

Droplet-induced stretch effects on lean premixed hydrogen-air flame front

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The interaction between a single water droplet and a lean premixed hydrogen-air flame is investigated using two-dimensional detailed-chemistry simulations in an Eulerian-Lagrangian framework. A single cusp flame configuration is employed to impose a controllable curvature to the flame and isolate the effects of droplet-induced stretch. When the water droplet evolves in an inertia-dominated regime, it acts as a localized momentum and heat sink, generating a transient deformation of the flame front and a reduction in the local displacement speed. It is observed that curvature gradient generated by the droplet-flame interaction, contributes to the decrease in flame speed and heat release rate by reducing the reactants focusing effect. This result is confirmed by comparison with an equivalent simulation performed under a unity Lewis number assumption, where curvature-induced differential diffusion effects are artificially suppressed. The analysis of droplet-induced stretch further shows that the interaction produces a local curvature inversion of approximately 40% of the initial flame shape, while the tangential strain rate component of stretch increases and counteracts this effect. After the interaction, the flame gradually recovers its original shape, and the curvature perturbation decays exponentially with a restoring time governed by the flame diffusion timescale. An analytical model using an analogy with a mass-spring-damper system is proposed to estimate the local flame displacement and displacement speed during the droplet-flame interaction.

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I. INTRODUCTION

The transportation and power generation sectors are increasingly seeking novel combustion systems and alternative fuels to mitigate the effects of climate change [1]. Among these, hydrogen has attracted significant attention thanks to its carbon-free emissions and its ability to burn under ultra-lean conditions, leading to lower flame temperatures and potentially reduced nitrogen oxide (NO_x) formation. However, the high reactivity and diffusivity of hydrogen introduce new challenges for its implementation in practical combustors, where thermodiffusive instabilities and flashback can arise [2]. Consequently, combustion systems must be redesigned to ensure stable and safe operation under such conditions. One strategy to mitigate the aforementioned challenges is the use of water injection (WI), which is recently gaining renewed interest as a potential method for NO_x mitigation in hydrogen combustion for gas turbines [3,4], particularly for aeroengine applications, for example, through the so-called water-enhanced turbofan concept [5]. In fact, unlike

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common hydrocarbons that can experience local extinction during water evaporation, resulting in increased CO and unburned hydrocarbons [6], the high reactivity of hydrogen mitigates the risk of local extinction when the injected droplets reach the flame front. Moreover, WI can serve as an effective strategy to mitigate the risk of autoignition-driven flashback, a common challenge in lean premixed combustion regimes [7]. Due to its relevance in modern combustion applications, greater research efforts are needed to shed light on the physics of water droplets and hydrogen flame interactions. From a fundamental perspective, the influence of water on the flame can be categorized into physical, thermophysical, and chemical effects [8]. The physical effect involves a reduction in the concentration of active species as a result of the dilution by water vapor. The thermophysical effect includes a decrease in the adiabatic flame temperature. The chemical effect is due to the active participation of water in the reactions, which shifts the chemical equilibrium and enhances three-body reactions. In general, when liquid water is added, the thermophysical effect is dominant [9,10], whereas in the case of steam injection, the chemical and physical effects become more important. Such effects have been extensively investigated for various fuels [11,12], including hydrogen [13]. In hydrogen combustion, water addition leads to a reduction in the concentration of H and O radicals within the flame [14], while simultaneously enhancing OH formation [4]. Moreover, the cooling effect induced by water has been shown to thicken the flame [10] and to attenuate both hydrogen's preferential diffusion and the associated nonunity Lewis number effects. Concetti *et al.* [15] have shown that, in lean premixed turbulent hydrogen flames, small water droplets mitigate the nonunity Lewis number phenomena typical of lean hydrogen combustion. For liquid droplets, however, all the discussed effects are strongly influenced by the droplet size, the flame structure, and the relative velocity between the droplet and the flame front. These dependencies have been highlighted in several studies on fire suppression and safety [16]. Moreover, recent direct numerical simulations (DNS) of statistically planar stoichiometric *n*-heptane/air flames interacting with mono-sized water droplets have shown that droplet inertia also plays an important role in modulating the residence time and, consequently, the extent of evaporation [17].

Despite the aforementioned research, several aspects of the influence of liquid water droplets on premixed flames remain unexplored. In particular, the perturbations induced on the flame front by evaporating droplets play an important role, as they can enhance flame wrinkling and local stretch. For instance, in the case of hydrocarbon fuel droplets, it has been shown that at high spray Peclet numbers, the droplet injection on an initially flat premixed flame front can trigger the Darrieus-Landau instability by creating holes of weak combustion, corresponding to low-temperature regions caused by droplet evaporation [18]. Moreover, for flames with fully developed Darrieus-Landau instabilities, the presence of fuel droplets was found to induce additional short-wavelength wrinkles on the flame front, thereby increasing the flame surface area and enhancing the overall flame speed [18]. Such flame speed enhancement has also been later observed numerically for hydrocarbon flames interacting with water droplets [19], where widely spaced droplets promoted enhanced flame wrinkling and increased burning rate, whereas densely distributed droplets led to localized extinction. Later on, Hasslberger *et al.* [9], by means of DNS of liquid water mists interacting with laminar and turbulent premixed stoichiometric *n*-heptane/air flames, identified the main interaction regimes of water droplet-flame interaction. These regimes, defined for hydrocarbon flames, have been classified according to the ratio between the evaporation and flame timescales and the ratio between the mean droplet separation distance and the flame thickness. They have shown that the regime in which the effective vapor cloud surrounding the droplets induces additional flame wrinkling occurs for large inter-droplet spacing and rapid droplet evaporation relative to the flame residence time. This regime is referred to as the *inhomogeneously perturbed* regime [9]. The effects of water injection on the flame surface topology and local flame propagation characteristics have also been analyzed for statistically planar turbulent *n*-heptane spray flames. It has been found that flame curvature variations and the probability of obtaining convex and concave flame front regions induced by fuel droplets in laminar cases decrease with water injection. This effect is particularly pronounced for small droplet diameters [20]. Furthermore, experimental evidence on isolated acetone droplets burning in a steady laminar methane counterflow flame has shown that

the fuel droplet flame interaction can lead to local flame extinction not only due to cooling but also as a result of high strain rates induced by droplet motion. The droplet-generated flow field distorts the flame front, increasing local strain and reducing the reaction rate ahead of the droplet [21]. Furthermore, experiments on uniformly dispersed spray flames of low-volatility fuels (Jet A and ATJ-8) have shown that droplet size strongly influences flame stretch and curvature. Large droplets promote localized reactions that generate regions of negative curvature and slow flame propagation, while increased evaporation at smaller Sauter mean diameters leads to a smoother, more gaseous-like front with reduced curvature effects and higher burning velocities [22].

In the case of lean hydrogen-air premixed flames, several recent studies have shed light on the details of flame-droplet interactions, mainly through investigations of spherically expanding flames [23], planar [20], and cylindrical flames [24]. For cylindrical flames, it was shown that the presence of water droplets induces pronounced corrugations of the flame surface, which distort the flow field ahead of the flame with perturbations of characteristic scale corresponding to the inter-droplet spacing. Consequently, the flame propagation speed was observed to increase by up to a factor of 2.2 in the presence of micro-droplets with diameters of about 200 μm as compared to the pure gaseous mixture. In contrast, as the droplet diameter decreases, the flame surface becomes progressively smoother, leading to reduced flame wrinkling and, ultimately, to slower flame propagation [24]. Similarly, it has been shown that adding large water droplets to spherically expanding hydrogen-air flames enhances both flame growth and the development of cellular structures. In contrast, small droplets mitigate these effects by increasing cooling [23].

While previous studies have shown that water droplet-flame interaction involves a strong coupling between physical, thermophysical, and chemical effects, and that droplets can induce corrugations on the flame surface, the effect of droplet-induced stretch and its coupling with preferential diffusion is still unclear. This is partly due to the complex coupling between turbulence and flame dynamics, which makes it challenging to isolate the individual effects mentioned above. However, this aspect is particularly relevant for hydrogen flames because, first, H_2 premixed flames are highly sensitive to stretch due to strong preferential diffusion [25,26]. Second, hydrogen is much more reactive than conventional hydrocarbons [2], which makes these flames less prone to extinction when a water droplet evaporates near the flame front. In this context, the present work develops a numerical framework designed to isolate and control the local interaction between a water droplet and a premixed hydrogen-air flame front. Specifically, the interaction of a single droplet with the positively curved region of a cusp flame is analyzed to provide physical insight into how droplet-flame interactions locally influence flame stretch, chemical reactivity, and flame propagation and how the combined effect of the droplet-induced stretch and differential diffusion alters the flame dynamics. Eventually, all these effects are incorporated into an analytical model for estimating the local variation of the flame speed due to flame-water droplet interactions.

The paper is organized as follows. Section II presents the governing equations, while the computational setup is described in Sec. III. The main results are discussed in Sec. IV, with details on the characteristic timescales provided in Sec. IV A. The effects of droplet-flame interaction on the flame displacement speed, flame stretch, and local reactivity are examined in Secs. IV B, IV C, and IV D, respectively. The flame response to the droplet induced perturbation is further analyzed in Sec. IV E. A simplified model to predict the variation of flame displacement speed due to the droplet-flame interaction is presented in Sec. V. The main conclusions are summarized in Sec. VI.

II. MATHEMATICAL MODEL

The interaction between a single water droplet and a planar premixed hydrogen-air flame is studied using two-dimensional direct numerical simulations with detailed chemistry. The chemical mechanism proposed by Sanchez and Williams [27] is employed to model the hydrogen oxidation. This mechanism includes 8 species and 14 reactions. A two-way coupling Eulerian-Lagrangian approach is employed, where the carrier multi-component reacting gaseous phase is solved in the Eulerian framework, while the liquid water droplets are tracked in the Lagrangian reference frame.

For the gaseous phase (subscript g), the governing equations are the Navier-Stokes equations with the low Mach approximation, which read

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial(\rho_g u_{g,i})}{\partial x_i} = \dot{S}_m, \quad (1a)$$

$$\frac{\partial(\rho_g u_{g,i})}{\partial t} + \frac{\partial(\rho_g u_{g,i} u_{g,j})}{\partial x_j} = -\frac{\partial p_d}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \dot{S}_u, \quad (1b)$$

$$\frac{\partial(\rho_g Y_k)}{\partial t} + \frac{\partial(\rho_g u_{g,i} Y_k)}{\partial x_i} = -\frac{\partial J_k}{\partial x_i} + \dot{\omega}_k + \dot{S}_y, \quad (1c)$$

$$\frac{\partial(\rho_g h_s)}{\partial t} + \frac{\partial(\rho_g u_{g,i} h_s)}{\partial x_i} = -\frac{\partial J_{h_s}}{\partial x_i} + \sum_{k=1}^N \Delta h_{f,k}^0 \dot{\omega}_k + \dot{S}_h, \quad (1d)$$

where ρ_g is the gaseous-mixture density, $u_{g,i}$ is the velocity component in the i direction, Y_k is the mass fraction of the k th species, h_s is the mixture sensible enthalpy, and p_d is the hydrodynamic pressure arising from the low-Mach-number approximation. In this formulation, the total pressure is decomposed as $p'(\mathbf{x}, t) = p + p_d(\mathbf{x}, t)$, where p denotes the constant thermodynamic pressure. The enthalpies of formation $\Delta h_{f,k}^0$ and specific heat capacities, required to recover the temperature from the sensible enthalpy, are evaluated using JANAF polynomials. The species diffusion fluxes J_k are computed using a mixture-averaged diffusion model including Soret diffusion for H_2 and H [28], and, for comparison, a unity-Lewis number model is also employed to isolate the differential diffusion effects. In the case of the mixture-averaged diffusion model, including Soret diffusion for H_2 and H (DD), the species diffusion flux is computed as

$$J_k^{DD} = \rho Y_k V_k = -\rho_g D_k^M \frac{\partial Y_k}{\partial x_i} - \rho_g D_T^M \frac{Y_k}{X_k T} \frac{\partial T}{\partial x_i}, \quad (2)$$

while for the unity-Lewis number (UL) case the species diffusion flux is computed as

$$J_k^{UL} = \rho Y_k V_k = -\rho_g \alpha_g \frac{\partial Y_k}{\partial x_i}. \quad (3)$$

The mixture sensible enthalpy diffusion fluxes for the two cases, J_{h_s} , are computed respectively as

$$J_{h_s}^{DD} = -\alpha_g \frac{\partial h_s}{\partial x_i} + \frac{\partial}{\partial x_i} \left[\sum_{k=1}^N h_k \left(\alpha_g \frac{\partial Y_k}{\partial x_i} - J_k \right) \right], \quad (4)$$

$$J_{h_s}^{UL} = -\alpha_g \frac{\partial h_s}{\partial x_i}, \quad (5)$$

where the second term on the right-hand side of Eq. (4) represents the inter-diffusion flux and α_g is the thermal diffusivity of the gaseous mixture.

The single liquid particle is in this framework tracked along its path in the domain, and its evolution affects the dynamics of the gaseous phase via coupling terms. The equations for the droplet (subscript d) velocity $u_{d,i}$ and position $x_{d,i}$ read

$$\frac{dx_{d,i}}{dt} = u_{d,i}, \quad (6a)$$

$$\frac{du_{d,i}}{dt} = \frac{18\mu_g C_u \text{Re}_d}{\rho_d d^2} (u_{g,i} - u_{d,i}), \quad (6b)$$

where μ_g is the gaseous mixture dynamic viscosity, ρ_d is the droplet density and Re_d is the droplet Reynolds number $\text{Re}_d = \rho_g (u_{g,i} - u_{d,i})(u_{d,i} - u_{g,i})d/\mu_g$. C_u is the droplet drag coefficient

computed according to the Schiller and Neumann correlation:

$$C_u = \begin{cases} \frac{24}{\text{Re}_d} (1 + 0.15 \text{Re}_d^{0.687}), & \text{for } \text{Re}_d \leq 1000, \\ 0.44, & \text{for } \text{Re}_d > 1000. \end{cases} \quad (7)$$

The evaporation of the droplet is modeled under the assumption of phase equilibrium, and the temporal evolution of its diameter is described by the simplified d^2 law [29]:

$$\frac{dm_d}{dt} = \pi d \text{Sh} D_s \rho_s \ln(1 + B), \quad (8)$$

where B is the mass Spalding number $B = \frac{Y_s - Y_\infty}{1 - Y_s}$ with Y_s being the vapor mass fraction at the droplet surface and Y_∞ its far-field value. The surface vapor mass fraction Y_s is computed under the assumption of thermodynamic equilibrium with Rault's law, based on the knowledge of the saturation pressure p_{sat} , which is evaluated using the NSRDS empirical correlation [30]. The Sherwood number Sh is computed using the Ranz-Marshall correlation [31] as $\text{Sh} = 2 + 0.552 \text{Re}_d^{1/2} \text{Sc}_g^{1/3}$, where Sc_g is the Schmidt number of the carrier gaseous phase. D_v is the water vapor mass diffusivity coefficient.

In absence of radiative heat transfer, the droplet temperature T_d evolution is determined by the balance of convective heating and evaporative cooling as

$$m_d c_{p,d} \frac{dT_d}{dt} = h \pi d^2 (T - T_d) f_b - L_v \frac{dm_d}{dt}, \quad (9)$$

where h is the heat transfer coefficient of the carrier phase determined via $h = (\text{Nu} \alpha_g)/d$, and the Nusselt number is computed via the Ranz-Marshall correlation [31] as $\text{Nu} = 2 + 0.552 \text{Re}_d^{1/2} \text{Pr}_g^{1/3}$, with Pr_g being the carrier's Prandtl number. L_v is the latent heat of vaporization of the liquid. To account for the reduction of heat transfer due to evaporation, the Bird's correction f_b is applied, where $f_b = \beta/(e^\beta - 1)$ with $\beta = -c_{p,\text{vap}} \dot{m}_d / \pi d \lambda_g \text{Nu}$ [32].

The coupling between gaseous and liquid phases is represented by the coupling terms $\dot{S}_j$, which are expressed as

$$\dot{S}_j = \frac{1}{V_{\text{cell}}} \sum_{i=1}^{N_d} \frac{d}{dt} (m_d \psi), \quad (10)$$

where $j = \{m, u, y, h\}$ [see Eqs. (1)] and $\psi = \{1, u_{g,i}, Y_{\text{H}_2\text{O}}, h_s\}$. The source term $\dot{S}_j$ is linearly interpolated from the droplet position to the eight surrounding grid points. Here, V_{cell} denotes the cell volume. It is worth noting that, throughout this work, two distinct definitions of the progress variable c are employed: a hydrogen-based progress variable, denoted as c_{H_2} , and a temperature-based progress variable, denoted as c_θ . In the remainder of this paper, both definitions are used depending on the specific analysis considered.

III. COMPUTATIONAL SETUP AND NUMERICAL METHODS

The setup consists of a freely propagating flame in a two-dimensional domain of dimensions $20\delta_{\text{th}}^0 \times 12\delta_{\text{th}}^0$, where δ_{th}^0 is the unstretched laminar thermal flame thickness. At very lean conditions, such flames are known to exhibit intrinsic hydrodynamic and thermodiffusive instabilities [33,34], which complicate the interpretation of flame response in the presence of a droplet. To mitigate this, a single-cusp flame configuration is studied to achieve a controllable curvature. Specifically, a prescribed curvature profile is imposed on the flame front following the procedure outlined as follows. A reference solution is first constructed using the one-dimensional code CHEM1D [35], providing a steady, unstretched flame profile. This solution is then mapped onto the two-dimensional domain, and a controlled spatial perturbation of the form $F(x) = A_0 \sin(-2\pi y/L_y)$ is imposed on the flame front. Here, x and y denote the streamwise and transverse directions, respectively, and

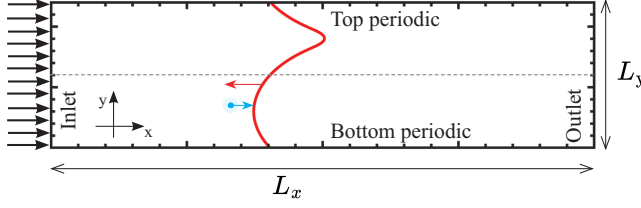


FIG. 1. Sketch of the computational domain with width of $L_x = 20\delta_{th}^0$ and $L_y = 12\delta_{th}^0$. The reactant mixture is injected left to right from the inlet section. The water droplet (cyan filled circle) is placed to a distance at an initial position of $(x_d = 7\delta_{th}^0, y_d = 3.3\delta_{th}^0)$ and it propagates with a velocity u_d across the flame (note the droplet size is out of scale). The gray dashed line indicates the region of the domain selected for analysis, restricted to the positively curved flame region.

$A_0 = 0.04\delta_{th}^0$ is the perturbation amplitude. This approach introduces controlled curvature on the flame front, enabling a systematic investigation of the interaction between flame curvature and the injected water droplet.

Following the pioneering works of Réveillon and Vervisch [36], Borghi [37], and the more recent extension to turbulent flames by Hasslberger *et al.* [9], droplet-flame interactions can be classified into different regimes based on two characteristic scales. The first is the ratio between the droplet evaporation timescale τ_v , and the flame timescale τ_f^0 , which quantifies the relative rate of droplet evaporation with respect to the characteristic flame timescale. The second is the ratio between the droplet inter-distance δ_s , and δ_{th}^0 , which quantifies the degree of spray dilution and therefore the level of droplet-droplet interaction. For a single droplet, the interaction dynamics depend primarily on the ratio τ_v/τ_f^0 . Under these conditions, two main regimes can be identified. The first is the preevaporation regime, corresponding to $\tau_v/\tau_f^0 \ll 1$, in which the droplet completely evaporates before reaching the flame front, thereby producing mainly thermal, chemical, and dilution effects on the flame. The second is the liquid-droplet/flame interaction regime, corresponding to $\tau_v/\tau_f^0 \gg 1$, in which the vapor cloud surrounding the droplet directly interacts with the flame. The present study focuses on the latter regime, where evaporation occurs in the vicinity of the flame front. Figure 1 shows a sketch of the computational domain, where the droplet is initialized at a y axis position of $y_d = 3.3\delta_{th}^0$, and a streamwise location of $x_d = 7\delta_{th}^0$. The initial droplet position along the y direction is chosen such that the droplet interacts with the positively curved position of the flame front. The streamwise position x_d , the droplet injection velocity u_d , the initial droplet diameter d_0 , and the reactant temperature T_r (see Table I) are instead chosen to obtain the aforementioned liquid-droplet/flame interaction regime. These parameters are determined through a series of preliminary simulations of a single evaporating droplet injected into a quiescent hot premixed hydrogen-air environment characterized by the same thermodynamic conditions as those encountered ahead of the flame front. The initial droplet temperature T_d^0 is fixed at 330 K, close to the wet-bulb temperature of water at the chosen gas temperature [38], consistent with the steady-state evaporation assumption

TABLE I. Overview of the performed simulation parameters. ϕ is the mixture equivalence ratio, T_r is the reactant temperature, δ_{th} is the thermal thickness, s_L is the laminar flame speed, d is the droplet diameter, and u_d is the droplet speed. Parameters marked with the superscript 0 refer to the corresponding values of a laminar, freely propagating reference flame without a droplet, whereas parameters marked with the subscript 0 refer to the initial droplet conditions.

	ϕ	T_r	δ_{th}^0	s_L^0	d_0 / δ_{th}^0	u_{d_0} / s_L^0
Value	0.6	400	0.36	1.15	0.15	0.25
Unit	mm	K	m/s	—	—	—

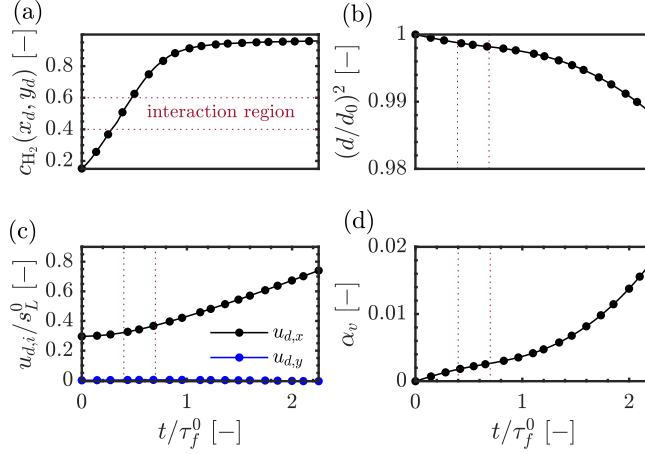


FIG. 2. Evolution in time of a water droplet crossing the flame front in the streamwise direction: (a) hydrogen-based progress variable; (b) droplet diameter d ; (c) droplet velocity components $u_{d,i}$; and (d) vapor mass fraction due to droplet evaporation α_v . The red dotted lines represents the droplet-flame front interaction interval.

(see Sec. II). The Navier-Stokes equations with low-Mach approximation are discretized using the finite volume method (FVM) implemented within the software OPENFOAM [39]. The simulations are performed with an in-house code developed within the OPENFOAM framework, namely a modified version of reactingParcelFoam [39]. Second-order central schemes are employed for all gradients, and second-order Cranck-Nicholson time integration is used. The numerical grid accounts for 2839×1703 cells, corresponding to 150 cells within the flame thermal thickness δ_{th}^0 . Periodic boundary conditions are applied to the top and bottom boundaries of the computational domain, while at the lateral boundaries, inflow and outlet boundary conditions are prescribed. At the outlet boundary, Neumann boundary conditions are imposed on temperature, species, and velocity, while pressure is set to $p = 1$ bar. At the inlet boundary, the velocity of the reactants equals that of the laminar unstretched flame speed s_L^0 plus a small contribution to allow the flame to remain within the boundaries of the computational domain. The mass fractions of hydrogen, oxygen, and nitrogen are specified to obtain a premixed mixture with an equivalence ratio of $\phi = 0.6$. The choice of $\phi = 0.6$ is motivated by two considerations. On the one hand, it is representative of operating conditions where water injection can be employed for pollutant-emission mitigation. On the other hand, this equivalence ratio is particularly relevant to one of the objectives of the present study, namely the investigation of droplet-induced stretch effects on flame dynamics. At such lean conditions, unlike most hydrocarbon flames, hydrogen-air premixed flames have a negative Markstein length. Therefore, the stretch perturbations induced by the droplet are expected to locally modify the flame reactivity.

IV. RESULTS AND DISCUSSION

A. Water droplet propagation across the flame and characteristic timescales evaluation

The trajectory of the water droplet across the positively curved region of the flame front is tracked over time by computing the hydrogen-based progress variable, c_{H_2} , at the droplet's instantaneous position, (x_d, y_d) , as shown in Fig. 2(a). The time origin ($t = 0$ s) corresponds to the droplet injection, and time is normalized using the timescale of a laminar, unstretched flame $\tau_f^0 = \delta_{th}^0/s_L^0$, at the nominal equivalence ratio. Since the droplet is initialized in proximity to the flame front, it rapidly crosses it and subsequently remains within the combustion products region.

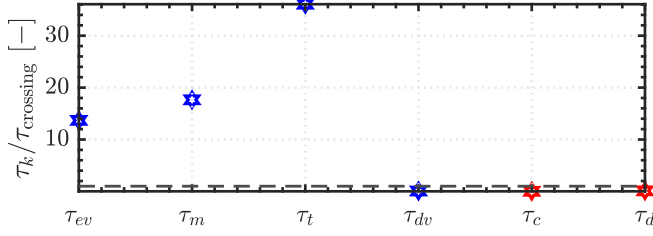


FIG. 3. Characteristic timescales τ_k associated with droplet evaporation τ_v , momentum response τ_m , heating τ_t , and vapor diffusion τ_{dv} , together with the flame chemical τ_c and diffusion τ_d timescales. All timescales are normalized by the droplet crossing time, τ_{crossing} . The horizontal dashed line separates processes faster than the droplet crossing from those occurring over longer timescales.

Figures 2(b)–2(d) show the evolution in time, respectively, of the droplet diameter, the streamwise and transverse velocity components $u_{d,x}$ and $u_{d,y}$, and the fraction of evaporated water vapor with respect to the total mass in the liquid phase α_v . It can be seen that, upon injection, the droplet follows a quasi-linear trajectory, which results from the higher streamwise acceleration due to the thermal expansion as compared to the transverse one [see blue circle line in Fig. 2(c)]. As a consequence, the droplet velocity gradually increases until reaching approximately 70% of the reference speed s_L^0 after about $2\tau_f^0$. Moreover, during the flame crossing, the water droplet experiences convective and conductive heat transfer from the surrounding hotter gases. As a result, the droplet temperature progressively rises, eventually triggering vaporization. At later stages, the evaporation leads to saturation of the combustion zone with inert water vapor, which can affect the oxidation kinetics of the hydrogen-air mixture [40].

Focusing on the progress variable range $0.4 \leq c_{H_2} \leq 0.6$, which delimits the flame front region [red dotted lines in Fig. 2(a)], and on the time interval $0.28 \leq t/\tau_f \leq 0.48$, the local droplet-flame front interaction can be characterized. Figure 2(b) shows the droplet diameter as a function of time. It can be noticed that during the interaction, the evaporation rate remains relatively low, as indicated by the limited decrease in the droplet diameter [Fig. 2(b)]. As a result, the amount of water vapor resulting from droplet evaporation [Fig. 2(d)] is insufficient to induce a significant chemical effect on hydrogen oxidation or a noticeable dilution of species concentrations. This is because droplet heating and evaporation primarily occur within the combustion product region, where their influence on flame dynamics is minimal. Given the multiple physical phenomena occurring during the droplet crossing time, τ_{crossing} , it is essential to identify the dominant effects influencing both the droplet and flame-front dynamics throughout the droplet-flame interaction. Thus, a time-scale analysis is performed to determine which processes take place on timescales comparable to the droplet's crossing time across the flame front. For this purpose, the characteristic timescales associated with the main physical processes governing both the droplet and the flame are computed. Specifically, the droplet evaporation timescale is defined as $\tau_v = (d_0)^2/K$, the droplet momentum relaxation time as $\tau_m = \rho_d d_0^2/(18\mu_g)$, and the thermal relaxation timescale as $\tau_t = \rho_d c_{p,d} d_0^2/(12\alpha_g)$. Here, $K = 8\lambda_g \rho_d c_{p,d} Sh/(d_0 \ln(1+B))$ represents the evaporation constant, and the vapor diffusion timescale is estimated as $\tau_{dv} = \pi d_0^2/D_v$ [41]. All timescales are normalized by the reference time corresponding to the mean droplet crossing time, τ_{crossing} , and are reported in Fig. 3 together with the flame characteristic chemical τ_c and diffusive τ_d timescales. It is observed from Fig. 3 that droplet evaporation occurs over timescales shorter than the droplet crossing time, consistent with the simulated interaction regime (see discussed in Sec. III). In contrast, the momentum and thermal relaxation timescales are much larger than τ_{crossing} , indicating the droplet's high inertia and high heat capacity. In fact, the water droplet exhibits stronger thermal inertia due to its large specific heat and latent heat of vaporization. Note that, because of their relatively large size and density, a water droplet responds slowly to variations in the gas flow velocity, retaining its momentum for longer and thereby interacting with the surrounding gas in an inertia-dominated regime. As shown in Fig. 2(d),

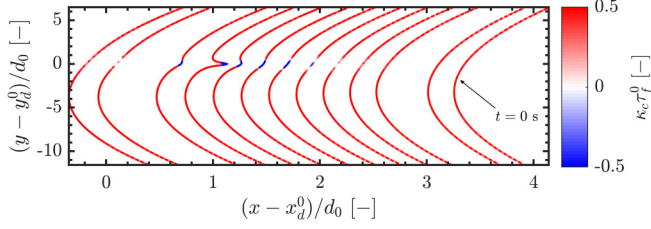


FIG. 4. Superimposed snapshots of the positively curved portion of the flame front, identified by the isoline of the temperature-based progress variable $c_\theta = 0.58$ and colored by the normalized curvature $\kappa_c \tau_f^0$.

during flame crossing, the droplet is gradually accelerated by the incoming reactant flow in the direction opposite to flame propagation. This slow acceleration modifies the local gas velocity field ahead of the flame and can, in turn, influence the local propagation of the flame front. The droplet's high inertia is therefore expected to introduce both momentum loss and thermal perturbations both ahead of and along the flame surface, potentially altering the flame dynamics. Together with this, Fig. 3 shows that vapor diffusion also occurs on a timescale comparable to the flame-crossing time. Although evaporation is slow, the resulting vapor cloud surrounding the droplet is still expected to interact with the flame front during the droplet crossing. Finally, Fig. 3 shows that the flame chemical and diffusive timescales are comparable to the droplet crossing time. This indicates that, while the droplet affects the local flow field, the flame evolves on a much shorter timescale and promptly responds to the induced perturbations in temperature and mixture composition, which in turn affect the flame speed. These effects will be discussed in more detail in the next sections.

B. Effect on the flame displacement speed

To characterize the effect of the water droplet on the flame front dynamics, the isoline corresponding to the temperature-based progress variable $c_\theta = 0.58$ is considered, and its temporal evolution is shown in Fig. 4. This isoline approximately coincides with the location of the peak H_2 reaction rate $\dot{\omega}_{\text{H}_2}$, and it is color coded in Fig. 4 with the value of the local curvature, which quantifies the degree of flame front deformation induced by the interaction with the droplet. The flame curvature is computed according to [42]

$$\kappa_c = -s_d \left(\frac{\partial n_i}{\partial x_i} \right), \quad (11)$$

where n_i is the normal vector to the isolevel of c_θ pointing toward the fresh gases. It can be seen from Fig. 4 that, as the flame propagates toward the reactants, the amplitude of the positively curved portion of the flame front increases due to the development of the imposed global perturbation. The droplet moves in the opposite direction relative to the flame front. Upon interaction, the flame front becomes locally distorted, exhibiting a dimple in the interaction region and a consequent inversion of the local curvature. The dimple exhibits a characteristic size comparable to the droplet's effective diameter. As illustrated qualitatively in Fig. 5, the cold vapor cloud generated by evaporation diffuses toward the flame front and interacts with it, producing a localized heat sink as well as a reduction of the gas velocity caused by the outward Stefan flow released at the droplet surface. A similar shape of a flame front interacting with a liquid droplet has been observed in experimental investigations of fuel droplet-flame interactions [21].

To characterize the formation of the droplet-induced dimple on the flame front and its influence on the local flame dynamics, the spatial distribution of the flame displacement speed s_d is analyzed for the cases with and without the droplet. The displacement speed s_d represents the propagation

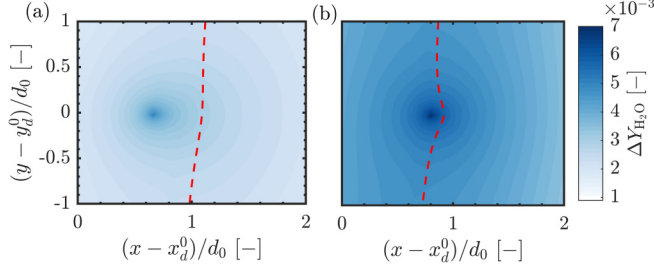


FIG. 5. H_2O vapor cloud produced by droplet evaporation. Panels (a), (b) show the spatial distribution of the excess water-vapor mass fraction relative to the corresponding dry flame at two representative time instants of the droplet-flame interaction, namely $t/\tau_f^0 = 0.436$ for panel (a) and $t/\tau_f^0 = 0.545$ for panel (b). These snapshots illustrate the perturbation induced by the evaporating droplet. The red dashed line marks the progress-variable isocline $c_\theta = 0.58$. The coordinates (x_0, y_0) denote the initial droplet position.

velocity of the flame front relative to the gas flow, and it is computed as [33,43]

$$s_d = \frac{1}{|\nabla c_\theta|} \left(\frac{\partial c_\theta}{\partial t} + u_{g,i} \frac{\partial c_\theta}{\partial x_i} \right). \quad (12)$$

The instantaneous variation of the normalized displacement speed s_d along the flame front (see Fig. 1) is shown in Fig. 6(a) for the cases with and without the droplet. In the baseline dry case (i.e., without the droplet), s_d slightly increases as compared to the reference unstretched 1D value along the flame crest (positively curved region of the front). This behavior is well known and results from the local acceleration of the flame due to the nonunity Lewis number, also known as the differential diffusion effect. However, for the case with the droplet [filled circles in Fig. 1(a)], the interaction with the flame leads to a local reduction of s_d in the vicinity of the droplet, where a negative curvature gradient is induced by the droplet. To shed light on the observed local reduction of the flame displacement speed due to the water droplet, the effect of the modification of flow field velocity, flame reactivity, and temperature on s_d is analyzed in the next. Given that the displacement speed is defined as the flame speed relative to the flow velocity, $s_a = s_d + u_{g,i} n_i$, where s_a is the absolute flame front velocity (i.e., the flame speed relative to a fixed reference frame), variations in the displacement speed are associated with changes in both the flow velocity and the absolute flame speed. To analyze the effect of the droplet motion on the flow velocity and its influence on the flame propagation, Fig. 6(b) shows the instantaneous gas velocity component normal to the flame surface, $u_{g,i} n_i$, along the isocline $c_\theta = 0.58$. Since the flame normal n_i is positive toward the reactants, the velocity component along the latter is negative according to the chosen reference frame (see Fig. 1). It can be seen that the droplet acts as a local momentum sink, reducing the gas-velocity component normal to the flame front and such reduction is about 2% of s_L^0 . Thus, under the investigated conditions, the effect of the droplet-induced gas-velocity reduction on s_d is expected to be of secondary importance. However, during the flame front crossing, the droplet is subjected to both convective and conductive heating, which locally affect the mixture reactivity and the diffusive fluxes across the flame front, ultimately influencing the flame propagation speed. To further analyze such effects on s_d , the latter can be expressed in terms of the overall energy conservation equation for the mixture [33]:

$$s_d = \frac{1}{\rho_g c_{p,g} |\nabla T|} \left[\underbrace{\dot{\omega}_T}_{s_d^{\text{chem}}} + \underbrace{\frac{\partial}{\partial x_i} \left(\lambda_g \frac{\partial T}{\partial x_i} \right)}_{s_d^{\text{cond}}} - \underbrace{\frac{\partial T}{\partial x_i} \left(\rho_g \sum_k c_{p,k} Y_k V_{k,i} \right)}_{s_d^{\text{cp}}} \right], \quad (13)$$

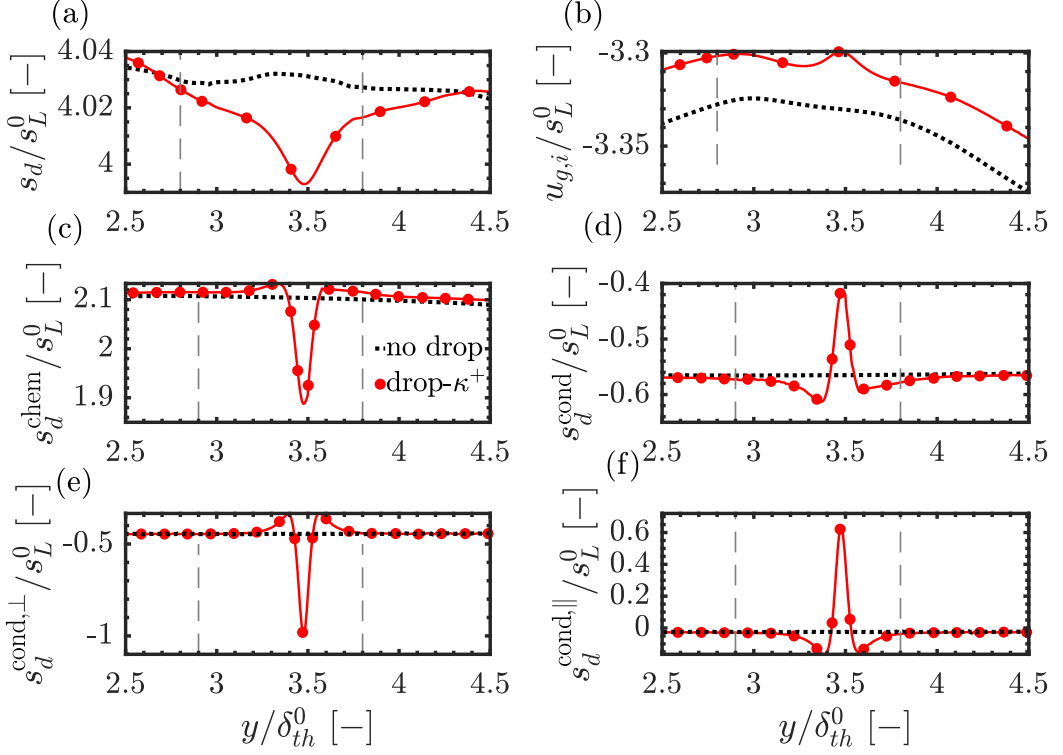


FIG. 6. (a) Distribution of the normalized flame displacement speed, s_d/s_L^0 . (b) Normal gas velocity component, $u_{g,i}/s_L^0$. (c) Chemical, s_d^{chem} , and (d) conductive, s_d^{cond} , contributions to the flame displacement speed obtained from the energy-based decomposition in Eq. (13). Each contribution compares the cases with and without the droplet. (e), (f) Spatial distribution of the normal and tangential components of the conductive term, $s_d^{\text{cond},\perp}$ and $s_d^{\text{cond},\parallel}$, as defined in Eq. (14). All the quantities are computed along the isoline $c_\theta = 0.58$.

where the right-hand side of Eq. (13) is reformulated to separately account for the contributions to the variation of the displacement speed arising from the heat-release rate s_d^{chem} , heat conduction s_d^{cond} , and species diffusion s_d^{cp} . The latter term is typically one order of magnitude smaller than the other two [43] and is therefore not considered in the present analysis. Figures 6(c) and 6(d) show the profiles of s_d^{chem} and s_d^{cond} along the flame transverse direction for the cases with and without the droplet. It can be observed that for both cases, the component of the displacement speed associated with the heat-release rate is not constant along the flame crest. For the case without the droplet, the slight increase in heat release originates from nonunity Lewis-number effects. Since under the present conditions the Lewis number is $\text{Le} < 1$, the reaction zone is replenished by fresh reactants more rapidly than heat can diffuse away from it. This enhances the local reactivity and, consequently, increases s_d^{chem} . In contrast, in the presence of the droplet, a local reduction in s_d^{chem} is observed within the interaction region. This reduction results from both the thermal effect of the droplet and the stretch effect induced by the droplet on the flame. Specifically, the droplet acts as a local heat sink, thereby lowering the gas temperature and consequently reducing the mixture reactivity. In addition, the curvature gradient generated by the droplet-flame interaction further promotes reactant defocusing and modifies the local balance between diffusive transport and heat conduction.

One can notice that the heat conduction contribution to the displacement speed [s_d^{cond} in Fig. 6(d)] is negative for the case without the droplet, indicating that heat is conducted toward this region. In the presence of the droplet, this contribution locally decreases (i.e., becomes less negative),

suggesting that the net conductive flux is lower than in the baseline case without the droplet. This behavior is consistent with the fact that the droplet locally absorbs energy, thereby reducing the net amount of heat available in this region. In addition, the deformation of the flame front induced by the droplet introduces local curvature variations that modify the orientation of the conductive heat flux components to the flame. Accordingly, s_d^{cond} can be further decomposed into normal and tangential contributions with respect to the flame surface as

$$s_d^{\text{cond}} = -\frac{1}{\rho_g c_{p,g} |\nabla T|} \left[\underbrace{n_i \frac{\partial}{\partial x_i} (\lambda_g |\nabla T|)}_{s_d^{\text{cond},\perp}} + \underbrace{\lambda_g |\nabla T| \frac{\partial n_i}{\partial x_i}}_{s_d^{\text{cond},\parallel}} \right], \quad (14)$$

where $s_d^{\text{cond},\perp}$ and $s_d^{\text{cond},\parallel}$ represent the variations of the flame displacement speed s_d associated with the components of the conductive heat flux normal and tangential to the flame front, respectively. As shown in Fig. 6(e), in the droplet region, the local negative curvature realigns the tangential heat flux, causing the tangential component $s_d^{\text{cond},\parallel}$ to change direction from negative (heat conducted outward from the reaction zone) to positive (heat directed inward). Simultaneously, the normal component $s_d^{\text{cond},\perp}$ becomes more negative as the local temperature gradients steepen in response to the cooling induced by droplet heating. These two effects act together to locally focus the conductive heat flux toward the reaction zone, partially compensating for the droplet-induced cooling. Overall, by comparing the magnitude of the heat-release-rate term [s_d^{chem} in Fig. 6(c)] with that of the conductive term [s_d^{cond} in Fig. 6(d)], it is evident that the former is larger, indicating that the reduction in the local displacement speed primarily follows the local decrease in heat release. As already mentioned, this reduction can be attributed to both the local negative curvature induced by the droplet and the associated decrease in the local temperature, which together lower the chemical reactivity, and this effect will be further discussed in Sec. IV D. Finally, as discussed above, the droplet-induced curvature also modifies the tangential heat flux along the flame front.

C. Effect on the flame front stretch

The effect of droplet-induced flame front local deformation is here quantified by looking at the variation of the stretch rate κ components, namely curvature κ_c and strain rate κ_S along the flame front. The stretch rate is here computed as

$$\kappa = \kappa_c + \kappa_S, \quad (15)$$

where the tangential strain rate κ_S is defined as

$$\kappa_S = (\delta_{i,j} - n_i n_j) \frac{\partial u_{g,i}}{\partial x_j}. \quad (16)$$

Figure 7 shows the instantaneous distributions of flame curvature and tangential strain rate for both cases with and without the water droplet. It can be seen that, before the droplet reaches the flame front [Figs. 7(a)–7(c)], the curvature remains weakly positive and approximately constant along the flame transverse direction. These profiles closely match those observed in the baseline case without the water droplet [dotted lines in Figs. 7(a) and 7(c)], indicating that the flame curvature is initially unaffected by the droplet dynamics. However, as the droplet approaches and begins to interact with the flame front, it induces a negative curvature gradient [Figs. 7(e), 7(g), and 7(i)], marking the onset of a localized deformation. This deformation, which resembles a dimple (see Fig. 4), becomes increasingly pronounced as the droplet penetrates the flame front [Fig. 7(i)], modifying the local flame front curvature by about 40%. As a result, the initially smooth and positively curved front becomes progressively distorted in the region surrounding the droplet, with the curvature becoming locally negative. At later stages, this negative curvature region gradually smooths out until it disappears, and the flame recovers its initial shape. Furthermore, a comparison of the strain rate and curvature profiles along the flame front [Figs. 7(b), 7(d), 7(f), 7(h), and 7(l)]

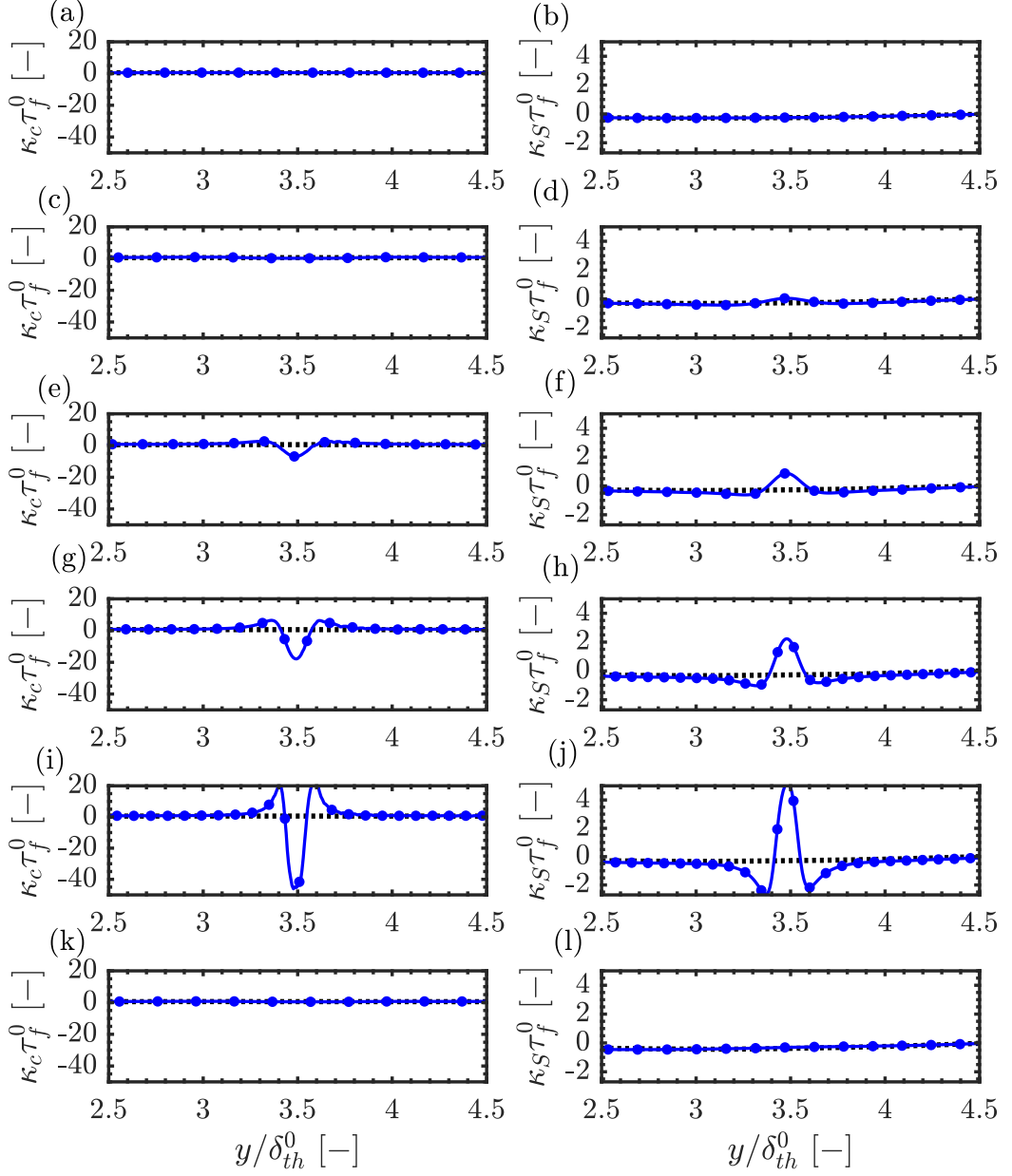


FIG. 7. Spatial evolution of the flame front curvature κ_c (left) and strain rate κ_s (right) at various time steps. The nondimensional time t/τ_f^0 ranges from 0 (a) to 0.71 (f), with increments of approximately 0.05 between consecutive frames: (a), (b) 0.000, (c), (d) 0.436, (e), (f) 0.491, (g), (h) 0.545, (i), (j) 0.600, (k), (l) 0.709.

indicates that the variation in strain rate induced by the droplet interaction is less pronounced than the corresponding variation in curvature. However, a minor deviation of κ_s is observed during the interaction interval, during which the strain rate increases to approximately 40% of its initial magnitude [Fig. 7(j)]. Additionally, similar to the curvature profile, the region of increased strain rate smooths out once the droplet has crossed the flame front. Moreover, variations in the tangential strain rate occur in the opposite sense to those of the curvature, i.e., their gradients have opposite

sign. As discussed previously, the curvature and tangential strain contributions to flame stretch are negatively correlated [33,44]. In particular, regions of negative curvature (concave toward the unburnt gases) are associated with expansive tangential strain. Thus, tangential strain tends to act in a restorative manner, partially re-establishing the initial total stretch rate along the flame front. It is worth noting that in the interaction regime analyzed, the droplet acts as an impulsive forcing applied over the short time interval τ_{crossing} , similar to the impulsive disturbances used to model noiselike perturbations in previous studies (see Fig. 2 in Ref. [45]). In earlier works, it has been shown that small perturbations on the flame front are convected along the crest and gradually dissipate as the flame restores its single cusp configuration [44,46]. In contrast, in the present case, the droplet-induced perturbation remains localized in the vicinity of the droplet position until the flame eventually recovers its original crest shape.

D. Effect on the local reactivity

In Sec. IV C, it was shown that, in the liquid-drop regime, the high droplet inertia induces local momentum losses and cooling, which distort the flame surface and lead to spatial variations in the flame stretch rate. These variations directly influence the local displacement speed, whose reduction has been observed to be primarily driven by the corresponding decrease in heat release rate [see Fig. 6(c)].

It is well known that curvature-induced stretch, combined with nonunity Lewis number effects [2,25], leads to localized modifications of the reaction rate, in addition to those caused by the temperature decrease associated with droplet heating. This effect is illustrated in Fig. 8(a), which shows the instantaneous hydrogen reaction rate $\dot{\omega}_{\text{H}_2}$, normalized by the peak value. It can be seen that, in the presence of the droplet, a spatial reduction of the hydrogen production rate occurs in the region surrounding the droplet. This reduction results from the combined influence of droplet-induced cooling and the locally negative stretch rate (see Fig. 7), which together act to decrease the hydrogen consumption along the droplet trajectory.

To qualitatively decouple these two effects, an additional simulation was performed to assess whether the observed reduction in reaction rate is solely caused by droplet-induced cooling or whether the stretch induced by the interaction also contributes by modifying the local reactivity through curvature variations. For this purpose, a UL model was employed. This way, the flame is insensitive to stretch effects [25], allowing the isolation of the influence of droplet cooling. The results were then compared with those obtained using the Mixture-Averaged + Soret (DD) model (Sec. II) for the same initial droplet parameters. To ensure a consistent comparison, the two simulations were analyzed at time instants at which the droplet induces the same local temperature reduction and has the same instantaneous diameter and velocity. Figure 8(b) shows the instantaneous normalized hydrogen reaction rate obtained with the UL diffusion model. As just noted, although the flame-front position shifts slightly when switching diffusion models, the reduction in reaction rate compared to the peak value is smaller than that observed in the DD case [Fig. 8(a)]. The higher reduction observed in the DD case, therefore, indicates the presence of an additional mechanism associated with differential diffusion, which further contributes to decreasing the flame reactivity. When comparing the normalized $\dot{\omega}_{\text{H}_2}$ values along the $c_\theta = 0.58$ isoline for both cases in Fig. 8(c). Specifically, the reaction rate for the DD case exhibits a stronger decrease in reaction rate in regions of negative curvature, and it is not constant away from the droplet region as it follows the local variation of the flame curvature [see red solid line in Fig. 8(c)]. In the UL case, the reaction rate remains essentially uniform along the flame isoline. The only decrease occurs in the vicinity of the droplet and is solely due to droplet heating and evaporation [see black dotted line in Fig. 8(c)]. This difference highlights the contribution of the droplet-induced stretch effect to the modulation of the local reaction rate, which represents a further effect beyond the well-known chemical, thermophysical, and physical influences of droplets on flames. Although the effect is small in the present single-droplet simulations, it is expected to become significant in spray configurations where multiple droplets interact simultaneously with the flame.

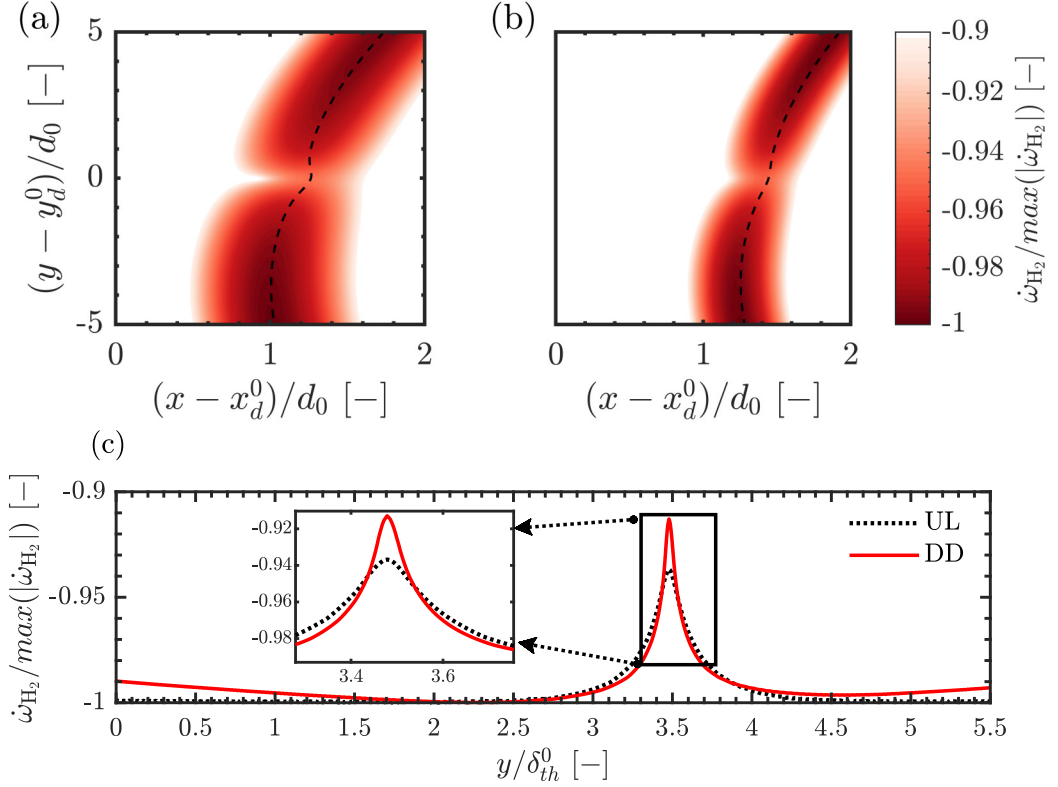


FIG. 8. Instantaneous reaction rate of hydrogen, $\dot{\omega}_{H_2}$, normalized by their peak value computed using (a) the Mixture-Averaged + Soret (differential diffusion, DD) transport model and (b) Unitary Lewis number (UL) model. The black dashed lines indicate the isolines of the progress variable at $c_\theta = 0.58$. (c) Normalized $\dot{\omega}_{H_2}$ obtained with Mixture Averaged + Soret (DD) and UL diffusion models along the isoline $c_\theta = 0.58$.

E. Relaxation of the droplet-induced perturbation

As shown in Fig. 7, during the droplet-flame interaction, the vapor cloud surrounding the droplet induces a localized perturbation of the flame front, which progressively decays with time until it recovers its initial shape. From the standpoint of flame stability, it is worth noting that the present flame is characterized by an effective Lewis number of $Le_{\text{eff}} = 0.628$, which is lower than the critical Lewis number Le_c for the onset of thermodiffusive instability $Le_c = 0.785$ and is therefore prone to thermodiffusive instability [47]. Nevertheless, the characteristic wavelength of the droplet-induced deformation, estimated as $\Lambda \approx 8d_0 \approx 1.2\delta_{th}^0$ [see Fig. 9(a)], is significantly smaller than the thermodiffusive cutoff wavelength reported for lean hydrogen-air flames under similar conditions, $\lambda_c \approx 3.18\delta_{th}^0$ [33]. Given that the perturbation lies outside the range of unstable modes, it is not expected to be amplified. In fact, as discussed in Ref. [48], when the perturbation wavelength becomes comparable to, or smaller than, the flame thickness, finite-thickness stabilization mechanisms become dominant. These mechanisms, associated with tangential heat conduction and species diffusion along the flame front, damp the perturbation and promote the recovery of the original flame shape, as observed in Fig. 4.

To gain further insight into this behavior, the characteristic wavelength of the droplet-induced flame-front deformation can be compared with the instability cutoff wavelength predicted by linear stability theory. Using the results of Berger *et al.* [34], the cutoff wavelength for thermodiffusive instability is plotted over a range of reactant temperatures and equivalence ratios and reported

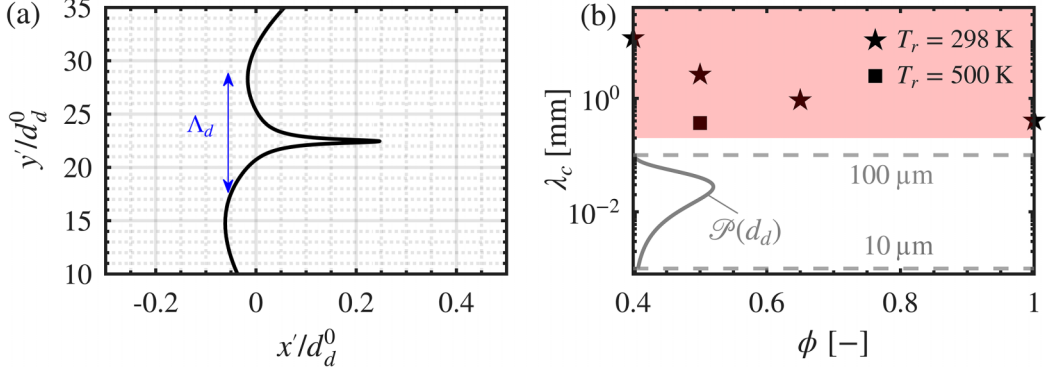


FIG. 9. (a) Estimated wavelength, Δ_d , of the droplet-induced flame-front deformation, computed from the difference between the flame-front shapes obtained with and without the droplet. The characteristic wavelength is found to be approximately $\Delta_d \approx 8d_d^0$. (b) Cutoff wavelength as a function of reactant temperature T_r and equivalence ratio ϕ , based on the linear stability analysis of Berger *et al.* [34]. The gray curve shows a representative Rosin-Rammler droplet-size distribution, while the red shaded region identifies the range of unstable wavelengths. The vertical axis in panel (b) is logarithmic.

in Fig. 9(b). It can be seen that the smallest unstable wavelength remains of the order of $\lambda_c \approx 1 \times 10^{-4} \text{ m} \approx \delta_{\text{th}}^0$. Assuming that the characteristic wavelength of the droplet-induced flame-front deformation remains of the order of the droplet diameter, as observed in the present simulations, comparison with a representative Rosin-Rammler droplet-size distribution typical of spray applications [gray curve in Fig. 9(b)] indicates that the perturbation wavelengths associated with most droplets lie below the instability cutoff wavelength. Although only qualitative, this comparison suggests that the response of a lean hydrogen premixed flame to droplet interaction identified in the present study may remain relevant over a broader range of droplet diameters than the specific value considered here.

To quantify the time required for the flame to recover its original shape, hereafter referred to as the flame restoring time, τ_{rest} , the instantaneous curvature perturbation amplitude is computed as the L_2 -norm of the spatial difference between the flame-front curvature fields obtained with and without the droplet:

$$A_{\kappa_c}(t) = \left[\int_{l_a} (\kappa_c^{\text{drop}, \kappa^+}(l_a, t) - \kappa_c^{\text{no, drop}}(l_a, t))^2 dl_a \right]^{1/2}, \quad (17)$$

where l_a is the arc-length coordinate along the flame front. As shown in Fig. 10, the perturbation amplitude initially grows, reaches a maximum, and subsequently decays as the flame recovers its original shape. The corresponding restoring time is about $\tau_{\text{rest}} = 0.5\tau_f^0$. The fast recovery relative to the characteristic flame time can be attributed to the small wavelength of the droplet-induced perturbation compared to δ_{th}^0 , for which tangential heat and species diffusion along the flame front efficiently smooth flame-front distortions, providing a strong stabilizing effect [33, 48]. It is interesting to note that the temporal decay of $A_{\kappa_c}(t)$ (i.e., the curvature restoring) is well fitted with an exponential law of the form $A_{\kappa_c}(t)/A_{\kappa_c, \text{max}} = \exp[-(t - t_{\text{max}})/\tau_{\text{rest}}]$, where t_{max} denotes the time at which the perturbation reaches its maximum amplitude and τ_{rest} is the corresponding restoring time. For the present configuration, the fitted restoring time is found to scale with the flame diffusion timescale as $\tau_{\text{rest}} = c_1 D_{\text{H}_2} / (s_L^0)^2$, where D_{H_2} denotes the hydrogen diffusion coefficient, and $c_1 = 0.17$ is an empirical proportionality constant which may depend on the droplet diameter.

This result is particularly significant because it may serve as a characteristic timing parameter for spray injection. Indeed, since the flame restores its shape with a frequency of $1/\tau_{\text{rest}}$, this timescale can be exploited in a spray-injection control system to modulate the local flame curvature.

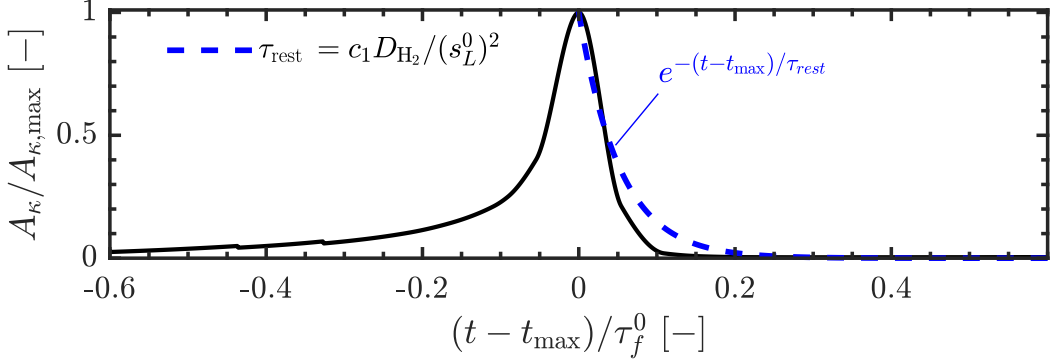


FIG. 10. Temporal evolution of the normalized curvature amplitude, $A_{k_c}(t)$. The blue dashed line shows the exponential fit, $A_{k_c}(t)/A_{k_c,\max} = \exp[-(t - t_{\max})/\tau_{\text{rest}}]$, with $\tau_{\text{rest}} = c_1 D_{\text{H}_2}/(s_L^0)^2$ and the fitted coefficient is $c_1 = 0.17$.

This aspect is especially relevant for hydrogen flames, where flame stretch strongly affects NO_x formation [49].

V. SIMPLIFIED MODEL FOR FLAME DISPLACEMENT AND VELOCITY DUE TO DROPLET-FLAME INTERACTION

This section presents a phenomenological reduced-order model for describing the local modification of the flame displacement and propagation speed induced by droplet-flame interaction. The model is motivated by the flame front dynamics observed in the numerical simulations and aims to capture the dominant features of the droplet-induced perturbation and the subsequent recovery of the flame motion following the droplet passage. For this purpose, the flame front is represented as a single curved surface propagating through the reactant mixture with an initial constant velocity u_f , which represents the velocity of the surface relative to a fixed coordinate system. The gas density is assumed constant and equal to the reactant density ρ_g^1 . Similarly, the gas viscosity ν_g^1 , thermal conductivity α_g^1 , and the mass diffusivity of hydrogen $D_{\text{H}_2}^1$ are taken as constant and equal to their value at the reactant temperature. The water droplet, of diameter d_0 , is assumed to propagate at a constant velocity u_{d_0} relative to the flame front. Since for an isolated droplet the region of the flame that is significantly affected by droplet-flame interaction is confined to the immediate vicinity of the droplet itself, the analysis focuses on the motion of a representative flame element on the flame front within this region.

The motion of the flame element, denoted by $\psi(t)$, is expressed as the superposition of a uniform base motion $\psi_\ell(t)$ and a perturbed component $\psi_p(t)$:

$$\psi(t) = \psi_\ell(t) + \psi_p(t)H(t - t_0), \quad (18)$$

where H is the Heaviside step function and t_0 is the time at which the droplet-flame interaction takes place. The uniform base displacement $\psi_\ell(t)$ corresponds to the trajectory that this point on the flame front would follow in the absence of the droplet, and it is expressed as

$$\psi_\ell(t) = \psi_0 + u_f t, \quad (19)$$

while the perturbed component is $\psi_p(t)$, and it accounts for the modification of the base motion induced by the droplet-flame interaction. To obtain the temporal evolution of $\psi_p(t)$, an analogy with a mass-spring-damper system subjected to an external forcing is proposed. This analogy is motivated by the droplet-flame interaction dynamics observed in the numerical simulations, where the droplet induces a localized perturbation that develops while it remains in the vicinity of the flame (see Fig. 4). Once the droplet has crossed the flame front, the perturbation amplitude progressively

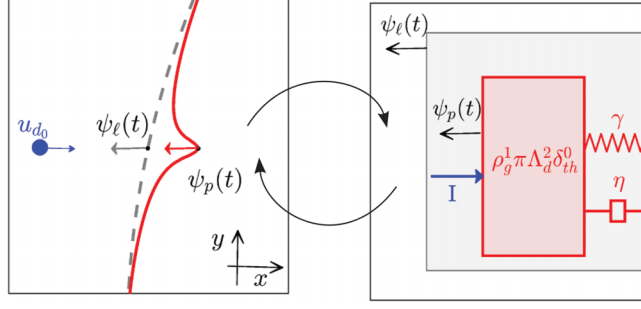


FIG. 11. Schematic illustration of the mass-spring-damper analogy used to model the local flame displacement $\psi(t)$ in the vicinity of a droplet. The displacement is decomposed into a uniform base motion $\psi_\ell(t)$ and a perturbed component $\psi_p(t)$ due to droplet-flame interaction. The perturbed component $\psi_p(t)$ is governed by a linear second-order differential equation analogous to a forced mass-spring-damper system, where γ is the effective stiffness, η is the damping, and the impulse I is the instantaneous forcing induced by the droplet.

decreases (see Fig. 10) and the flame relaxes toward its unperturbed configuration. This transient response resembles the behavior of a dynamical system subjected to an impulsive forcing and subsequently evolving toward its initial equilibrium state. Based on this observation, the perturbed displacement $\psi_p(t)$ is assumed to be analogous to the response of a mass-spring-damper system subjected to an impulsive forcing at $t = t_0$, and its temporal evolution is therefore described as

$$\begin{aligned} \frac{d^2 \psi_p}{dt^2} + \eta \frac{d \psi_p}{dt} + \gamma \psi_p &= F(t - t_0), \\ \psi_p(0) &= 0, \\ \left. \frac{d \psi_p}{dt} \right|_{t=0} &= 0. \end{aligned} \quad (20)$$

In Eq. (20), η denotes the pseudodamping coefficient, γ represents the square of a characteristic frequency, and $F(t - t_0)$ is an impulsive forcing term. To establish the mass-spring-damper analogy shown in Fig. 11, each term in Eq. (20) requires explicit specification which follows from the physical arguments introduced in Secs. IV B–IV D and from a dimensional analysis as follows. From a mechanical point of view, the damper dissipates energy and opposes the motion of the mass. In the proposed analogy, this effect is assumed to be equivalent to the viscous diffusion effects within the gaseous phase, which attenuate the flame-front perturbation induced by the droplet. Since the pseudodamping coefficient η has dimensions of an inverse of time [s^{-1}], it can be defined as $\eta = \nu_g^1 (2\pi/\Lambda_d)^2$, where $\Lambda_d = 8d_0$ represents the characteristic length scale of the spatial deformation induced by the droplet, as estimated from the simulation data. This term therefore characterizes the damping at the droplet of the local flame-front displacement and velocity generated by the droplet-flame interaction. It is worth noting that the mathematical form is similar to the stabilizing influence of viscosity on the linear growth rate [50,51]. Moreover, the coefficient γ in Eq. (20) represents the spring stiffness per unit mass, with dimensions [s^{-2}]. In a classical mechanical oscillator, this quantity corresponds to the square of the natural oscillation frequency associated with the restoring action of the spring. By analogy, in the present flame–droplet interaction problem, γ is interpreted as the square of a characteristic frequency describing the rate at which the perturbed flame-front element tends to recover its unperturbed configuration after being displaced by the droplet-induced forcing. The restoring term is assumed to be governed by the characteristic relaxation timescale of the droplet-induced perturbation. As discussed in Sec. IV E, the recovery of the flame front following the droplet passage was observed to follow an exponential decay with a characteristic time given by: $\tau_{\text{rest}} = c_1 D_{H_2}^1 / (u_f)^2$ where c_1 is a proportionality constant

determined from the numerical simulations. Since the spring coefficient represents the tendency of the flame front to recover its unperturbed configuration, it is modeled as the square inverse of this characteristic relaxation timescale $\gamma = (1/\tau_{\text{rest}})^2$.

The effect of the droplet is introduced through an impulsive forcing term of the form $F(t) = I\delta(t - t_0)$, where δ denotes the Dirac δ function. This formulation is equivalent to imposing an instantaneous jump in the flame-element displacement velocity $\dot{\psi}_p$ at $t = t_0$, while the displacement remains continuous: $\dot{\psi}_p(t_0^+) - \dot{\psi}_p(t_0^-) = I$, with $\psi_p(t_0^+) = \psi_p(t_0^-)$. It is noted that I has the dimensions of a velocity, $[I] = [\text{kg m/kg s}] = [\text{ms}^{-1}]$. However, the masses appearing in the numerator and denominator do not have the same physical meaning. The numerator corresponds to the droplet mass, $m_{d_0} = \rho_d \pi d_0^3/6$, which provides the impulse, whereas the denominator represents the effective inertia of the system being displaced, namely the portion of the flame that responds to the forcing. This effective flame inertia is modeled as $m_p = \rho_g^1, \pi, \Lambda_d^2, \delta_{\text{th}}^0$. Moreover, the analyses presented above have shown that the droplet modifies the flame both by reducing the local propagation velocity through momentum losses and by lowering the temperature through heating and evaporation. Consequently, the impulse I is expressed as the sum of two distinct contributions reflecting the aforementioned effects, namely,

$$I = I_{u_d} + I_{\text{th}} = \frac{2\rho_d(d_0)^3}{3\rho_g^1\Lambda_d^2\delta_{\text{th}}^0}(u_{d_0} + u_{d,\text{th}}). \quad (21)$$

The term I_{u_d} in Eq. (21), represents the instantaneous displacement of the flame front resulting from the transfer of momentum from the droplet to the flame. The second contribution, I_{th} , accounts for the apparent displacement of the flame front associated with the reduction in flame propagation speed induced by droplet heating and evaporation.

The apparent velocity reduction $u_{d,\text{th}}(T)$ is modeled using the classical Zel'dovich-Frank-Kamenetski (ZFK) high-activation-energy asymptotic theory for a first-order Arrhenius reaction rate, whose derivation and details can be found in Ref. [[52], pp. 49–50], as

$$u_{d,\text{th}}(T) = \sqrt{\frac{2\alpha_g^1|B_1|T_u^n}{\beta^2} \exp\left(-\frac{E_a}{RT_b}\right)}, \quad (22)$$

where α_g^1 is the thermal diffusivity of the unburned gas, $B_1 = v_F A_1$ where $v_F = -1$ is the coefficient of the global one-step reaction, while A_1 is the preexponential constant of the one-step Arrhenius reaction rate, and T_u is the unburned-gas temperature with n the corresponding temperature exponent. The parameter β is the Zel'dovich number $\beta = E_a(T_b - T_u)/(RT_b^2)$, E_a is the activation energy and R the universal gas constant. Finally, T_b is the highest temperature within the flame without the droplet. Under the assumptions of adiabatic, constant pressure, and complete combustion, T_b can be computed as

$$T_b = T_u + \frac{Q Y_{\text{H}_2}^1}{c_{p,g}^1}, \quad (23)$$

and, in the presence of the droplet as

$$T'_b = T_u + \frac{Q Y_{\text{H}_2}^1 - L_v \alpha_w}{c_{p,g}^1}, \quad (24)$$

where Q is the low heating value of hydrogen (≈ 120 MJ/kg), α_w is the fraction of evaporated water assumed equal to ≈ 0.01 [see Fig. 2(d)] and, $c_{p,g}^1$ is the heat capacity of the reactants mixture. By substituting, in turn, Eqs. (23) and (24) into Eq. (22) and taking the difference between the two resulting expressions, the apparent velocity jump can be expressed as

$$u_{d,\text{th}} = \sqrt{C} \left[\frac{1}{\beta(T'_b)^2} \exp\left(\frac{E_a}{2RT'_b}\right) - \frac{1}{\beta(T_b)^2} \exp\left(\frac{E_a}{2RT_b}\right) \right], \quad (25)$$

with $C = 2\alpha_g^1|B_1|T_u^n$. By explicitly substituting the expression of each coefficient into Eq. (20), the perturbed flame element equation becomes

$$\frac{d^2\psi_p}{dt^2} + 2\left(\frac{\nu_g\pi^2}{\Lambda_d^2}\right)\frac{d\psi_p}{dt} + \left(\frac{1}{\tau_{\text{rest}}}\right)^2\psi_p = \frac{2\rho_d(d_0)^3}{3\rho_g^1\Lambda_d^2\delta_{\text{th}}^0}(u_{d_0} + u_{d,\text{th}})\delta(t - t_0). \quad (26)$$

It is worth noting that Eq. (26), which describes the evolution of the displacement perturbation of a flame-front element during its interaction with a droplet, has the same mathematical structure as the model of Clavin and Williams for the linear evolution of a perturbed weakly wrinkled premixed flame front [48,53]. A similar damped-oscillator structure is also obtained when considering an intrinsically stable flame interacting with weak incoming perturbations, such as turbulent velocity fluctuations or standing waves [53–55]. Although both the present reduced model and those based on the Clavin-Williams stability analysis describe the temporal evolution of a flame-front displacement, their physical meaning is different. In the classical stability framework, the equation describes the evolution of perturbations of the flame front as a whole, decomposed into spatial Fourier modes of given wave number. Its coefficients are obtained from a linear stability analysis and include hydrodynamic and thermodiffusive effects. In contrast, the present simplified model is phenomenological and describes the local displacement and velocity of a single flame-front element during its interaction with a water droplet, which acts as a thermal and a momentum sink [see the right-hand side of Eq. (26)]. Therefore, the coefficients in Eq. (26) should not be interpreted as direct counterparts of those appearing in the classical Clavin-Williams linear stability equation.

It is also important to note that, since the Markstein length is not included in the present model, stretch effects on the flame element displacement are not explicitly accounted for. Phenomenologically, this effect could be incorporated by modifying the recovery timescale τ_{rest} through an additional contribution whose sign and magnitude depend on the Markstein length and on the local stretch rate on the flame induced by the droplet.

The solution of the system of equation Eq. (20) admits a closed-form expression, and can be derived by solving the characteristic equation associated with the linear second-order system as

$$\lambda^2 + \frac{2\nu_g^1\pi^2}{\Lambda_d^2}\lambda + \frac{1}{\tau_{\text{rest}}^2} = 0, \quad (27)$$

with roots

$$\lambda_{1,2} = -\frac{\nu_g^1\pi^2}{\Lambda_d^2} \pm \sqrt{\left(\frac{\nu_g^1\pi^2}{\Lambda_d^2}\right)^2 - \frac{1}{\tau_{\text{rest}}^2}}. \quad (28)$$

For the present conditions, $(\frac{\nu_g^1\pi^2}{\Lambda_d^2})^2 < \frac{1}{\tau_{\text{rest}}^2}$, which implies a negative discriminant with the eigenvalues forming a complex-conjugate pair and the system exhibits an underdamped response characterized by exponentially decaying oscillations with a damping ratio of $\zeta = 2\nu_g^1\pi\tau_{\text{rest}}/\Lambda_d^2 = 0.21$.

The solution of Eq. (26) can then be arranged as

$$\psi(t) = \psi_0 + u_f t + \left[\frac{I}{\sqrt{\gamma - \eta^2/4}} \exp\left(-\frac{\eta}{2}(t - t_0)\right) \sin\left(\sqrt{\gamma - \frac{\eta^2}{4}}(t - t_0)\right) \right] H(t - t_0). \quad (29)$$

The flame-element displacement velocity, $\dot{\psi}_p$, can also be obtained analytically as follows:

$$\begin{aligned} \dot{\psi}(t) = u_f + I \exp\left[-\frac{\eta}{2}(t - t_0)\right] & \left[\cos\left(\sqrt{\gamma - \frac{\eta^2}{4}}(t - t_0)\right) \right. \\ & \left. - \frac{\eta}{2\sqrt{\gamma - \eta^2/4}} \sin\left(\sqrt{\gamma - \frac{\eta^2}{4}}(t - t_0)\right) \right] H(t - t_0). \end{aligned} \quad (30)$$

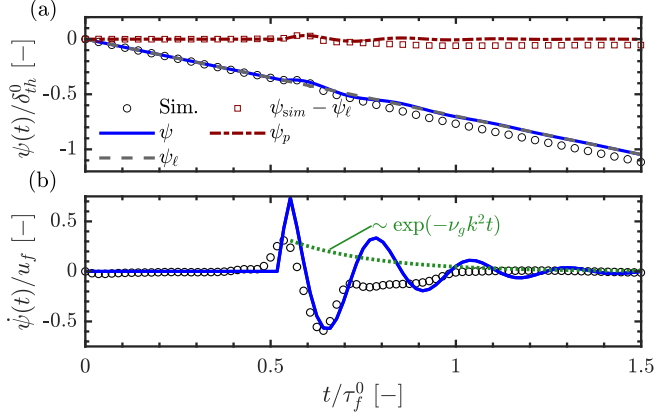


FIG. 12. Comparison between the numerical simulations and the derived simplified model for the local flame element displacement and velocity during the droplet-flame interaction. (a) Temporal evolution of the flame-element displacement $\psi(t)$. The gray dashed line denotes the unperturbed linear trajectory $\psi_\ell(t)$ while the red symbols and dashed line represent the perturbation displacement extracted from the simulations, $\psi_{\text{sim}} - \psi_\ell$ and the model prediction, ψ_p respectively. (b) Corresponding temporal evolution of the perturbation velocity $\dot{\psi}$. Note that both $\psi(t)$ and $\dot{\psi}$ are shifted to have zero as the initial value. The green dotted line denotes the exponential decay $\exp[-\eta/2(t - t_0)]$ with $\eta = \nu_g k^2$.

The comparison between the model solution in terms of displacement $\psi(t)$ and velocity $\dot{\psi}(t)$ is shown in Fig. 12. It can be seen that, as the flame front propagates from left to right (see Fig. 11), the resulting displacement $\psi(t)$ is negative in the adopted reference frame. The interaction with the droplet produces a local deceleration of the flame front in the direction opposite to its propagation [see Fig. 12(a)]. This effect is modeled as an impulsive forcing proportional to the droplet's linear momentum, associated with its effective impact speed ($\propto m_{d_0} u_{d_0}$), together with an apparent momentum transfer generated by droplet heating and evaporation ($\propto m_{d_0} u_{d,\text{th}}$). Although the quantitative agreement is limited, the proposed model captures the main features of the observed dynamics. In particular, it reproduces the onset and magnitude of the droplet-induced flame-front displacement around $t/\tau_f^0 \approx 0.5$ [see square markers and the red dotted-dashed line in Fig. 12(a)]. The underprediction of the cumulative displacement at later times reflects the model assumption that, after the droplet passage, the flame element relaxes toward its unperturbed linear trajectory ψ_ℓ . In contrast, in the numerical simulations, the flame element remains embedded within a growing positively curved portion of the flame front, whose global evolution continues to displace the flame element upstream. Furthermore, the velocity response [Fig. 12(b)] shows that the proposed model predicts a transient oscillatory motion of the flame element around its unperturbed linear trajectory, followed by a progressive attenuation of the perturbation due to the damping term. A similar behavior can be identified in the numerical simulations immediately after the droplet passage, approximately within the interval $0.5 \leq t/\tau_f^0 \leq 0.7$. However, the simplified model tends to overpredict the amplitude of the first velocity peak associated with the droplet crossing event. Since, according to the analytical solution, the initial velocity response satisfies $\dot{\psi}_p(t_0) \propto I$, this discrepancy suggests that the present formulation may overestimate the effective droplet-induced forcing or underestimate the effective inertia of the perturbed flame element. In addition, the model predicts a more pronounced oscillatory relaxation than observed in the numerical simulations. This is because the model assumes that the flame element displacement relax to ψ_ℓ once the droplet-induced perturbation has decayed. In addition, the model predicts a more pronounced oscillatory relaxation than observed in the numerical simulations. As discussed above, this occurs because the flame element remains embedded within a positively curved region of the flame front, where the local flame displacement speed is enhanced. This effect promotes a faster recovery of the perturbation and is not accounted for in the present low-order model.

Eventually, the model captures the decay rate of the perturbation [see Fig. 12(b)]. According to Eq. (30), for $t > t_0$ the decay is governed by the term $\exp[-\eta/2(t - t_0)]$. Being $\eta = \nu_g k^2$, this suggests that the attenuation of the droplet-induced disturbance becomes stronger with increasing wave number, consistent with the observation in Sec. IV E.

VI. CONCLUSIONS

The interaction between a single water droplet and a lean premixed hydrogen-air flame front has been investigated through two-dimensional detailed-chemistry simulations using an Eulerian-Lagrangian framework. To examine droplet-induced stretch effects on the flame front, a single-cusp flame configuration has first been obtained and subsequently perturbed by initializing a single water droplet near its positively curved region. This setup has enabled the imposition of a controlled curvature on the flame and a systematic analysis of the resulting interaction dynamics.

The droplet initial velocity and diameter have been selected such that the droplet evolves within an inertia-dominated regime, in which it acts as a localized momentum and heat sink. As a result, it has been observed to induce a local deceleration of the surrounding gas and transient thermal perturbations near the flame front. A time-scale comparison has shown that the flame responds rapidly to these droplet-induced disturbances, restoring its shape without significant modification of its global structure, apart from transient local effects. During the transient, the droplet has been observed to locally distort the flame front, producing a dimple-like deformation due to the combined effects of droplet inertia and interaction with the cold vapor cloud surrounding the droplet. This deformation has been found to cause a local reduction in the displacement speed, primarily associated with a decrease in heat release within the reaction zone. The reduction in flame reactivity has been attributed partly to local cooling induced by droplet heating and evaporation, and partly to the curvature gradient generated by the droplet-flame interaction, which reduces reactant focusing and weakens local reactivity.

Furthermore, the analysis of droplet-induced stretch and flame-front deformation has shown that the interaction produces a localized curvature inversion, whose amplitude reaches approximately 40% of the initial curvature. In contrast, the tangential strain-rate component acts in the opposite direction: it increases during the interaction and partially counteracts the curvature inversion, thereby contributing to the recovery of the original total stretch rate on the flame.

The curvature inversion induced by the droplet has been treated as an initial perturbation, and its temporal evolution has been examined. This analysis has revealed that the perturbation amplitude first increases and then decays exponentially, with a restoring time proportional to the flame diffusion timescale. Furthermore, a qualitative comparison with the results from the linear stability analysis present in the literature suggests that the flame response to droplet interaction identified in the present study may extend to a broader range of droplet diameters relevant to spray applications.

As the droplet modifies the local stretch field, the flame reactivity has also been observed to be affected through both cooling and stretch-induced effects. Specifically, while the droplet heating and evaporation have been shown to lower the local temperature and slow down the reaction rate, the curvature inversion has additionally been shown to influence the local reactivity through differential diffusion effects. The comparison with the unity-Lewis-number model has confirmed that these variations cannot be attributed solely to thermal effects, showing a direct coupling between droplet-induced curvature and local flame reactivity. Although the impact is minor for a single droplet, the results suggest that in water sprays interacting with premixed flames, droplet-flame interactions is expected to significantly influence the global flame reactivity. Furthermore, while the present study considers a single droplet diameter, injection velocity, and equivalence ratio, the trends observed suggests that variations in these parameters would primarily affect the magnitude of the droplet-induced perturbation of the flame dynamics and local reactivity, rather than altering the underlying interaction mechanisms. Future work will be devoted to quantitatively assessing the influence of these parameters on the flame response.

A simplified model has finally been proposed to estimate the displacement of the flame element subjected to the droplet-flame interaction. The model describes the flame response as the superposition of a uniform base motion and a perturbation generated by an impulsive forcing associated with the droplet's velocity and with the reduction in local propagation speed caused by droplet heating and evaporation. Additionally, the model has been shown to represent the decay rate of the perturbation well. Specifically, the obtained analytical expression for the displacement flame element further indicates that this decay becomes faster as the wave number associated with the droplet-induced disturbance increases.

Future studies will focus on identifying whether a critical droplet size exists that can trigger unstable thermodiffusive wavelengths, as well as extending the present analysis to several droplet diameters to achieve a more robust characterization of the flame restoring timescale.

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DATA AVAILABILITY

The data supporting the findings of this study were generated through numerical simulations. The numerical data underlying the figures and the custom scripts used for data analysis and post-processing are available from the corresponding author upon request.

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