consumed locally. Conversely, when the droplet size is large, the post-flame evaporation zone is large, leading to a reduced gradient of fuel vapor from liquid droplets.

### 5. Conclusions

Propagation of one-dimensional laminar planar flames laden with fuel droplet mists is investigated theoretically. Localized homogeneous and heterogeneous flames are considered, which are characterized by different relative locations of dispersed fuel droplets and flame front. Within the framework of large activation energy, correlations describing flame propagation speed, flame temperature, evaporation onset and completion fronts are derived. With this correlation, the influences of droplet (e.g. diameter and droplet mass loading) and fuel (e.g. latent heat of vaporization) parameters on propagation of fuel-droplet-laden planar flames are assessed.

The results indicate that fuel droplets affect the flame propagation differently for fuel-lean and fuel-rich conditions. Under fuel-lean conditions, the flames are enhanced by the evaporating droplets. The burned gas temperature of homogeneous flame is slightly higher than the purely gaseous flame due to the fuel vapor addition. For fuel-lean heterogeneous flames, residual fuel vapor and considerable temperature gradient exist in the post-flame evaporation zone. However, under fuel-rich conditions, the droplets suppress the flame propagation. The tendencies of temperature and droplet mass loading distributions are similar to those from the fuel-lean cases. However, the burned gas temperature is much lower than that of fuel-lean case, due to the off-stoichiometric compositions. In addition, the foregoing effects on fuel-rich and fuel-lean flames under respective conditions are intensified with increased droplet mass loading. Our results also show that evaporation completion front location is largely affected by the droplet diameter, instead of mass loading. Conversely, the evaporation onset front varies little with droplet properties. Bifurcation and multiplicity are observed for large droplet loading and fuel-rich gas composition, in terms of the propagation speed and droplet evaporation onset/completion front locations.

It is also shown that for different values of latent heat, the droplet evaporative heat loss effects on the flame propagation are different. This is particularly pronounced for the fuel-lean conditions, where increasing latent heat leads to variations from flame enhancement to weakening relative to the droplet-free flames. The normalized evaporative heat loss in different flame and evaporation zones are also calculated. In general, for homogeneous flames, the heat loss only occurs in the pre-flame zone. However, for heterogeneous flames, heat loss in the post-flame evaporation zone become dominant for relatively large droplets. Furthermore, the effect of Lewis number on laminar planar spray flames is also studied, and it is found that Lewis number influences heterogeneous flame propagation speed under fuel-lean conditions when the droplet diameter is intermediate.

### **Declaration of Competing Interest**

None.

### **CRediT** authorship contribution statement

**Qiang Li:** Conceptualization, Methodology, Validation, Formal analysis, Writing - original draft, Visualization. **Huangwei Zhang:** Conceptualization, Methodology, Writing - review & editing, Supervision, Project administration, Funding acquisition. **Chang Shu:** Writing - review & editing, Supervision.

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#### Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ijmultiphaseflow.2020. 103452.

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