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Rich Spray-Flame Propagating through a 2D-Lattice of Alkane Droplets in Air

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Abstract

In a recent numerical paper (Nicoli *et al. Combust. Sci. Technol. vol. 186, pp. 103-119; 2014*) [1], a model of isobaric flame propagation in lean sprays has been proposed. The initial state of the monodisperse mists was schematized by a system of individual alkane droplets initially located at the nodes of a face-centered 2D-lattice, surrounded by a saturated mixture of alkane and air. In the present study, the previous model is complemented with an original chemical scheme that allows us to study the combustion of rich alkane/air mixtures.

The main parameters of this configuration are S , the lattice spacing (in reactive-diffusive length units), φ_L , the liquid loading (or equivalence ratio relative to the fuel under liquid phase), and φ_G (with $\varphi_G \leq 0.8$), the gaseous equivalence ratio (i.e. that corresponding to the saturated vapour pressure in the fresh spray). We presently focus on sprays, the overall equivalence ratio of which is within the range $1 \leq (\varphi_L + \varphi_G) \leq 1.85$.

For a large set of parameters, we retrieve a feature often observed on the rich side in the experiments: flame propagation in the presence of droplets can be faster than the pure premixed flames with the same overall equivalence ratio. This is mainly observed when the lattice spacing is sufficiently large. However, the study underlines the role played by the velocities of two particular single-phase premixed flames: the “initial vapour flame” that only burns (if any) the mixture due to the saturated vapour and the “all fuel flame” that propagates (if any) in a mixture where all fuel is vaporized and mixed. When the “initial vapour flame” is too slow (i.e. a feeble spray Peclet number), the spray-flame speed results from the competition between two mechanisms: a speed chemically enhanced due to some enrichment coming from vaporization (possibly bounded by the “all fuel flame” speed) and a slowing down in flame velocity because the vaporization time scale sets the pace on combustion. On the other hand, for large spray Peclet number, the upper flammability limit is found to be strongly enlarged, and the spray-flame propagates with the velocity of the “initial vapour flame”.

Moreover, the flame structure deeply depends on lattice spacing: for a large lattice, the combustion stage mainly corresponds to a triple flame, with the diffusion flame that develops around the oxygen pocket located behind the lean wing of the flame front (i.e. far from the droplets). On the other hand, as S decreases, this diffusion flame tends to be more and more incorporated into the flame front.

Keywords : spray-flame; two-phase combustion; heterogeneous combustion; stratified combustion; droplet array combustion, flamelet model.

Nomenclature

D_{th}	thermal diffusivity
$F(\varphi_u)$	heat of reaction depending on unburnt mixture equivalence ratio
I_W^-	marker of diffusion flame (i.e. the negative part of the indexed reaction rate)
L	latent heat of fuel vaporisation
Le_i	Lewis number of species i in the mixture
P	pressure
p_F	partial pressure of fuel
Pe_s	spray Peclet number
Q^*	effective heat of reaction at stoichiometry
R	droplet radius
s	lattice spacing
T_A	activation temperature
T_b^*	adiabatic flame temperature for stoichiometric gaseous mixture
T_u	temperature of the fresh gaseous mixture
$U_L(\varphi)$	adiabatic flame speed for the single-phase premixture of equivalence ratio φ
$U_L^* = U_L(\varphi = 1)$	adiabatic flame speed for the stoichiometric single-phase premixture
W	reaction rate
Y_i	mass fraction of species i in the mixture
Z_F	fuel mixture fraction (that follows the fuel atoms)
Z_O	oxygen mixture fraction (that follows the oxidizing atoms)
Ze	Zeldovich number for stoichiometric gaseous mixture
δ_L^*	adiabatic flame thickness for the stoichiometric gas mixture
φ	equivalence ratio
φ_u	local estimate of the unburnt mixture equivalence ratio
φ_L	liquid equivalence ratio of the fresh spray (or liquid loading)
φ_G	(initial) gaseous equivalence ratio of the fresh spray (a function of the saturated vapour pressure)
φ_T	overall equivalence ratio of the fresh spray
$\lambda(T)$	thermal conductivity (here, a function of temperature)
ψ_i	reduced mass fraction of specie i
ρ	density
θ	reduced temperature

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4 “*” (resp. “^”) superscript indicates the value at stoichiometric (resp. saturated vapour) conditions
5 “u” (resp. “b”) subscript indicates the value for fresh (resp. burnt) mixture
6 “L” (resp. “G”) subscript indicates the value for liquid (resp. gaseous) phase
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12 **1. Introduction**

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15 Combustion spreading through a spray concerns a large number of applications, such as Diesel engines or
16 rocket engines, gas turbines or industrial furnaces. In a recent study [1], it has been performed numerical
17 simulations of isobaric flames propagating through a face-centred 2D-lattice of droplets. The lattice was
18 conceived as a schematization of a particular initial state of the fresh spray. Since the purpose was the lean
19 sprays, it has been observed that the results very weakly depended on the chemical scheme: the classical one-
20 step irreversible chemistry with a global exothermic reaction was found to be sufficient for exhibiting the
21 main features of the combustion spread in a lean mist.
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25 Contrarily to that previous work on lean sprays, we are now interested in rich spray combustion. In [2], we
26 have shown that the results of numerical simulations in rich sprays can strongly depend on the selected
27 chemical scheme. Although the overall spray composition is supposed to be rich, the local equivalence ratio
28 can be found lean far from the droplets, if the saturated vapour pressure of fuel is low. To study the
29 combustion in such a heterogeneous medium, we have implemented a chemical scheme, which is a
30 composition-corrected one-step global reaction. To obtain satisfactory properties we have proposed to adapt
31 the heat release to the equivalence ratio of the fresh gaseous mixture, that results from droplet vaporization
32 and the subsequent mixture of fuel with air. This chemical scheme introduces two progress variables that
33 allow us to adapt heat release to fresh composition. This procedure gives satisfaction on both lean and rich
34 sides [2].
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39 The problem of flame speed enhancement by droplets has a long history; an interesting summary of the
40 early works has been carried out by Myers and Lefebvre (1986) [3]. Let us particularly quote the works by
41 Cekalin (1961) [4] and by Mizutani and Nakajima (1973) [5-a, 5-b], who added kerosene droplets to a
42 propane air mixture and saw an increase in propagation speed. We also have to mention the pioneering works
43 of Hayashi and Kumagai (1975) [6] and Hayashi et al. (1976) [7], who used a Wilson cloud chamber to
44 produce a nearly monodisperse spray. For polydisperse kerosene sprays, Polymeropoulos and Das (1975) [8]
45 observed that burning velocity reaches a maximum for a certain domain of droplet size.
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49 The situation concerning the velocity increase is, however, not completely clear. For ethanol and isooctane
50 sprays, Hayashi and Kumagai (1975) [6] and Hayashi et al. (1976) [7] reported velocity enhancement for rich
51 sprays, and for lean sprays with large droplets. But, Ballal and Lefebvre (1981) [9] for isooctane, and Myers
52 and Lefebvre (1986) [3] with six different fuels, did not observe the enhancement effect for lean sprays. Our
53 recent numerical study on flames propagating in a lean droplet lattice [1] tends to confirm the latter
54 observations: no increase in spray-flame velocity were noticeable for lean alkane sprays. There are
55 nevertheless other experiments reported in the literature where a velocity increase occurs: for instance, in the
56 lean spray case, a more recent experimental study by Nomura et al. (2000) [10] on ethanol sprays in
57 microgravity indicates larger propagation speeds in a spray than in the equivalent premixed flame, when the
58 droplet size belongs to some interval.
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6 Because it focuses on the droplets, our small scale DNS study does not contain an important effect
7 observed in the experiments: the role of the flame front instabilities (see, for instance, the recent works by
8 Bradley et al. (2014) [11] and by Nassouri et al. (2013) [12] in the case of the expanding spherical spray-
9 flames). Given the importance of these effects in numerous experiments, we now discuss this question more
10 deeply.
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13 Various experiments have revealed that flame spreading in a rich spray has a propagation velocity larger
14 than that of the equivalent premixed flame. In a number of these experiments, the flame front was found
15 corrugated, with a large number of cells. Therefore, spray-flame speed enhancement could possibly be
16 explained by instabilities of the front. As a matter of fact, the interplay between instabilities and droplets
17 seems to have a peculiar importance for the spherical flames, a case that has extensively been studied in the
18 recent years [11-13]: due to gas expansion and droplet inertia, front acceleration modifies vaporization which
19 in turn modifies combustion spreading. Moreover, even for the pure gaseous flame, we know that the
20 spherical flame is subject to highly non-linear effects, leading to the creation of a lot of cells and even to an
21 acceleration of the flame speed (called self-acceleration), see the experiments by Bradley et al. (2001) [14]. In
22 this regard, the experiments with droplets lead more or less to the same effects, except that the inhomogeneity
23 seen by the flame front is here caused by droplets, and not by turbulence.
24

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26 On the theoretical side, similar conclusions can be drawn. The creation of many cells in spherical
27 premixed flames (without droplets) has long been modeled in the case of the hydrodynamic instability with
28 the Sivashinsky equation, namely in 2D by Karlin and Sivashinsky (2007) [15], Fursenko et al. (2008) [16],
29 (see also the simulations of D'Angelo et al. (2000) [17] in the 3D case, which could be compared to the
30 experiments with droplets). This model equation contains the two main effects, creation of many cells and
31 self-acceleration. In the related case of the Sivashinsky equation close to a parabolic shape, it has been shown
32 in Denet and Joulin (2011) [18] that, as the stretch is reduced (as the front is less and less curved), solutions
33 with a lot of cells appear, the same effect as the one observed in the spherical configuration. Every theoretical
34 approach stresses on the major role played by high-level noise, which can here be triggered by the droplets.
35

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37 A droplet lattice, as depicted by the left (unburnt) parts of the various fields drawn in Fig.1, is a manner of
38 controlling the spray initial conditions. Other attempts exist in the literature. For instance, Mikami et al.
39 (2006) [19] measured the flame spread along an array of anchored n-decane droplets. In this microgravity
40 experiment, droplet size and transverse interdroplet distance were fixed, only the interdroplet distance in the
41 direction of spreading was changed. The purpose was to investigate different modes of droplet combustion,
42 from individual to group combustion. The domain of overall equivalence ratio considered in [19] is much
43 higher than the one studied here.
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46 In what concerns the recent spherical spray-flames as studied in [11-12], we would warn the Reader that
47 such experiments cumulate many physical effects, and consequently are not easy to interpret. For instance,
48 the self-acceleration of flame is observed in [11], but the effect of instabilities seems to be limited to a
49 relatively mild increase of 50% in the reported flame velocity; it could be more in other experiments,
50 particularly at high pressure. Our present DNS study being performed in a small domain to focus on droplet-
51 flame interplay, we hence do not pretend to reproduce the features observed in the above-mentioned
52 experiments, especially the front instabilities.
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55 Let us finally note that the present DNS -as described in detail below- solves the vaporization and the
56 combustion of "thick" individual droplets. This is in contrast to simulations that use point droplets, such as all
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4 1D numerical studies on spray-flame, as in Aggarwal and Sirignano (1985) [20], Silverman et al. (1993) [21],
5 Suard, et al. (2004) [22] and Neophytou and Mastorakos (2009) [23], or in the 2D analysis by Reveillon and
6 Vervisch (2005) [24]. By contrast, the present DNS fully resolves the droplets as in the numerical approach
7 by Kikuchi et al. (2005) [25]; here, we additionally allow the droplets to be moved by the gas expansion.
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10 The paper is structured as follows. First, the spray-flame modelling is presented, the chemical scheme
11 being briefly described. Second, the flame spread through the lattice of droplets is numerically studied. The
12 spray-flame speed is defined, and the flame structure is discussed. Finally, the role played by the various
13 parameters is described.
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16 17 18 19 20 **2. Heterogeneous modelling of spray flames** 21 22

23 At low pressure, flame thickness in standard sprays appears large in comparison with droplet interspacing.
24 In the recent years, this property allowed us to resort to a homogenization process for developing an
25 appropriate numerical modelling [22, 26-27]. In such an approach which also neglects droplet inertia, liquid
26 fuel appears as an additional species only allowed to enter into the chemical scheme after a vaporization step.
27 Several spreading regimes have been predicted [22], in particular an intrinsic oscillatory regime, which had
28 been observed experimentally by Hanai *et al.* [28] and by Atzler [13]. The existence of this regime, which
29 occurs as a Hopf bifurcation, does not require the presence of differential diffusivity effects [26-27].
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32 At moderate and high pressures, spray-flame thickness can no longer be large enough -in comparison with
33 droplet interspacing- to allow any process of homogenization. In such a system where both phases are
34 initially in equilibrium, the spray-flame tends to be controlled by vaporization, the chemical heat release
35 permitting the vaporization of the droplets one after another. Therefore, the spray-flame propagates within a
36 heterogeneous (or stratified) mixture with droplets. The mist initial structure is represented as a face-centred
37 2D-lattice of alkane droplets in a pre-mixture of alkane-air (see Fig.1). Then, the droplets can move as the
38 flame propagates.
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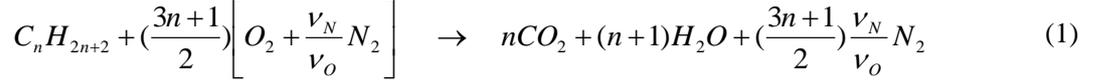
41 This work is hence devoted to spray with droplet inter-distance not small in comparison with the
42 characteristic combustion scales (at least, of the same order). Our numerical modelling starts from the usual
43 set of conservation laws: mass, momenta, energy and species. The non-dimensional form of the conservation
44 laws is performed with the use of the units related the stoichiometric (gaseous) premixed flame, flame
45 thickness, flame velocity, as already used in [1]. A brief description of the overall approach is provided in
46 Appendix A.
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49 50 *2.1 General considerations* 51

52 Since the accurate chemical schemes for alkane are too complex for efficient numerical simulations, a
53 simplified chemical kinetics is generally recommended. It is long known that the classical one-step Arrhenius
54 law (equipped with constant heat release) largely overestimates the adiabatic flame temperature on the rich
55 side. To overcome the difficulty to assess the main rich flame characteristics (as speed and temperature), we
56 have considered [29] a simple modification of the one-step chemical scheme: heat release becomes a
57 function, denoted by $F(\varphi_u)$, of the fresh mixture equivalence ratio φ_u (see below the definition of φ_u). In
58 practice, this model is able to correctly mimic the premixed single-phase flame characteristics (adiabatic
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4 flame temperature and flame speed). As a matter of fact, this adaptation accounts for all the species in
5 equilibrium at the actual flame temperature. This approach of flamelet type requires to know –for any point
6 within the computational domain- the actual composition of the corresponding fresh premixture, already
7 denoted φ_u . Section 2 is mainly devoted to the description of this flamelet approach.
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10
11 Let us first introduce the irreversible single-step reaction for alkane-air combustion
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15 This single reaction allows us to characterize the local mixture composition by φ , the field of equivalence
16 ratio, which reads
17

$$18 \quad \varphi = \frac{Y_F}{Y_O} \times \frac{\nu_O M_O}{\nu_F M_F} \quad (2)$$

19
20 where ν_i stands for the stoichiometric coefficient of species i , M_i , the molar mass of species i . In fresh air,
21 $\nu_N/\nu_O = 3.76$ is the molar ratio of nitrogen to oxygen, while the mass ratio is $\nu_N M_N/\nu_O M_O = 3.29$.
22 At stoichiometry, let us denote by Q^* , the combustion heat related to the flame temperature (i.e. T_b^*), in
23 accordance with
24

$$25 \quad T_b^* = T_u + \frac{(Y_F)_u Q^*}{C_p \nu_F M_F} \quad (3)$$

26
27 We denote by U_L^* , the laminar (single-phase) flame speed, that characterizes the combustion of a premixed
28 fresh mixture of unity equivalence ratio (i.e. $\varphi = 1$). In what follows, the subscript “u” [resp. “b”] is
29 associated with gaseous fresh [resp. burnt] mixture. Thus, $D_{th,b}^*$ denotes the thermal diffusivity coefficient of
30 the burnt gases in the stoichiometric (gaseous) flame. The non-dimensioning process described in Appendix
31 A uses $l_{RD}^* = D_{th,b}^*/U_L^*$ and $\tau_{RD}^* = D_{th,b}^*/(U_L^*)^2$ as length and time scales, respectively.
32

33 Furthermore, we handle temperature and species mass fractions under the reduced forms
34

$$35 \quad \theta = (T - T_u)/(T_b^* - T_u) \quad ; \quad \psi_i = Y_i/Y_{i,u}^* \quad (4.a-b)$$

36
37 (i=f for the alkane fuel, i=o for oxygen and i=p for combustion products)
38

39 Appendix A recalls the system (A.14-A.17) of governing equations that are derived from the general laws of
40 conservation. Equation (A.14) deserves a particular attention
41

$$42 \quad \frac{\partial \theta}{\partial t} + \bar{V} \cdot \bar{\nabla} \theta = \frac{1}{\rho} \text{div}(\rho D_{th} \bar{\nabla} \theta) + F(\varphi_u) W(\rho, \psi_i, \theta) \quad (5)$$

43
44 where W , the reaction rate, is defined in (A.11), and D_{th} is a strongly non-linear function of temperature,
45 which prohibits the diffusion phenomena at low temperature. Vector \bar{V} stands for the velocity field that is
46 governed by the Navier-Stokes equations (A.16-A.17).
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In Equ. (5), appears $F(\varphi_u)$, a quantity adjustable to the fresh mixture composition φ_u , which will allow us to tackle the problem of flame propagation in stratified medium. Let us first propose the following definitions.

The (initial) overall equivalence ratio of the spray is given by the normalized ratio of the total amount of fuel to the total amount of oxygen in the lattice

$$\varphi_T = \frac{\nu_O M_O \int_{\text{initial lattice}} \rho_F dv}{\nu_F M_F \int_{\text{initial lattice}} \rho_O dv}, \quad (6)$$

while the quantity φ_L [resp. φ_G] takes account of the fuel density under liquid phase [resp. gas phase], only. We obviously have $\varphi_T = \varphi_L + \varphi_G$. In the present study, the range selected for φ_T is limited to $1 \leq \varphi_T \leq 1.85$. In Appendix B, it is show how φ_G (or the saturated vapour pressure) can in practice be controlled without affecting the scalings of the paper.

Before combustion reaches a certain locus of the fresh spray, the local equivalence ratio φ_u is an unsteady quantity since it depends on vaporization and mass transfer: it can vary from φ_G (far from the droplets) to a very high value (nearly pure fuel close to the droplets). Two particular single-phase flames can be considered in this context. On the one hand, if all fuel is mixed before burning, we can be faced with a rich premixed flame, the laminar velocity of which is denoted by $U_L(\varphi_T)$. On the other hand, if the initial saturated fuel vapour (mixed with air) is flammable, a combustion spreading can occur rapidly, so that the fuel in the droplets has no time to vaporize. In this case, we are concerned with the propagation of a premixed flame, the laminar velocity of which is $U_L(\varphi_G)$. To discuss the importance of the latter situation, let us now consider τ_{vap} , the characteristic time to vaporize (and mix) the droplets. Supposing that τ_{vap} follows the ‘‘D2-law’’, we obtain $\tau_{vap} \propto \rho_L / \rho_G \times (2R)^2 / D_{th}$. Furthermore, we introduce τ_{prop} , the characteristic time of propagation in the lattice (without resorting to the liquid fuel), which behaves like $\tau_{prop} \propto s / U_L(\varphi_G)$. The comparison of both characteristic times invites us to define Pe_s , the Peclet number of spray combustion, as

$$Pe_s = \frac{\rho_L (2R)^2}{\rho_G D_{th}^*} \times \frac{U_L(\varphi_G)}{s} \quad (7)$$

where ρ_L , ρ_G , R and s are respectively the density of the liquid, the density of the gas, the droplet radius and the lattice spacing. In the case of large Pe_s , we expect that $U_L(\varphi_G)$ will provide us with the spray-flame speed.

2.2 Flamelets in stratified medium

When the assumptions $D_F \approx D_{O_2} \approx D_P$ hold for the diffusivities of fuel, oxygen and products, the literature on premixed flames considers that certain combinations of variables are preserved from the fresh

gases to the burnt gases. In the present work, we select two mixture variables which involve either fuel and products mass fractions, or oxidant and products mass fractions, namely:

$$Z_F = \frac{Y_F}{\nu_F M_F} - \frac{Y_P}{\nu_P M_P} \quad \text{and} \quad Z_O = \frac{Y_{O_2}}{\nu_{O_2} M_{O_2}} - \frac{Y_P}{\nu_P M_P} \quad (8.a-b)$$

Note that ν_p is a negative coefficient in equations (8.a-b) and (A.2) for $i=p$. Consequently, under the above assumptions of equal diffusivity of the species, the Z_F and Z_O fields are obviously governed by the non-reactive equation

$$\frac{\partial Z}{\partial t} + \bar{V} \cdot \bar{\nabla} Z = \frac{1}{\rho} \text{div}(\rho D \bar{\nabla} Z) \quad (9)$$

which results from combinations of equations (A.2).

Hence, at the flame characteristic length scale, which is supposed much smaller than the droplet interspacing, Z_F and Z_O can be considered as conserved when crossing the flame front. Since Z_F and Z_O are conserved through the flame, their ratio Z_F/Z_O is also conserved.

$$Z_F/Z_O = \left\{ [Y_F - (\nu_F M_F / \nu_P M_P) Y_P] / [Y_{O_2} - (\nu_{O_2} M_{O_2} / \nu_P M_P) Y_P] \right\} \times \left\{ \nu_{O_2} M_{O_2} / \nu_F M_F \right\} \quad (10)$$

where $Y_P = 1 - Y_F - Y_{O_2} - Y_{N_2}$ and $Y_{N_2} = (\nu_{N_2} M_{N_2}) / (\varphi_T \nu_F M_F + \nu_{O_2} M_{O_2} + \nu_{N_2} M_{N_2})$

Now, in the fresh gases, Z_F reduces to $Z_F = (Y_F)_u / (\nu_F M_F)$, whereas Z_O to $Z_O = (Y_{O_2})_u / \nu_{O_2} M_{O_2}$.

Therefore, Z_F/Z_O is nothing but φ_u , the equivalence ratio of the fresh gases, since Z_F/Z_O reduces in the unburnt gases of the flamelet to

$$Z_F/Z_O = \left\{ [Y_F]_u / [Y_{O_2}]_u \right\} \times \left\{ \nu_{O_2} M_{O_2} / \nu_F M_F \right\} = \varphi_u \quad (11)$$

Thus, as given by equation (10), the ratio $Z_F(x, y, t) / Z_O(x, y, t)$ allows us to derive an estimate of φ_u , the upstream mixture equivalence ratio, from any local composition within the flame (especially in the reaction zone). Heat release inside the flame thickness can then be adapted to φ_u (within some uncertainties nevertheless since the assumption of equal diffusivities does not exactly hold). This approach will be used throughout the paper, which consequently considers the spray-flame as a set of local flamelets propagating in a heterogeneous medium. This concept requires that the characteristic length scale of composition variations is much larger than the flame thickness, which is the main assumption ruling the paper. Let us remark that in [30-31] is used another ‘‘invariant’’ which allows the authors to adapt heat release and activation energy in pace with the composition variation; the resulting one-step kinetics is implemented and checked with respect to a counter-flow diffusion flame.

From the quantitative point of view, it has been shown in [2] that the following general form of the adjustable quantity $F(\varphi_u)$ gives reliable results for the single-phase premixture in what concerns the alkane/air flame speed and temperature

$$\begin{cases} F(\varphi_u) = [1 - \alpha(\varphi_u - 1)] & \text{if } \varphi_u \in [0.5, 2] \\ W = 0 & \text{if } \varphi_u \notin [0.5, 2] \end{cases}, \quad (12)$$

where α is a coefficient depending on the fuel. The Zeldovich number has been determined theoretically for the studied fuel and more or less appeared as independent of the equivalence ratio. More precisely, for heavy alkane-air premixtures, it has been obtained $\alpha = 0.33$ and $Ze = 7$ [2, 29]. The quantitative comparison with experimental data (conducted in Ref. [2]) indicates that the model describes alkane spray combustion quite reasonably.

3. Numerical experiments

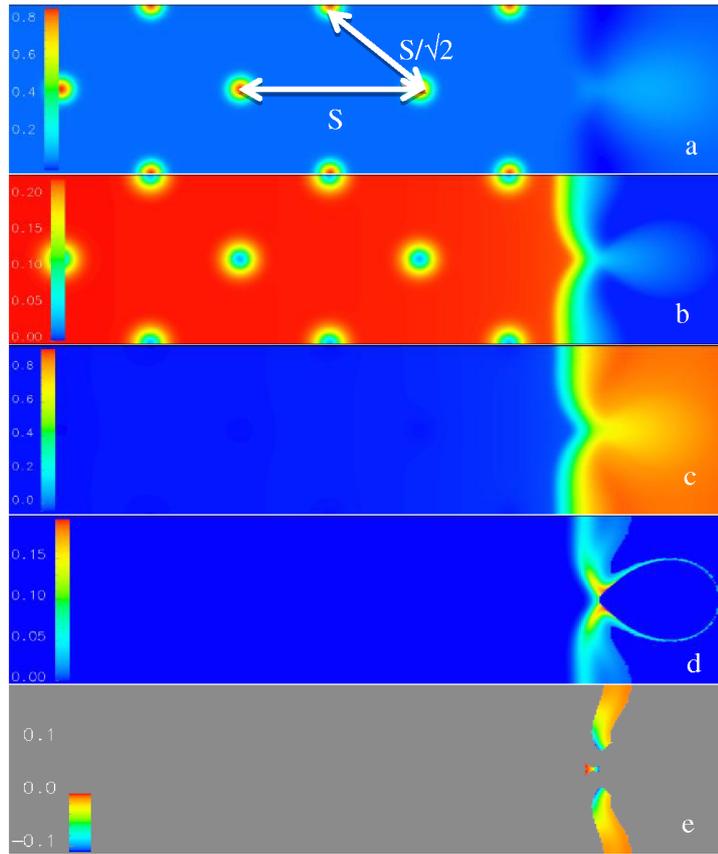


Figure 1: Simultaneous contour plots of fuel mass fraction (a), oxygen mass fraction (b), temperature (c), reaction rate (d), I_w^- negative part of indexed reaction rate (e) ($s = 6$, $\varphi_G = 0.60$, $\varphi_T = 1.25$)

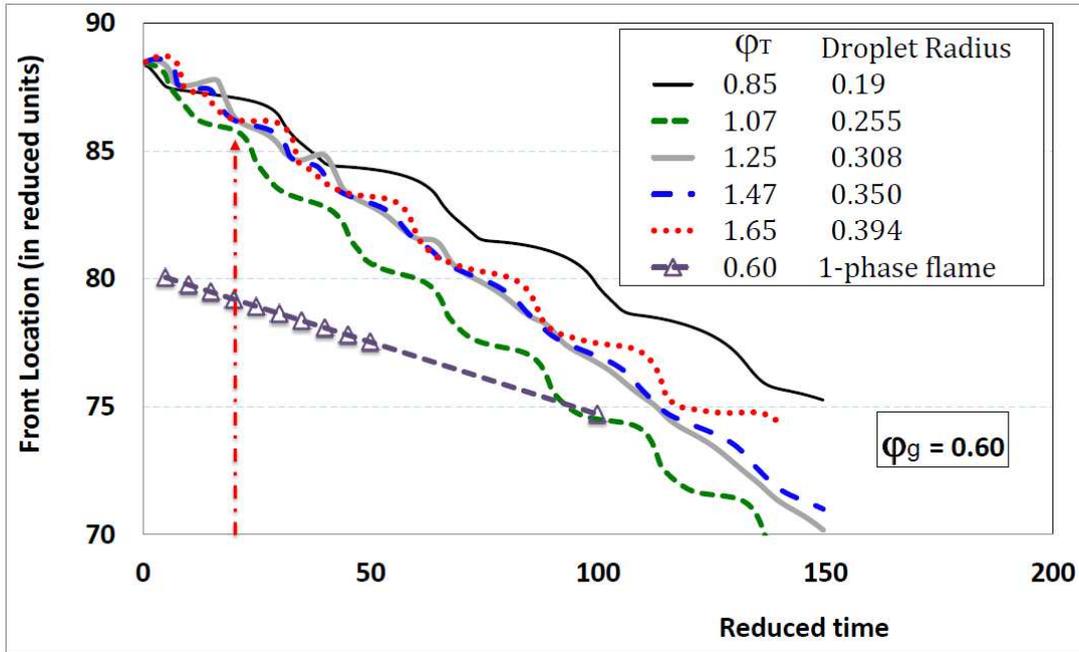
The numerical experiments consist in solving the whole set of conservation laws, as presented in Appendix A. The numerical method [32] is briefly described in Appendix A. As mentioned before, the initial conditions correspond to a lattice of individual droplets surrounded by a mixture of fuel and air in equilibrium. Fig.1 presents the main characteristics of the numerical experiments. A spray-flame propagates from the right to the left. Note the snapshots correspond to the time when both triple flames meet and mark the

end of a rapid stage in the spray-flame propagation process (the instant of the snapshots is indicated in Fig.2 by a vertical arrow). Spray-flame periodically consumes the droplets, which remain at rest until they start to vaporize as indicated in Fig.1.a, where the field of fuel mass fraction is represented. It also indicates that a certain amount of fuel is unburnt behind the (rich) spray-flame. Fig.1.b presents the field of oxygen mass fraction, while Fig.1.c corresponds to the temperature field. Fig.1.d shows the field of heat release. As for Fig.1.e, the negative part of the indexed reaction rate [33] is plotted for displaying the diffusion flames (see below); different elementary flames are noticeable, and will be discussed below.

The numerical experiments aim at determining the flame speed when combustion propagates through an array of fuel droplets positioned at the nodes of the face-centered lattice for a given rich spray. We are interested in the influence of the spray composition (i.e. φ_T , φ_G) and s , the lattice spacing. Droplet radius is obviously a function of liquid loading and lattice spacing. Three dimensionless lattice spacings are investigated: $s = 3$, $s = 6$ and $s = 12$ (in units of stoichiometric premixed flame thickness, as described in Appendix A). Five different initial premixtures surrounding the droplets are considered: $\varphi_G = 0$, $\varphi_G = 0.2$, $\varphi_G = 0.4$, $\varphi_G = 0.6$ and $\varphi_G = 0.8$. Evidently, when φ_G is fixed, the amount of fuel initially under liquid phase increases as φ_T increases. In the same manner, for fixed s and φ_G , droplet radius increases as φ_T increases.

For initiating combustion in the lattice, we follow the same procedure than that used in our previous works [1-2]: close to the open (right) end of the lattice, the temperature field is imposed with the profile of a single-phase flame. This allows us to vaporize and ignite the first droplet of the spray. To follow the combustion spread, we compute $\langle \theta \rangle_y(x)$, the mean temperature averaged in the periodic (y-)direction (i.e. transversally to the propagation). Then, we decide to define x_{sf} , the spray-flame position, as the locus where $\langle \theta \rangle_y(x_{sf}) = 0.5$.

3.1 Spray-flame speed



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4 **Figure 2: Front position vs. time for various liquid loading** ($\varphi_L = 0, 0.25, 0.47, 0.65, 0.87, 1.05$; $\varphi_G = 0.6$;
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6 $s = 6$ and iso-octane/air spray; droplet radius corresponding to each φ_L is provided in units of stoichiometric premixed
7 flame. Vertical arrow indicates the instant of the snapshots of Fig.1)
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10 In this section, we present results on spray-flame speed at constant gaseous equivalence ratio φ_G . In
11 other words, this numerical experiment considers a constant (saturated) vapour pressure; as the initial two-
12 phase mixture is supposed in equilibrium at a given temperature, the initial temperature is a logarithmic
13 function of φ_G thanks to the Clausius-Clapeyron relation of the considered fuel, as described in Appendix B.
14 φ_T is then modified by changing φ_L , the initial liquid loading. Considering the intermediate lattice spacing
15 $s = 6$, Figs. 2 and 3 show the flame front position for $\varphi_G = 0.6$ and $\varphi_G = 0.8$, respectively. Note that a
16 single-phase premixed flame can propagate in both initial premixtures, slowly at $\varphi_G = 0.6$ and more rapidly at
17 $\varphi_G = 0.8$.
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24 In Figure 2, we can observe the actual way the flame propagates in the lattice for $\varphi_G = 0.6$. The front
25 position (defined as the transversally averaged isotherm $\langle \theta \rangle_y (x_{sf}) = 0.5$) is plotted versus time for
26 various overall equivalence ratios (i.e. for increasing liquid loading). The lower (marked) curve corresponds
27 to the front position of a single-phase premixed flame with the (initial) gaseous equivalence ratio (i.e.
28 $\varphi_L = 0$, $R = 0$). The mean slope of each curve is here negative and its absolute value determines the flame
29 speed for a given φ_T . It can be seen that, for this lattice spacing ($s=6$), the single-phase premixed flame with
30 the overall (gaseous) equivalence ratio of 0.6 propagates significantly slower than all the considered spray-
31 flames. One also observes that combustion propagates through the lattice in an unsteady manner [1], since it
32 results from successive stages of droplet vaporization, species mixing, and reaction. Fig. 2 includes a lean
33 case with the overall equivalence ratio $\varphi_T = 0.85$ (i.e. $\varphi_L = 0.25$): this is the slowest spray-flame. It can be
34 observed that the increase of the slope is not monotonous with the overall equivalence ratio. The maximum in
35 slope is more or less obtained for the stoichiometric spray (i.e. $\varphi_T = 1.07$). When liquid loading further
36 increases the spray-flame speed decreases and seems to rapidly reach an asymptotic value.
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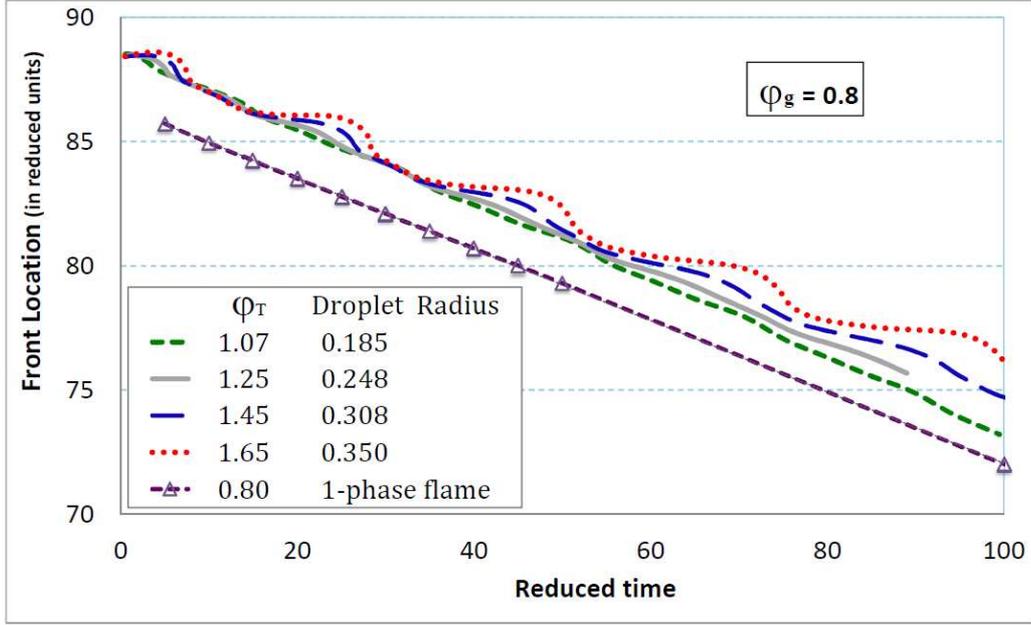


Figure 3: Front position versus time for various liquid loadings $\varphi_L = 0, 0.27, 0.45, 0.65, 0.85$.
 ($\varphi_G = 0.8$ and lattice spacing $s=6$, iso-octane/air spray)

Let us now consider Fig. 3, where the vapour pressure is chosen higher (i.e. $\varphi_G = 0.8$). $U_L(\varphi_G = 0.8)$, the speed of the single-phase flame that spreads in the initial saturated vapour is large. Then, unlike the previous case, the liquid loading is of little help in terms of propagation. The maximum spray-flame speed is again achieved for stoichiometric overall equivalence ratio. If the liquid loading is still increased the spray-flame speed slightly decreases. This slowdown with increasing equivalence ratio is, however, very weak in comparison with the single-phase premixed flame. This observation shows that fuel under liquid phase does not play the same role as the fuel under vapour. As we shall see, this role depends on the droplet size (i.e. mainly on the lattice spacing) and the initial vapour pressure. The fact that the droplet size plays a role in spray-flame propagation can already be seen for instance in Fig.3, where the fluctuations in flame front position increase as the liquid loading increases, i.e. as the droplet size increases. As studied in the previous contribution [1], those fluctuations in front position are due to the vaporization stage (if needed), which depends on the droplet radius squared.

We now investigate the role played by the saturated vapour (i.e. by φ_G) for the same intermediate lattice spacing $s = 6$. In Fig. 4, the non-dimensional spray-flame speed is plotted with respect to φ_T , the overall equivalence ratio of the spray, for various equivalence ratios related to the vapour. In other words, the spray-flame speed is plotted for various (gaseous) equivalence ratio φ_G . In Fig.4, the curves of spray-flame speed are again compared with the single-phase premixed flame velocity.

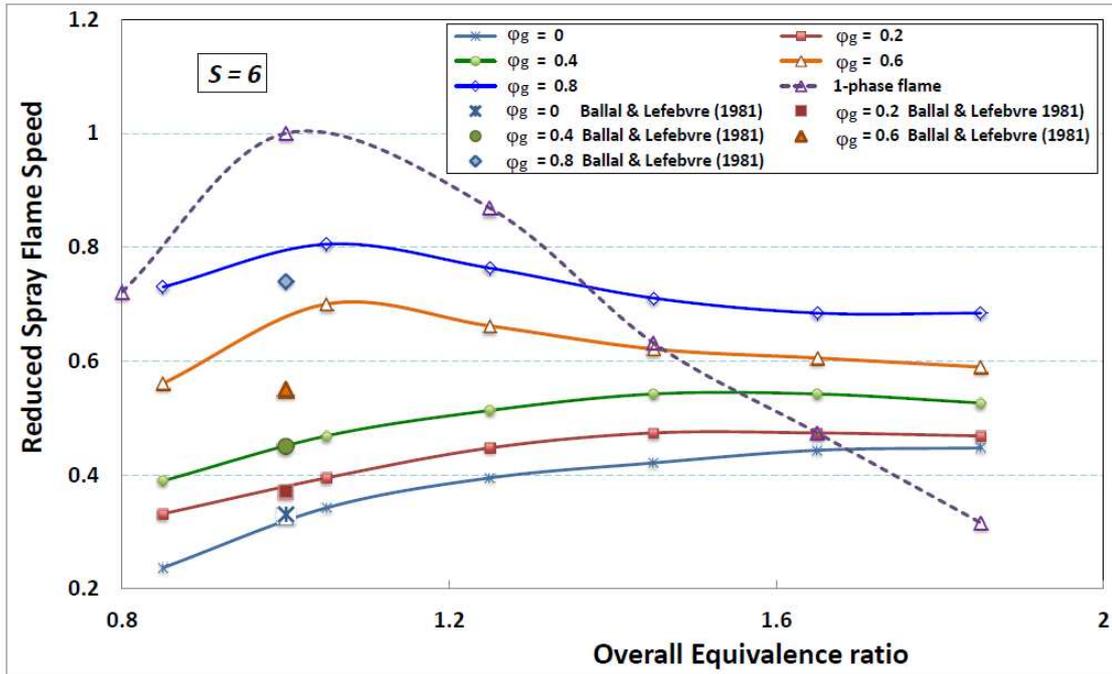


Figure 4: Spray-flame speed versus overall equivalence ratio of the spray for different gaseous equivalence ratios ($s = 6$, heavy fuel oil/air spray;

numerical predictions are compared with the experiments by Ballal & Lefebvre for $\varphi_T = 1$)

For the sake of validating the numerical approach, it can be checked that the experimental observations made in [9,11,12] are retrieved by our numerical results:

- for moderately lean or stoichiometric sprays, the flame velocity is higher without droplets (the overall equivalence ratio being given). In Fig.4, we have added five experimental points from Ballal & Lefebvre [9] for $\varphi_T = 1$ (Sauter mean diameter in the experiment being in link with the lattice spacing used in our numerical predictions). The agreement between experiment and present modelling appears reasonably satisfactory.

- for rich sprays (say $\varphi_T \geq 1.6$), this situation reverses for all values of φ_G : rich spray-flame speed is always higher than single-phase flame speed.

It is worth noting that for very low vapour pressure (i.e. $\varphi_G = 0$) a spray-flame does exist, even though its velocity is quite low. In other words, combustion ensures vaporization at a pace that allows its own propagation! From Fig.4 (i.e. for $s = 6$), we additionally have to underline another trend: for $\varphi_G = 0, 0.2, 0.4$, i.e. when φ_G corresponds to a non-flammable single-phase mixture (in other words, combustion needs droplets to propagate), the spray-flame speed is an increasing function of φ_T . Otherwise, for higher φ_G , the spray-flame speed exhibits a maximum in the vicinity of the (overall) stoichiometry. Lastly, we observe that, when the overall equivalence ratio still increases, the spray-flame velocity does not

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4 vary so much. In other words, on the far rich side, it seems that a constant amount of liquid fuel is involved in
5 spray-flame propagation.
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8 9 *3.2 Role of the lattice spacing*

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12 In the previous paragraphs, increasing the liquid loading led us to slightly increase the droplet radius
13 (in 2D, as the square root of φ_L). A more efficient increase in droplet radius is achieved when the lattice
14 spacing is enhanced: for fixed φ_L , the droplet radius increases linearly with s . For three different values of
15 gaseous equivalence ratio ($\varphi_G = 0.2 ; 0.6 ; 0.8$), the role played by the lattice spacing is now studied.
16
17 More precisely, for each φ_G , the spray-flame velocity is estimated as a function of the overall equivalence
18 ratio for three lattice spacings ($s=3, 6$ and 12). Figure 5 (resp. 6 and 7) plots the spray-flame speeds for
19 $\varphi_G = 0.2$ (resp. for $\varphi_G = 0.6$ and $\varphi_G = 0.8$). On each figure, the dashed line recalls the 1-phase flame
20 speed versus gaseous equivalence ratio (since $\varphi_G = \varphi_T$), while the experimental data from Ballal & Lefebvre
21 [9] are reported for $\varphi_T = 1$ [Note the Sauter mean diameter studied in the experiment corresponds to
22 $s = 10$ and not to $s = 12$].
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29 The spray-flames characterized by $\varphi_G = 0.2$ need to vaporize droplets, previously to any propagation.
30 Hence, Fig. 5 indicates an important role played by lattice spacing on the spray-flame speed. For small lattice
31 spacing (say, $s = 3$), droplet radius being small, the droplets quickly vaporize and contribute to achieve a
32 rather rapid propagation. For larger lattice spacings ($s=6 ; s=12$), droplet radius being higher, the
33 vaporization is slower and imposes its pace to the combustion. When the overall equivalence ratio is high, Fig.
34 5 indicates that propagation velocity of the spray-flame with small lattice spacing [i.e. $s = 3$] follows the same
35 trend as the single-phase flame: spray-flame speed decreases as equivalence ratio increases. This feature is due
36 to the rapid vaporization and mixing of the fuel, which then burns accordingly with the chemical scheme.
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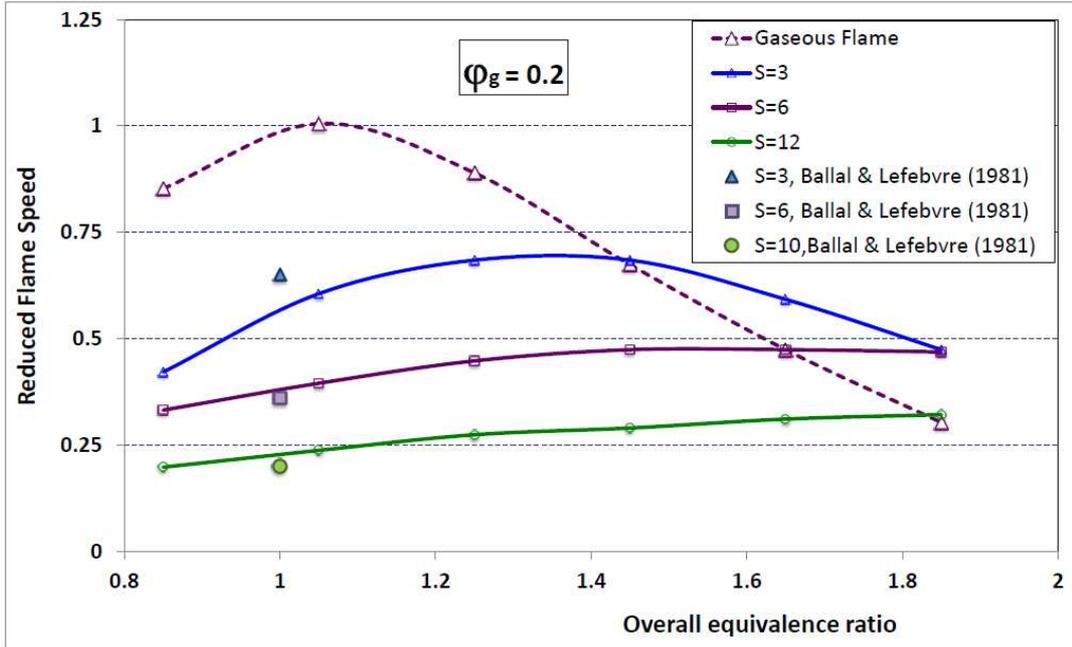


Figure 5: Lattice spacing effect on spray-flame velocity:
spray-flame speed versus overall equivalence ratio for $s=3, 6$ and 12 and $\varphi_G = 0.2$
 (comparison with the experiments by Ballal & Lefebvre for $\varphi_T = 1$, heavy fuel oil/air spray)

Figure 6 treats of a slightly different situation since vapour pressure is high enough ($\varphi_G = 0.6$) to obtain a flammable (initial) single-phase premixture. The spray-flame now requires a smaller amount of fuel coming from the liquid loading to reach the near-stoichiometric conditions in the premixture. Therefore, for relatively small droplet size (cases $s=3$ or $s=6$), the spray-flame presents a maximum of its velocity. The intensity of the maximum is nevertheless lower than the maximum single-phase flame speed, since non-zero vaporization time scale impacts on combustion. The latter impact is weaker for small lattice spacing: for $s = 3$, the curve of spray-flame speed roughly adopts the same pattern than that of the single-phase flame.

On the very rich side of the overall equivalence ratio, spray-flame with small lattice spacing again experiences the rich chemistry, whereas the spray-flame with large lattice spacing, i.e. with a large radius, maintains a large part of the liquid fuel non reacting. In other words, although vaporization of large droplets is a slow process, the rich spray-flame with large droplets propagates faster than the rich spray-flame with small droplets.

Figure 7 presents the spray-flame speed when the vapour pressure is large (i.e. $\varphi_G = 0.8$). If the lattice spacing (or the droplet size) is small, the liquid loading rapidly participates to the spray-flame propagation. In this case (say, $s = 3$), the spray-flame shares the same trends as the single-phase flame: the maximum flame speed occurs at (overall) stoichiometry, and a flammability limit occurs on the rich side, too. Otherwise, for large droplets (say, $s = 12$), the spray-flame propagation ignores the liquid loading and propagates at the same speed as would propagate a single-phase flame in the saturated vapour [since $U_L(\varphi_G = 0.8) = 0.76$, as discussed below].

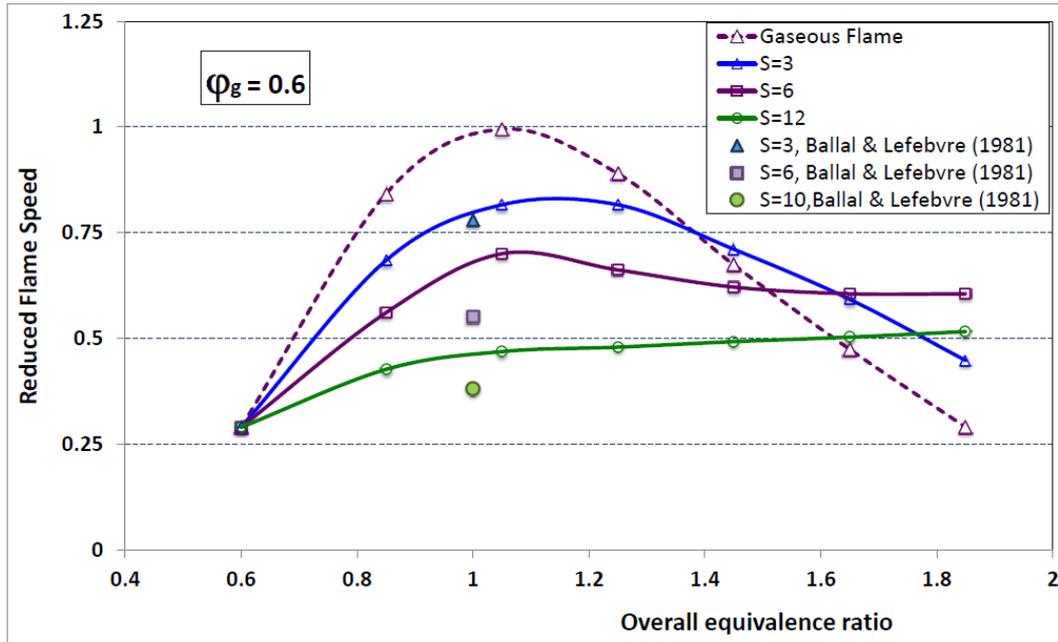


Figure 6: Lattice spacing effect on spray-flame velocity:
spray-flame speed versus overall equivalence ratio for $s=3, 6$ and 12 , and for $\varphi_G = 0.6$
 (comparison with the experiments by Ballal & Lefebvre for $\varphi_T = 1$, heavy fuel oil/air spray)

The previous comments on Figs. 5-7 invite us to stress on the following features, that have already been observed in numerous experimental and numerical studies [11, 12, 20, 21, 23, 34] :

- spray with small droplets (i.e. short vaporization time scale) tends to burn with the same trends as the single-phase premixture.
- when the overall equivalence ratio is large enough (say, $\varphi_T \geq 1.5$) spray-flame speed is always higher than the single-phase flame which tends to extinguish according to the single-step chemical scheme. The difference between spray-flame and single-phase flame becomes more pronounced as droplet size increases. In other words, the presence of large droplets causes some amount of fuel (i.e. under liquid phase) to be maintained out of the combustion. This point will be clarified below.

Furthermore, the vaporization time scale of the droplets undoubtedly plays a role in the spray-flame propagation. Since droplet radius depends on both lattice spacing and liquid loading, the point deserves to be studied specifically. This is the object of the next paragraph.

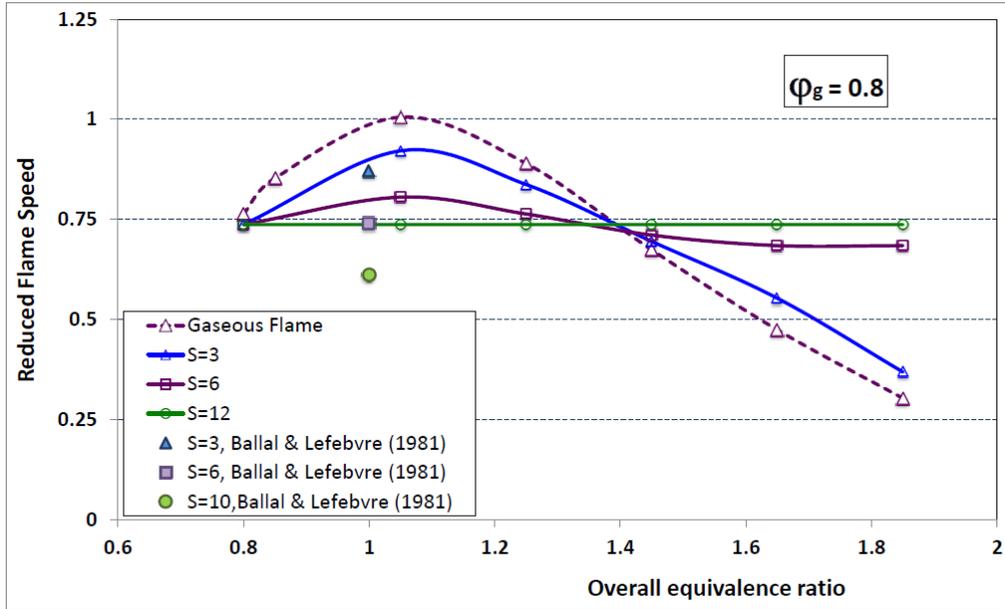


Figure 7: Lattice spacing effect on the spray flame velocity:
velocity versus overall equivalence ratio for $s=3, 6$ and 12 and $\varphi_G = 0.8$

(comparison with the experiments by Ballal & Lefebvre for $\varphi_T = 1$, heavy fuel oil/air spray)

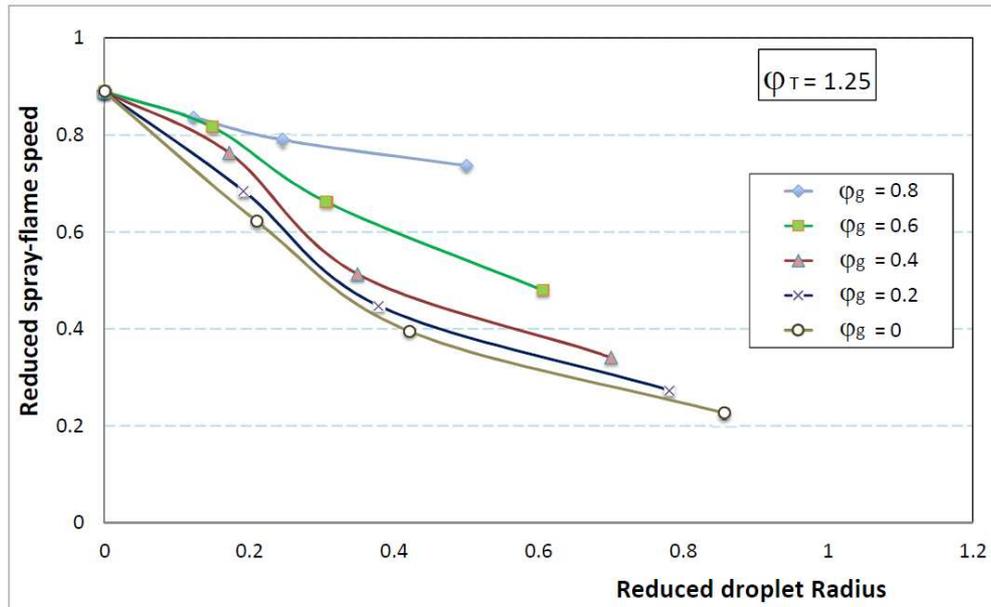
3.3 Detailed role of droplet radius

We now consider a spray with fixed temperature and given chemical composition: φ_T , its overall equivalence ratio, is hence determined, as well as φ_G , the equivalence ratio related to its saturated vapour. Different lattice spacings are considered. We present a series of figures (i.e. Figs. 8-10) for sprays with a fixed overall equivalence ratio. In each figure, a certain amount of fuel is supposed in vapour form and the rest under liquid state; the size of the corresponding fuel droplet is a parameter still free. Our numerical study then consists in computing the spray-flame speed dependence on the radius of these fuel droplets.

Figure 8 concerns a slightly rich spray ($\varphi_T = 1.25$). It presents the spray-flame speed versus droplet radius for various gaseous equivalence ratios (or various vapour pressures). For this case of overall equivalence ratio, the results show that the single-phase flame speed (i.e. $U_L(\varphi_T = 1.25) = 0.89$) is always larger than any two-phase flame of the same overall composition. Let us observe additionally that three curves (i.e. for $\varphi_G = 0., 0.2, 0.4$) correspond to a non-flammable gaseous surrounding of the droplets. It is noticeable that these curves are close to each other. In other words, the spray-flame needs to resort to vaporization of some liquid fuel. In that case, vaporization rules propagation, and the spray-flame speed behaves in inverse ratio to droplet radius (as already studied in lean spray, see Ref. [1]).

Furthermore, let us recall that the initial vapour (in fig.8) is only flammable for $\varphi_G = 0.6$ and $\varphi_G = 0.8$, for which the corresponding single-phase flame speeds are $U_L(\varphi_G = 0.6) = 0.29$ and $U_L(\varphi_G = 0.8) = 0.76$,

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4 respectively. Therefore, from Fig.8, it is clear that droplet vaporization enhances flame speed, whatever the
5 droplet size and the considered vapour pressure. But, this enhancement reaches the single-phase flame speed of
6 the same overall composition, only for vanishing droplet size. To sum up, Fig. 8 is characteristic of the situation
7 for $U_L(\varphi_T) > U_L(\varphi_G)$, where $U_L(\varphi_T)$ represents the laminar flame speed of the single-phase premixture
8 obtained for $\varphi = \varphi_T$ (which is also the spray-flame speed for a spray with infinitely small droplets)
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Figure 8: Spray-flame speed versus droplet radius for various φ_G (and $\varphi_T = 1.25$).

Figure 9 now concerns a moderately rich spray ($\varphi_T = 1.45$). Spray-flame speed is again plotted versus droplet radius for various vapour pressures in this figure, which exhibits two different behaviours. The first case corresponds to the results obtained for $\varphi_G = 0.8$, for which we have $U_L(\varphi_G = 0.8) = 0.76$ and $U_L(\varphi_T = 1.45) = 0.67$. This situation [i.e. for $U_L(\varphi_G) > U_L(\varphi_T)$] exhibits a flame speed enhancement with droplet radius. This behaviour is explained thanks to the following rationale: for very small droplets ($R \rightarrow 0$), vaporization and mixing are immediate so that we start from the rich single-phase case with the speed $U_L(\varphi_T = 1.45) = 0.67$. On the other hand, for large droplets we retrieve the single-phase with the speed $U_L(\varphi_G = 0.8) = 0.76$. In other words, the droplets are large enough to have no time to fully vaporize during the spray-flame propagation. This is the sense of the upper curve of Fig. 9 (i.e. for $\varphi_G = 0.8$), where spray-flame speed increases with droplet radius: the larger the droplets, the lesser liquid fuel is involved in combustion.

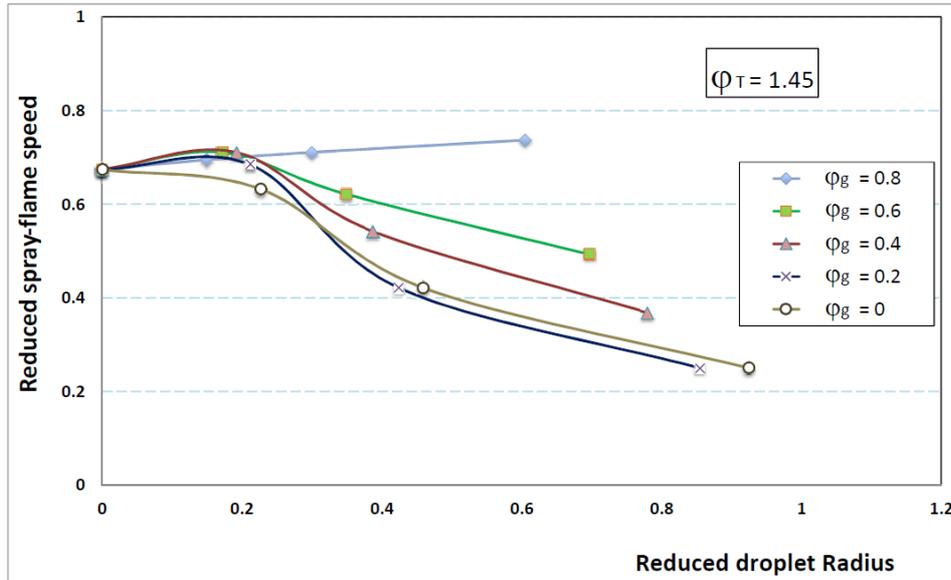


Figure 9: Spray-flame speed versus droplet radius for various φ_G (and $\varphi_T = 1.45$).

In fig.9, the second case considers the other four curves ($\varphi_G = 0., 0.2, 0.4, 0.6$), for which $U_L(\varphi_G) < U_L(\varphi_T)$. These curves are non-monotonic as droplet size increases: if droplet radius slightly increases, less liquid fuel is involved in combustion, and the spray-flame speed slightly increases; now, if the droplet radius is too large, the spray-flame speed asymptotically tends to $U_L(\varphi_G)$, since the vaporization time tends to infinity; therefore, each curve reaches a maximum for an intermediate droplet radius, and afterwards decreases to the asymptotic flame speed $U_L(\varphi_G)$ [which can be a zero value].

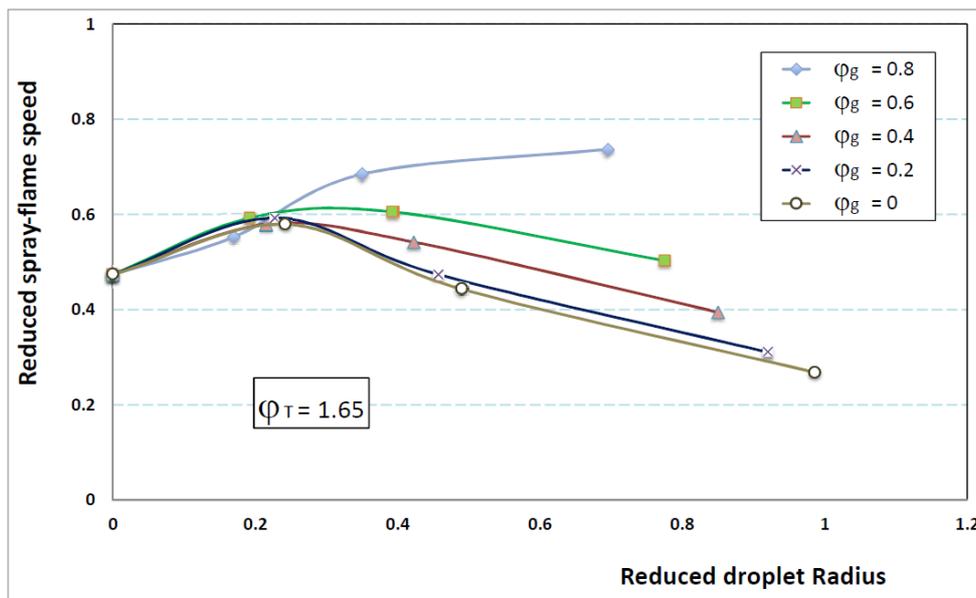


Figure 10: Spray-flame speed versus droplet radius for various φ_G (and $\varphi_T = 1.65$).

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4 It is interesting to still increase the overall equivalence ratio of the spray. Fig.10 is concerned with a rich
5 spray ($\varphi_T = 1.65$): it plots spray-flame speed versus droplet radius for various vapour pressures. In a more
6 marked manner, this case presents the same trends as those of Fig. 9. Initial configurations with feeble vapour
7 pressure need droplet vaporisation: if the droplets are vanishing, a very rich premixture burns; by contrast, if the
8 droplets are very large, only a lean vapour pressure is submitted to combustion. Both opposite trends explain why
9 spray-flame speed versus droplet radius here exhibits a maximum for an intermediate droplet radius. On the other
10 hand, if the initial configuration has an equivalence ratio of vapour background which does not require droplet
11 vaporisation for efficient burning, the presence of large droplets allows the actual mixture to ignore the liquid
12 loading; this is why the curve with $\varphi_G = 0.8$ is an increasing function of droplet radius, this curve starting from
13 $U_L(\varphi_T = 1.65) = 0.48$ (for vanishing droplets) and ending at $U_L(\varphi_G = 0.8) = 0.76$ (for large droplets). This
14 confirms that liquid loading does not intervene when the droplets are huge.

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21 To sum up, for fixed φ_T and φ_G (with $\varphi_T > 1 > \varphi_G$ in the present work), increasing the droplet radius can
22 have different effects :

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24 - if $U_L(\varphi_T) < U_L(\varphi_G)$
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26 and $U_L(\varphi_G) \square U_L^*$, spray-flame speed is enhanced (and tends to $U_L(\varphi_G)$ as $Pe_s \square 1$)
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28 and $U_L(\varphi_G) \square U_L^*$, spray-flame speed admits a maximum for an optimal droplet radius.
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30 - if $U_L(\varphi_T) > U_L(\varphi_G)$
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32 and $U_L(\varphi_T) \square U_L^*$, spray-flame speed diminishes (and tends to $U_L(\varphi_G)$ as $Pe_s \square 1$)
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34 and $U_L(\varphi_T) \square U_L^*$, spray-flame speed admits a maximum for an optimal droplet radius.

35 We now turn to a detailed description of how the flame propagates.
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4. Analysis of spray-flame structure

4.1 Large lattice spacing

In the case of lean sprays, it has been found [1] that the flame propagated from one droplet to the next in different ways, either with a very lean premixed flame, or with constant re-ignition of the next droplet in the case of very small equivalence ratio relative to initial vapour. Once the next droplet was ignited in one way or another, a triple flame propagated around the droplets, leaving behind the diffusion flame around the droplet. Such a propagation was found to correspond to the third propagation mode observed in [19].

In the rich case, however, Roland Borghi suggested -see the sketches in the book by Borghi and Champion [35] and also in Demoulin and Borghi [36] - that the diffusion flame should be around the oxidant; this was called pocket combustion. Let us see what we obtain in the present simulations.

In Fig. 11, we show different fields characteristic of the spray-flame at a particular instant for a the large lattice spacing $s=12$: fuel and oxygen mass fractions, temperature, heat release. The fifth field requires a particular comment: we have plotted I_w^- , the negative part of the indexed reaction rate, which is defined as follows [33]

$$\begin{cases} I_w^- = 0 & \text{if } I_T \geq 0 \\ I_w^- = W \times I_T / |I_T| & \text{if } I_T < 0 \end{cases} \quad \text{with } I_T = \bar{\nabla}\psi_F \cdot \bar{\nabla}\psi_O \quad (21)$$

where I_T is the so-called Takeno flame index [37]. I_T is expected negative when the species diffuse towards each other, as it occurs in a diffusion flame. In other words, plotting the negative part of I_w helps us to localize the diffusion flames. The chosen time in Fig. 11 corresponds to the late instants of the triple flame stage (i.e. just before both triple flames meet); we do not actually show the complete computational domain. As in the lean case [1], for a large value of s , we observe triple flames, the wings of which are connected here to lean and rich premixed flames. Fig. 11.e clearly exhibits the location of the diffusion flames. The first diffusion flame accompanies the triple flame, while the second one burns oxygen in excess between the previous vaporized droplets. As a result, the lean premixed flame does not burn all the oxidant available locally, and is followed by a diffusion flame surrounding the oxidant (and not the fuel as in the lean case), as suggested by Borghi. We are here at a late stage of droplet vaporization, it appears that a significant premixture exists close to the droplet (we recall that the diffusion coefficient is larger for the oxidant than for the fuel, i.e. a Lewis number of 0.9 for the oxidant and 1.8 for the fuel). As a matter of fact, the flame around the droplet is a (slow) rich premixed flame. This rich premixed flame does not burn all the fuel, since a significant amount of fuel is found at the right of the figure where the flame extinguishes. In the same manner, the premixed flame does not burn all oxygen: in Fig. 11.c, a feeble amount of oxygen is present at the right of the domain, and is slowly consumed thanks to the diffusion flame located at the right of the domain.

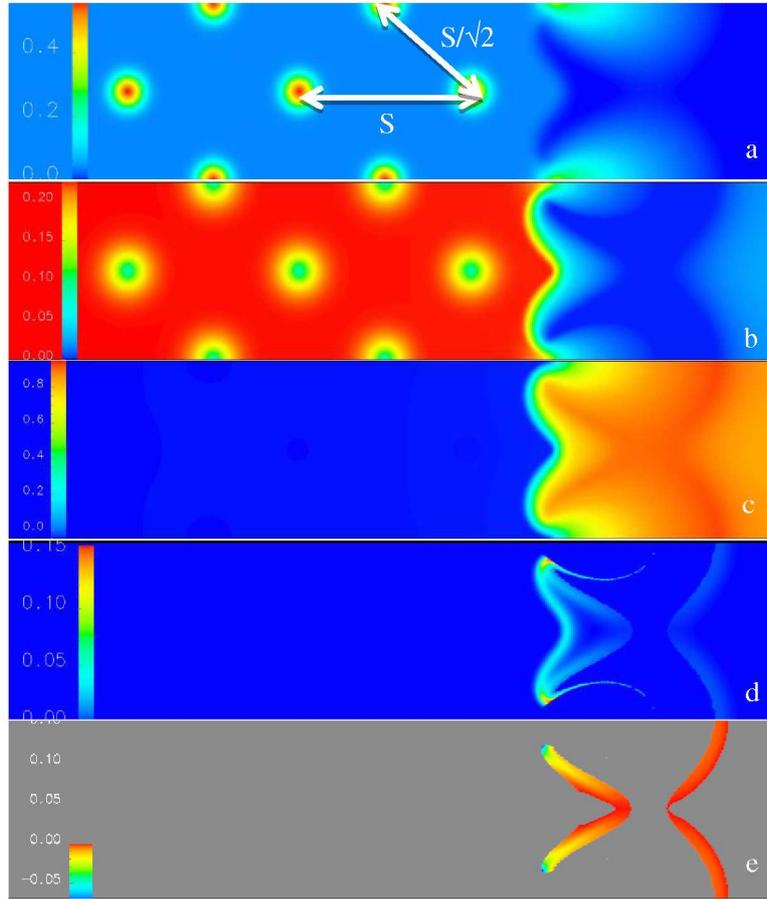


Figure 11: Simultaneous contour plots of fuel mass fraction (a), oxygen mass fraction (b), temperature (c), reaction rate (d), I_w^- negative part of indexed reaction rate (e) ($s=12$, $\varphi_G=0.60$, $\varphi_T=1.25$)

As in the case $s=6$ (the case presented in Fig.1), the case $s=12$ with a value of the vapour equivalence ratio low enough, the flame propagates from one droplet to the other by re-ignition of the next droplet, which Cekalin [4] called time relay combustion (see also the mode 3 in Ref.19). Note that this mechanism leads to a faster propagation velocity than the premixed flame for very rich φ_T (say $\varphi_T > 1.65$).

4.2 Small lattice spacing

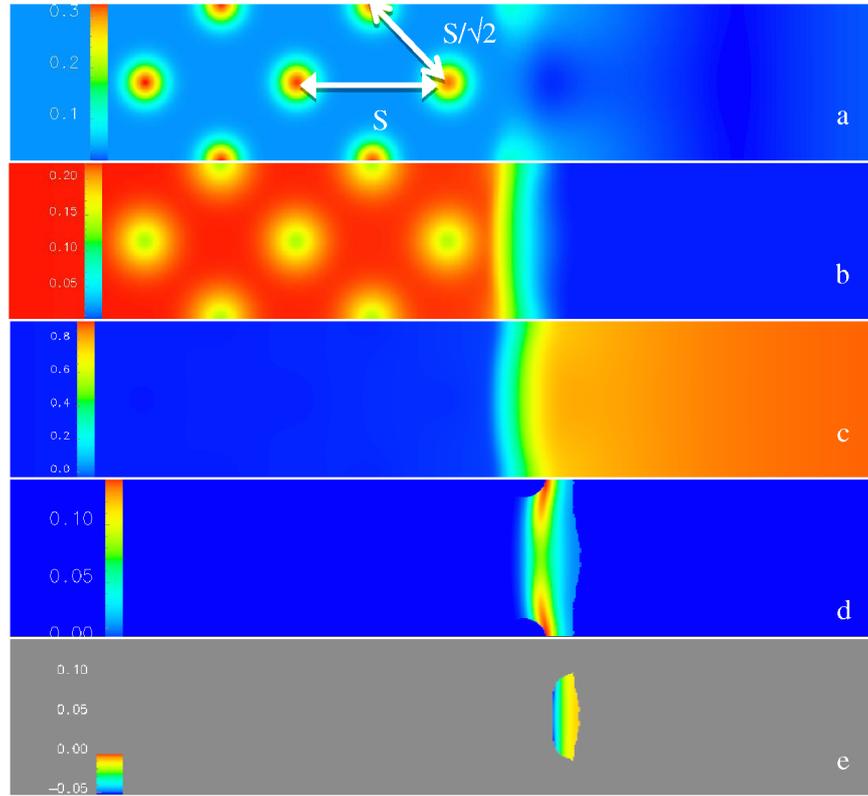


Figure 12: Simultaneous contour plots of fuel mass fraction (a), oxygen mass fraction (b), temperature (c), reaction rate (d), I_w^- , the negative part of indexed reaction rate (e) ($s = 3$, $\varphi_G = 0.60$, $\varphi_T = 1.25$)

In principle, for a very small lattice spacing [i.e. $s \approx 0$], the flame propagation is supposed to retrieve the homogenization regime as studied in [22] and [26-27]. Fig.12 presents the same plots as in Fig.11, fuel and oxidant mass fractions, temperature, heat release, and the negative part of indexed reaction rate, for the smallest value of s that we have studied (i.e. $s = 3$ in units of stoichiometric single-phase flame thickness). In Fig.12, we observe that combustion does not yet occur in a completely pre-vaporized case. If one only looks at both temperature and oxidant fields, it might be concluded that the flame appearance is that of a premixed flame. By contrast, heat release field is rather strange, with a reaction zone thickness very large, of the order of the flame thickness.

To better understand what happens, let us look at the fuel mass fraction. At the time step chosen here, we are in the late stage of burning of one droplet, and the reaction proceeds around the droplet, reminiscent of the triple flame in Fig.11. It seems actually (see the blue zone with almost no fuel mass fraction) that the diffusion flame exists but is not separated from the rest of the reaction. This is obviously corroborated by Fig. 12.e. The overall reaction zone thickness here appears very large: it corresponds to both premixed and

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4 diffusion flames. As a result, for $s=3$ there is no more complete separation between both types of flames, an
5 effect we have already observed in the lean case (see Fig. 8 of Ref. [1]).
6

7 **5. Conclusion**

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10 In the paper, which follows a previous article on lean sprays, we numerically study the propagation of
11 spray-flames in a rich spray, which is initially schematized by a regular lattice of droplets. The paper focus is
12 the spray-flames characterized with a rich overall equivalence ratio (i.e. $\varphi_T \geq 1$). The characteristics of the
13 spray-flames are expressed in units of the stoichiometric single-phase flame.
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15 We aim at comparing our results with the characteristics of the classical single-phase premixed flame
16 that has the same overall equivalence ratio, the speed of which has been denoted by $U_L(\varphi_T)$. This
17 corresponds to the “all fuel flame” that propagates (if any) in the mixture obtained when all fuel is vaporized
18 and mixed. Another single-phase premixed flame of reference is the flame which would exist if the saturated
19 (initial) vapour burns only. The latter single-phase flame is called “initial vapour flame”, and is characterized
20 by φ_G , the so-called gaseous equivalence ratio, and its velocity has been denoted by $U_L(\varphi_G)$. It has been
21 argued in the literature (see Ref. [7]) that the relevant propagation velocity in spray is precisely the single-
22 phase flame speed $U_L(\varphi_G)$. The whole set of our results do not corroborate this claim: it presents rather
23 intricate data that strongly depend on the three parameters φ_G , φ_T , and s , the lattice spacing. For the
24 studied situations (i.e. $0 \leq \varphi_G < 1 < \varphi_T \leq 1.85$), we can conduct the following discussion.
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33 Here, the simplest case to interpret is the case $Pe_s \gg 1$ (i.e. $\tau_{prop} \ll \tau_{vap}$): droplet vaporization does
34 not act on propagation. In other words, the liquid loading is maintained apart from the combustion that rules
35 propagation (a part of the liquid fuel possibly reacting with the remaining oxygen behind the leading front).
36 We here retrieve the situation described by Hayashi et al. [7], who claimed that the relevant propagation
37 velocity is $U_L(\varphi_G)$, i.e. the propagation due to the saturated vapour, only. In our present study, this is the
38 situation met for $\varphi_G = 0.8$ and large droplet radius.
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44 By contrast, if $Pe_s \leq O(1)$ (i.e. $\tau_{prop} \geq \tau_{vap}$), propagation uses (or must use) some part of the liquid
45 loading. Thus, propagation results from the following mechanisms: vaporization is needed to increase a too
46 lean φ_G , which diminishes τ_{prop} (since U_L increases); as soon as $\tau_{prop} < \tau_{vap}$, vaporization ceases to
47 contribute to propagation. Two subcases are then to be considered here: (a) if $U_L(\varphi_T)$ is of the same order as
48 U_L^* [i.e. $U_L(\varphi_T) \approx O(1)$ in our figures], spray-flame speed is a decreasing function of droplet radius, and
49 asymptotically reaches $U_L(\varphi_G)$ for large droplets; (b) if $U_L(\varphi_T)$ is small or moderate, there is an optimal
50 droplet radius for propagation, and, for radii larger than the optimal radius, the spray-flame speed presents a
51 minor dependence on φ_T . Subcase (b) includes the most striking situation: we have found propagation even
52 for $U_L(\varphi_G = 0) = U_L(\varphi_T = 2.2) = 0$ [i.e. neither “initial vapour flame”, nor “all fuel fame” exist], the
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optimal radius being on the order of 0.4 times the stoichiometric flame thickness, and the maximum spray-flame speed being found close to 0.45.

As for the comparison with the experimental literature, it must be conducted in terms of the fundamental laminar spray-flame speed, because our DNS carried out at the scale of the droplets is not able to simulate large scale instabilities, or spherical expansion instabilities as those occurring in the Wilson chambers. As mentioned in Introduction, those instabilities are very sensitive to perturbations: a change in geometry, pressure, can trigger those instabilities, and increase the measured propagation velocity. This is a possible reason for the conflicting results found in the experimental literature. Whatever the scattering in literature, our results corroborate an often observed feature on spray-flames: the rich flammability of spray-flames can be enhanced by a large extent, provided that droplet radius belongs to the appropriate range.

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Appendix A

This addendum is devoted to derive a non-dimensional form of the governing equations from the basis conservation laws, which read for energy and species

$$\frac{\partial(\rho C_p T)}{\partial t} + \text{div}(\bar{V}\rho C_p T) = \text{div}(\lambda \bar{\nabla} T) + Q w(\rho, Y_i, T) \quad (\text{A.1})$$

$$\frac{\partial Y_i}{\partial t} + \text{div}(\bar{V}\rho Y_i) = \text{div}(\rho D_i \bar{\nabla} Y_i) - \nu_i M_i w(\rho, Y_i, T) \quad (\text{A.2})$$

$$\text{where} \quad w(\rho, Y_i, T) = (\rho)^2 Y_F Y_O \exp[-T_A / T] \quad (\text{A.3})$$

is the reaction rate, and T_A the activation temperature. Non-dimensioning is carried out with the use of the characteristics of a flame of reference, which has been chosen as the stoichiometric single-phase premixed flame. Namely, these characteristics are: (a) the stoichiometric mass fractions denoted by $Y_{i,u}^*$ for species i [$i = F, O$ and p , for fuel, oxygen and products, respectively]; (b) the adiabatic flame temperature T_b^* ; (c) the corresponding thermal diffusivity in the burnt gases $D_{th,b}^* = \lambda(T_b^*) / (\rho_b^* C_p)$; (d) the laminar velocity of the stoichiometric flame U_L^* .

Within the framework of a single step chemical scheme, note that T_b^* , the adiabatic flame temperature, allows us to define Q^* , the heat of reaction associated to expression (A.1) at stoichiometry, as follows

$$Q^* = C_p (T_b^* - T_u) \nu_F M_F / (Y_F)_u \quad (\text{A.4})$$

As a matter of fact, the non-dimensioning we use resorts to the following theoretical expression of the laminar velocity, as derived by Joulin and Mitani [38] (see also Garcia-Ybarra et al. [39]).

$$(U_L^*)^2 = \frac{4}{Ze^3} \left(\frac{\rho_b^*}{\rho_u^*} \right)^2 \frac{\lambda_b}{\rho_b^* C_p} \left[(\rho_b^*)^2 v_F M_F Y_{O,u}^* \right] \exp(-T_A / T_b^*) \quad (\text{A.5})$$

Note that superscript “*” denotes a quantity related to the stoichiometric composition, while subscript “u” [resp. “b”] is associated with gaseous fresh [resp. burnt] mixture. As classically, $D_{th,b}^*$ and U_L^* allow us to define two scales for time and length, the so-called transit time and flame thickness, as follows

$$\tau_{RD}^* = D_{th,b}^* / (U_L^*)^2 \quad l_{RD}^* = D_{th,b}^* / U_L^* \quad (\text{A.6.a-b})$$

Hence, for the sake of simplifying the notations, $\{t, \mathbf{x}, \bar{V}, \rho, D_{th}, D_i, F(\varphi_u)\}$ stand hereinafter for

$$\{t/\tau_{RD}^*, \mathbf{x}/l_{RD}^*, \bar{V}/U_L^*, \rho/\rho_b^*, D_{th}/D_{th,b}^*, D_i/D_{th,b}^*, Q/Q^*\} \quad (\text{A.7.a-f})$$

Furthermore, temperature and species mass fractions are made dimensionless as follows

$$\theta = (T - T_u) / (T_b^* - T_u); \quad \psi_i = Y_i / Y_{i,u}^* \quad (i=F \text{ for the alkane fuel and } i=O \text{ for oxygen}) \quad (\text{A.8.a-b})$$

We are now able to write Equ. (A.1-3) in non-dimensional form as

$$\frac{\partial \theta}{\partial t} + \bar{V} \cdot \bar{\nabla} \theta = \frac{1}{\rho} \text{div}(\rho D_{th} \bar{\nabla} \theta) + F(\varphi_u) W(\rho, \psi_i, \theta) \quad (\text{A.9})$$

$$\frac{\partial \psi_i}{\partial t} + \bar{V} \cdot \bar{\nabla} \psi_i = \frac{1}{\rho} \text{div}(\rho D_i \bar{\nabla} \psi_i) - \mu_i W(\rho, \psi_i, \theta) \quad (\text{A.10})$$

$$\text{where} \quad W(\rho, \psi_i, \theta) = \frac{Ze^3}{4} \left(\frac{\rho_u^*}{\rho_b^*} \right)^2 \psi_F \psi_O \left(\frac{\rho}{\rho_b^*} \right)^3 \exp \left[Ze \frac{\theta - 1}{1 + \gamma(\theta - 1)} \right] \quad (\text{A.11})$$

$$\text{with the reduced coefficients} \quad \mu_i = v_i M_i / (v_F M_F) \quad (\text{A.12})$$

$$\text{and the classical parameters, } Ze = T_A (T_b^* - T_u) / (T_b^*)^2 \text{ and } \gamma = (T_b^* - T_u) / T_b^* \quad (\text{A.13.a-b})$$

It is worth noting that $F(\varphi_u)$, the reduced heat of reaction, is a quantity that is tuneable in function of the local composition of the fresh mixture, which is characterized by the field $F(\varphi_u)$ [see section 2]. This takes account of the heterogeneous composition of the mixture. Accordingly with the present non-dimensioning, we have $F(\varphi_u = 1) = 1$.

Finally, we assume that all Lewis numbers [$Le_i = D_{th} / D_i$] are constant (i.e. the ratio of thermal diffusivity to molecular diffusivity is supposed constant for each species I ; they are taken equal to $Le_F = 1.8$ for the fuel and $Le_O = 0.9$ for oxygen. The same hypothesis is set on the Prandtl number [$Pr = \nu / D_{th}$ is supposed constant]. So that, we obtain the following system of governing equations, that reads

$$\frac{\partial \theta}{\partial t} + \bar{V} \cdot \bar{\nabla} \theta = \frac{1}{\rho} \text{div}(\rho D_{th} \bar{\nabla} \theta) + F(\varphi_u) W(\rho, \psi_i, \theta) \quad (\text{A.14})$$

$$\frac{\partial \psi_i}{\partial t} + \bar{V} \cdot \bar{\nabla} \psi_i = \frac{1}{Le_i} \frac{1}{\rho} \text{div}(\rho D_{th} \bar{\nabla} \psi_i) - \mu_i W(\rho, \psi_i, \theta) \quad (\text{A.15})$$

coupled with the Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \bar{V}) = 0 \quad (\text{A.16})$$

$$\frac{\partial \bar{V}}{\partial t} + \overline{\nabla V} \cdot \bar{V} = \text{Pr} \frac{1}{\rho} \text{div} \left\{ \rho D_{th} \left[\overline{\nabla V} + (\overline{\nabla V})^T \right] \right\} - \frac{1}{\rho} \overline{\nabla} P \quad (\text{A.17})$$

where P stands for pressure.

System (A.14-17) has been solved numerically with a mixed numerical method that takes account of the y-periodicity, for which Fourier spectral methods is used. As for the x-direction, the numerical approach resorts to finite differences. A particular treatment for computing pressure has been implemented [32] and continuously improved [40], since the present isobaric combustion is characterized by low Mach number flows. As surface tension is neglected, the numerical approach can consider a single-fluid flow with very high variations of density, from the volumetric mass of a hot gas to that of a liquid fuel. In such a way, inertia of the dense phase is easily accounted for. To confine the liquid fuel into the droplets, diffusivity is frozen at low temperature [1]. Typical discretization is 3072 nodes in the (propagation) x-direction and 256 Fourier modes in the (transverse) y-direction. More precisely, about 15 nodes are at least present along a droplet radius. To check the numerical precision, this discretization has been doubled; no change in the observed features has been noticed.

The limitation of the numerical approach is that no immediate coupling with sound can be envisaged, since acoustic filtering is associated to low Mach number flow models, as well as highly compressible flow (or high speed combustion) cannot be considered. Another limitation is related to the absence of surface tension: if the length scale of the flow shears is smaller than the droplet size, freezing the diffusivity will be insufficient to confine the fuel inside the droplets.

Appendix B

This addendum is devoted to answer a practical question: is it possible to change φ_G without drastically affecting the characteristic quantities used for the non-dimensional stage that has been described in Appendix A? This point is an important issue in terms of interpreting our results with respect to laboratory experiments.

Our numerical experiments have considered spray-flames, which are determined by the set of parameters that characterizes the initial mixture: pressure P , temperature T_u , chemical composition (i.e. φ_G and φ_T given) and droplet geometry (i.e. S given). Evidently, such a spray-flame cannot generally exist from the experimental point of view, since P , T_u and φ_G are not independent. These quantities are linked by the Clausius-Clapeyron formula on saturated vapour.

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4 Furthermore, as flame of reference in the non-dimensional process, we have used the stoichiometric
5 single-phase flame defined by the set $\{P, T_u, \varphi_G = \varphi_T = 1\}$. Obviously, the latter only exists if the pair
6 $\{P, T_u\}$ belongs to a certain domain, which is delimited by the conditions of saturated vapour.
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10 Hence, instead of considering the spray-flame determined by $\{\varphi_G, \varphi_T, S\}$ for any $\{P, T_u\}$, the
11 experimentalist has to perform the experiment for $\{P, T_u, \varphi_G\}$ satisfying the conditions of saturated vapour.
12 For example, we can investigate two opposite cases: (a) we fix T_u and consider $P(\varphi_G)$, or (b) we fix P and
13 consider $T_u(\varphi_G)$. Both strategies are studied below, for the range $0.1 \leq \varphi_G \leq 1$, discarding the limit case
14 $\varphi_G = 0$.
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20 (a) we first consider that all spray-flames have the same initial temperature. Then, p_F , the saturated vapour
21 pressure of fuel, is given. Therefore, φ_G is experimentally controlled by the amount of air added to the
22 mixture that surrounds the droplets. We hence obtain the pressure of the experiment as
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$$27 \quad P(\varphi_G) = p_F + p_{O_2}(1 + \nu_{N_2}/\nu_{O_2}) = p_F \left[1 + (\nu_{O_2} + \nu_{N_2}) / (\nu_F \varphi_G) \right] \quad (B.1)$$

28 To fix the idea, P reads for isoootane
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$$30 \quad P(\varphi_G) = p_F [1 + 60/\varphi_G] \approx 60 p_F / \varphi_G \quad (B.2)$$

31 Expressions (B.1-2) recall us that -for heavy alkanes- the total pressure is essentially determined by the
32 amount of air. If we consider the range of variation $0.1 \leq \varphi_G \leq 1$, expression (B.2) indicates that total
33 pressure will vary by a factor 10. Although flame speed is known to vary mildly with pressure, this manner of
34 monitoring φ_G is not satisfactory, since flame thickness varies as P^{-1} . Therefore, using \hat{P} , a certain pressure
35 value independent of φ_G , instead of $P(\varphi_G)$, introduces a huge error in assessing the length scale. We must
36 turn to another manner of controlling φ_G .
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44 (b) we now question the role of $T_u(\varphi_G)$, the fresh mixture temperature, which allows the experimentalists to
45 monitor the fuel saturated vapour pressure for a given total pressure (i.e. a given amount of air, essentially).
46 In combustion, it is well-known that the most sensitive quantity to temperature is the reaction rate. More
47 precisely, it is known as an exponential function of the burnt gas temperature, which depends linearly on T_u
48 [as recalled in Eq.(3)]. In other words, the issue concerns the error committed by the fact of using \hat{T}_u , some
49 constant value of the equilibrium temperature, instead of $T_u(\varphi_G)$. To fix the ideas about the effects of such a
50 modification in reaction rate, let us estimate the error committed on the single-phase flame speed U_L^* by the
51 fact to use \hat{T}_u instead of $T_u(\varphi_G)$. Eq. (A.5) recalls that reaction rate and flame speed squared are in direct
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59 From the Clausius-Clapeyron formula, we relate T_u and φ_G as follows.
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$$\frac{L}{R_c \hat{T}_u} \left[1 - \frac{\hat{T}_u}{T_u} \right] = \ln\left(\frac{p_F}{\hat{p}_F}\right) = \ln\left(\frac{\varphi_G}{\hat{\varphi}_G}\right) \quad (\text{B.3})$$

where p_F , L and R_c are the saturated vapour pressure of fuel, the latent heat of fuel vaporization and the gas constant, respectively. Superscript “^” corresponds to the condition of saturated vapour for an intermediate value of φ_G , say $\hat{\varphi}_G = 0.3$. Now, from Eq. (A.4-5) and Eq. (B.3), we can derive the following relation between $U_L^*(T_u(\varphi_G))/U_L^*(\hat{T}_u)$ and φ_G as

$$\frac{U_L^*(T_u)}{U_L^*(\hat{T}_u)} \approx \exp\left\{ -\frac{Ze[\hat{T}_u - T_u(\varphi_G)]}{2\hat{T}_b^*} \right\} \approx \exp\{N_{VR} \ln(\varphi_G / \hat{\varphi}_G)\} = (\varphi_G / \hat{\varphi}_G)^{N_{VR}} \quad (\text{B.4})$$

where

$$N_{VR} = \frac{Ze}{2} \frac{R_c \hat{T}_u}{L} \frac{\hat{T}_u}{\hat{T}_b^*} \quad (\text{B.5})$$

Note that N_{VR} is a number that takes account of vaporization and reaction. For the isoctane flame under standard conditions, N_{VR} is as small as 0.03. In consequence, a ratio of $\varphi_G / \hat{\varphi}_G = 3$ is damped into $U_L^*(T_u(\varphi_G))/U_L^*(\hat{T}_u) = 1.034$ by expression (B.4). This corresponds to a relative error on the order of 3%. In other words, interpreting our results as obtained with the same initial temperature introduces an error on the reaction rate largely within the error bars of the experiments, as well as within those of the numerical methods.

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