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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., 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-centred 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 ares, 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 vaporised 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 vaporisation (possibly bounded by the "all fuel flame" speed) and a slowing down in flame velocity because the vaporisation 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.

1. Introduction

Combustion spreading through a spray concerns a large number of applications, such as Diesel engines or rocket engines, gas turbines or industrial furnaces. In a recent study [1], it has been performed numerical simulations of isobaric flames propagating through a face-centred 2D-lattice of droplets. The lattice was conceived as a schematization of a particular initial state of the fresh spray. Since the purpose was the lean sprays, it has been observed that the results very weakly depended on the chemical scheme: the classical one-step irreversible chemistry with a global exothermic reaction was found to be sufficient for exhibiting the main features of the combustion spread in a lean mist.

Contrarily to that previous work on lean sprays, we are now interested in rich spray combustion. In [2], we have shown that the results of numerical simulations in rich sprays can strongly depend on the selected chemical scheme. Although the overall spray composition is supposed to be rich, the local equivalence ratio can be found lean far from the droplets, if the saturated vapour pressure of fuel is low. To study the combustion in such a heterogeneous medium, we have implemented a chemical scheme, which is a composition-corrected one-step global reaction. To obtain satisfactory properties

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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
"$*$" (resp. "^")	superscript indicates the value at stoichiometric (resp. saturated vapour) conditions
"u" (resp. "b")	subscript indicates the value for fresh (resp. burnt) mixture
"L" (resp. "G")	subscript indicates the value for liquid (resp. gaseous) phase

we have proposed to adapt the heat release to the equivalence ratio of the fresh gaseous mixture, that results from droplet vaporisation and the subsequent mixture of fuel with air. This chemical scheme introduces two progress variables that allow us to adapt heat release to fresh composition. This procedure gives satisfaction on both lean and rich sides [2].

The problem of flame speed enhancement by droplets has a long history; an interesting summary of the early works has been carried out by Myers and Lefebvre [3]. Let us particularly quote the works by Cekalin [4] and by Mizutani and Nakajima [5(a), (b)], who added kerosene droplets to a propane air mixture and saw an increase in propagation speed. We also have to mention the pioneering works of Hayashi and Kumagai [6] and Hayashi et al. [7], who used a Wilson cloud chamber to produce a nearly monodisperse spray. For polydisperse kerosene sprays, Polymeropoulos and Das [8] observed that burning velocity reaches a maximum for a certain domain of droplet size.

The situation concerning the velocity increase is, however, not completely clear. For ethanol and isooctane sprays, Hayashi and Kumagai [6] and Hayashi et al. [7] reported velocity enhancement for rich sprays, and for lean sprays with large droplets. But, Ballal and Lefebvre [9] for isooctane, and Myers and Lefebvre [3] with six different fuels, did not observe the enhancement effect for lean sprays. Our recent numerical study on flames propagating in a lean droplet lattice [1] tends to confirm the latter observations: no increase in spray-flame velocity were noticeable for lean alkane sprays. There are nevertheless other experiments reported in the literature where a velocity increase occurs: for instance, in the lean spray case, a more recent experimental study by Nomura et al. [10] on ethanol sprays in microgravity indicates larger propagation speeds in a spray than in the equivalent premixed flame, when the droplet size belongs to some interval.

Because it focuses on the droplets, our small scale DNS study does not contain an important effect observed in the experiments: the role of the flame front instabilities (see, for instance, the recent works by Bradley et al. [11] and by Nassouri et al. [12] in the case of the expanding spherical spray-flames). Given the importance of these effects in numerous experiments, we now discuss this question more deeply.

Various experiments have revealed that flame spreading in a rich spray has a propagation velocity larger than that of the equivalent premixed flame. In a number of these experiments, the flame front was found corrugated, with a large number of cells. Therefore, spray-flame speed enhancement could possibly be explained by instabilities of the front. As a matter of fact, the interplay between instabilities and droplets seems to have a peculiar importance for the spherical flames, a case that has extensively been studied in the recent years [11–13]: due to gas expansion and droplet inertia, front acceleration modifies vaporisation which in turn modifies combustion spreading. Moreover, even for the pure gaseous flame, we know that the spherical flame is subject to highly non-linear effects, leading to the creation of a lot of cells and even to an acceleration of the flame speed (called self-acceleration), see the experiments by Bradley et al. [14]. In this regard, the experiments with droplets lead more or less to the same effects, except that the inhomogeneity seen by the flame front is here caused by droplets, and not by turbulence.

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

A droplet lattice, as depicted by the left (unburnt) parts of the various fields drawn in Fig. 1, is a manner of controlling the spray initial conditions. Other attempts exist in the literature. For instance, Mikami et al. [19] measured the flame spread along an array of anchored n-decane droplets. In this microgravity experiment, droplet size and transverse interdroplet distance were fixed, only the interdroplet distance in the direction of spreading was changed. The