EXPERIMENTAL AND NUMERICAL CHARACTERIZATION OF THE METHYL DECANOATE COMBUSTION IN LAMINAR COUNTERFLOW SPRAY PREMIXED FLAMES

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ABSTRACT
Biodiesel is a mixture of long chain fatty acid methyl esters used mainly in compression ignition engines. In order to improve engine performance, an understanding of its fundamental properties and the combustion pathways is required. A surrogate fuel: methyl decanoate (MD) is used in order to simplify the models and experiments. This study presents new data for MD combustion in a laminar counterflow premixed flame configuration (spray MD/air against methane/air) at atmospheric pressure, for different strain rate and equivalence ratio conditions. The visible and UV chemiluminescence of the excited radicals CH\(^*\)(A\(^2\Delta\)) and OH\(^*\)(A\(^2\Sigma^+\)) as well as Planar Laser-Induced Fluorescence (PLIF) of OH are employed experimentally to analyze the flame structure. The counterflow spray flame is simulated by choosing a MD skeletal reaction mechanism, to which we add CH\(^*\) and OH\(^*\) reactions. The numerical predictions of the CH\(^*\) concentration are very close to the experimental profiles along the central axis. The numerical and experimental results indicate differences in the OH\(^*\) production routes between MD and methane flames.

INTRODUCTION
In the context of reduction of fossil fuel consumption, the use of biodiesel is one of the strategies adopted by several countries around the world. However, changing the fuel in diesel engines induces changes in combustion behavior, which can impact pollutants emission.

Indeed, the use of biodiesel in diesel engines decreases emissions of pollutants such as carbon monoxide, unburned hydrocarbons, and particulate matter [1], although a slight increase in emissions of nitrogen oxides is observed in some cases [2]. Therefore, a better understanding of the biodiesel combustion is needed.

Previous studies have shown that methyl decanoate (MD) is a good surrogate for biodiesel combustion. Surrogate fuels are easier to study both experimentally and numerically because of their shorter hydrocarbon chain. Several kinetic schemes have been validated and permit to simulate the general behavior of premixed and diffusion flames of this synthetic fuel.

A very large chemical kinetic mechanism for MD consisting of 3012 species and 8820 reactions was developed by [3]. This mechanism is capable of reproducing, particularly, early CO\(_2\) formation. However, because of its large size, the simulation even for a laminar flame is very time consuming, as well as it requires enormous computing resources.

The directed relation graph (DRG) method [4] was used to reduce the detailed mechanism to a skeletal mechanism consisting of 125 species and 713 elementary reactions [5]. It has been validated with experiments studying the limits of ignition and extinction of MD in a counterflow gaseous diffusion flame.

A convenient way to experimentally study the flame behavior is to analyze space and time resolved emission of CH\(^*\) and OH\(^*\). Indeed, these two radicals are naturally present in the...
combustion zone and permit to determine important macroscopic properties such as flame location, flame speed and heat release rate fluctuations. However, these two radicals can only be considered as tracer because they have no significant influence on combustion reaction mechanisms. For this reason, CH* and OH* are generally not taken into account in reduced kinetic schemes, and comparison with experimental data are consequently not done.

Most of biodiesel surrogates chemical schemes validations were realized employing either homogeneous reactors or counterflow gaseous diffusion flames [5]. Spray counterflow diffusion flames have been studied by [6, 7], however in our knowledge, none of them concerns biodiesel surrogates. In the present work, we study a counterflow of spray MD/air against methane/air mixture to carry both experiments and simulations. The simultaneous presence of two different fuels in this configuration is an additional requirement so that the chemical scheme should be able to predict both flames. The skeletal MD kinetic scheme proposed by [5] was chosen to carry the simulations with reasonable CPU time. CH* and OH* formation, chemiluminescence and quenching reactions were added. The available literature data were recently summarized by [8]. Most CH* and OH* reactions and rate constants found in literature [8–11] are validated with experiments involving light hydrocarbon flames, such as methane but no validation of the data has yet been made for a biodiesel surrogate.

Measurements of CH* and OH* emissions, OH PLIF and temperature profiles have been realized for several MD laminar counterflow spray premixed flames for different equivalence ratio and strain rate conditions. Also, by comparing experimental and numerical OH and temperature profiles, we seek to verify that the current counterflow burner configuration permits to reproduce similar combustion as the one simulated with the chosen kinetic scheme. Then, we seek to validate the production and consumption reactions of CH* and OH* in the case of MD flames.

1 EXPERIMENTAL SETUP
1.1 Counterflow Burner Device

The experiments were carried out in a counterflow burner. The setup used will be described briefly. More information of the burner can be found in [12, 13].

The burner consists of two opposed axisymmetric convergent nozzles of 20 mm inner diameter. A premixed gaseous flow of methane and air is injected at ambient temperature through the lower side of the burner, while a spray flow of MD and air is transported at 400 K from the upper side. Two laminar flame fronts appear on each side of the stagnation point. The distance between the two nozzle exits was kept constant to 40 mm. Each nozzle is surrounded by a coaxial nozzle fed by nitrogen in order to protect the flames from ambient perturbations that could disturb the measurements.

The liquid fuel atomizer is the one used in [13]. The advantage of this system is that the size distribution of the spray is particularly narrow [14]. The inconvenience is that we were restricted to work with small air flowrates and with very lean MD flames.

The methane flame was kept constant throughout the study (φ = 0.62, Injection Temperature = 300 K). The methane/air flow velocity at the injector face is 50.1 cm/s and the mass flow rate per unit area (mass flux) is 5.9E-02 gcm⁻²s⁻¹.

We have performed experimental and numerical studies of nine different combinations (A-I) of equivalence ratio (φ) and strain rate (ε) gathered in Tab. 1. The corresponding MD and air mass flow rates at the upper burner are given in Tab. 2. The strain rates are estimated using the definition given by [15]. All gaseous mass flow rates are controlled by the mass flow meters with an accuracy of ±1.5% and a repeatability of ±0.5% of the full scale. The MD liquid mass flow was measured with an accuracy of ±10%. The overall uncertainty of strain rate, methane and MD flames equivalence ratios can therefore be estimated at ±2.5%, ±1.5% and ±12%, respectively.

| TABLE 1. NINE DIFFERENT EXPERIMENTAL CONDITIONS STUDIED (A-I), STRAIN RATES ARE IN s⁻¹, VELOCITIES ARE IN cm s⁻¹ |
|-----------------|-----|-----|-----|
| MD Flames References |  |  |  |
| φ \ ε | 42.5 | 45.1 | 49.2 |
| 0.2 | - | - | C |
| 0.22 | - | - | F |
| 0.26 | A | B | I |
| 0.28 | D | E | - |
| 0.31 | G | H | - |
| \Velocity | 29.5 | 34.4 | 42.2 |

1.2 Emission Spectroscopy

The visible and UV chemiluminescence of the excited radicals CH(A²Δ) denoted CH*, and OH(A²Σ+) denoted OH*, were measured by Optical Emission Spectroscopy (OES). The objective of these measurements is to determine the relative mole fractions of CH* and OH* emissions of MD flames with respect to those of methane flame. Thus, emission spectra were not quantitatively calibrated.

Two 500 – 6mm focal length UV lenses were used to focus the light emitted by the flame into the entrance slit of a spectrome-
TABLE 2. MASS FLOW RATES CORRESPONDING TO THE NINE CASES STUDIED (A-I), IN Kg/h.

<table>
<thead>
<tr>
<th>A-I MD Flames Conditions</th>
<th>Molar Mass flow rate / Air mass flow rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>φ</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>-</td>
</tr>
<tr>
<td>0.22</td>
<td>-</td>
</tr>
<tr>
<td>0.26</td>
<td>0.0070 / 0.307</td>
</tr>
<tr>
<td>0.28</td>
<td>0.0082 / 0.359</td>
</tr>
<tr>
<td>0.31</td>
<td>0.0099 / 0.437</td>
</tr>
</tbody>
</table>

As the MD flames are very lean, the emission is very low, then a compensation on the slit opening was made, always taking care of having a reasonable spectral resolution. So, for CH* and OH*, a slit width of respectively 750 µm and 500 µm were chosen, giving respectively a spectral resolution of 0.3 and 0.27 nm. The exposure time was kept constant to 100 ms. The CH* population was obtained by making an integration between 420 and 440 nm wavelength, while the OH* population was acquired between 300 and 320 nm wavelength.

For the CH* and OH* mole fractions in both flames, an average over 50 images was made. The uncertainty of the measurement was estimated from the CH* and OH* maximum mole fractions in the 50 images, in comparison to the average values. For the methane flame it was ±20% and for MD flames it was ±25%.

1.3 Visualization

Images of CH* and OH* emission have been recorded using a 512 × 512 pixels ICCD camera (Princeton Instruments) equipped with UV-lens (Nikkor 105 mm focal length).

Narrow-band interference filters were interposed along the optical path for capturing the CH* and OH* emission. The filter used for CH* has 60% transmission and a 10 – nm wide bandpass centered around 430 nm. The OH* filter is centered at 313 nm, 10 – nm bandpass and 68% transmission in the maximum.

As these results are complementary to the spectroscopy measurements, the exposure time was fixed to 100 ms and an average over 50 images was made.

Figure 1A presents a typical MD flame front obtained from CH* visualization. This figure shows that the flame front is slightly convex. The line of sight creates an integrated signal along its trajectory and increases the measured mole fraction. As the flame front is axi-symmetrical, Abel inversion is used to eliminate the effects of the integration and get the trace of the flame front in the symmetry plane of the burner as done in [11,16] (Fig. 1B). It should be noted that the Abel inversion has shifted slightly the location of the maximum CH* emission intensity.

The resolution of the CCD camera and the depth of field (about the flame length) limit the accuracy of the vertical positioning along the flame axis to ±0.2 mm. Then, due to the slight flames oscillation, the flame position was estimated with an accuracy of ±0.5 mm.

1.4 OH PLIF

Figure 3 presents the experimental setup used to realize OH PLIF measurements. The laser sheet dimension was about 30 ×
The kinetic modeling for methyl decanoate (MD) oxidation in the counterflow spray flame was performed using the SPRAY-COUNTERFLOW code of the REGATH package with detailed

The spatial resolution obtained by the optical arrangements was 120 µm. Considering the flames central axis and in order to determine the OH profiles from the images, the intensity values are summed up over each horizontal line (100 pixels or 12 mm), and the results will be represented as a function of the axial position.

1.5 Temperature measurements

We have determined the temperature along the axis with a commercial thermocouple Pt-30%Rh/Pt-6%Rh type B of 200 µm of wire diameter (Omega P30R-008) for MD Flames G, H and I only. This thermocouple supports temperatures up to 2100 K.

The temperature profiles were obtained by taking into account the perturbations produced by the thermocouple. Indeed, the flame attachment to the thermocouple can be minimized by introducing carefully the thermocouple in the flame. However, there was an attachment of the methane flame front, due to flame stabilization much like that on a bunsen flame, so this part of the profiles is not very accurate, however the rest is still comparable with the numerical results. The measured temperatures were corrected for radiation losses [18].

The temperature uncertainty in fresh gases is ±5 K, and close to the combustion zones is ±60 K. We have made the temperature profile measurements in the burner axial direction, using steps of 100 µm in the flame front.

2 NUMERICAL SIMULATION CONDITIONS

We consider an axisymmetric counterflow configuration shown in Fig. 4. A methane-air mixture is injected from the right side whereas mono-disperse spray MD fuel and air are injected from the left side. The gaseous and spray flow are described by the balance equations given in [6, 19]. The mass vaporization rate of a single droplet and the heat transferred from the gas to each droplet are modeled by the expression for a spherically symmetric single-component droplet obtained from the film temperature model [20].

In order to carry the simulations, liquid and gaseous boundary conditions are needed (see Table 3). The upper stream (MD/air) is at an initial temperature of 400 K. The droplet velocity matches the gas velocity at the injector exit. The initial droplet diameter is $D_0 = 30 \, \mu m$ and the droplet number density is $n_l = 820$ droplets per cm$^3$. The liquid fuel properties used for the simulations are: specific mass $\rho_f = 871 \, Kg/m^3$, latent heat of evaporation $L = 289.9 kJ/kg$, boiling temperature $T_{boil} = 497 K$ and the constant pressure heat capacity $c_{pl} = 2.05 kJ/(kg K)$ [21, 22].

The temperature profiles were corrected with the laser sheet energy profile fluctuations. An average over 100 OH PLIF images was done, taking into account the slight flames oscillation. As the LIF images were not corrected for quenching, the thermal distribution among energy levels, and saturation effects, the color scale in the resulting images represents pure fluorescence intensity, and does not directly correspond to OH mole fraction. Nevertheless, it was shown that quenching effects on the OH PLIF signals is constant along a counterflow flame [17]. For this reason, it may be considered that the OH LIF signals in our experiments are within a calibration constant linearly proportional to the OH mole fraction.

The OH radical is excited with a dye laser CONTINUUM (Rhodamine 590) pumped by a Nd: YAG laser CONTINUUM doubled (800 mJ @ 532 nm). The $Q_1(6)$ OH transition of the $Q''=0, Q'=1$ band of the ($A^2\Sigma, X^2\Pi$) system was excited at 283.043 nm with an energy of about 1 mJ.

The fluorescence images were collected on the same camera used for the visualization ($512 \times 512$ pixels ICCD). In this case, the camera gate was kept constant to 20 ns. This allows the CCD to drastically reduce the chemiluminescence signals. Furthermore, the same filter used for the OH$^*$ visualization was chosen to collect the OH fluorescence signal.

Measurements have been performed in linear regime of fluorescence, for this reason, an estimation of the laser sheet energy was carried out by directing the laser beam to a quartz cell, filled with dodecane, and then visualizing the fluorescence signal with the same ICCD camera. The images were then divided by the recorded laser intensity profiles to compensate for the laser profile fluctuations.

The OH profiles were corrected with the laser sheet energy profile on a single shot basis. An average over 100 OH PLIF images was done, taking into account the slight flames oscillation. As the LIF images were not corrected for quenching, the thermal distribution among energy levels, and saturation effects, the color scale in the resulting images represents pure fluorescence intensity, and does not directly correspond to OH mole fraction. Nevertheless, it was shown that quenching effects on the OH PLIF signals is constant along a counterflow flame [17]. For this reason, it may be considered that the OH LIF signals in our experiments are within a calibration constant linearly proportional to the OH mole fraction.
The methyl decanoate (MD) skeletal mechanism due to [5] including 125 species and 713 reactions was chosen to carry the simulations. We have validated this mechanism for the thermochemical and transport properties developed at EM2C laboratory [23]. The initial droplet diameter is 30 \( \mu m \). In this figure \( z = 0 \) corresponds to the upper burner edge and \( z = 40 \) to the lower burner edge. The premixed methane/air flame front is located at about \( z = 20.2 \) mm. At this point, the gas temperature increases very rapidly from 300 K to 1600 K within 1 mm. The \( CH^* \) profile at this point passes through a maximum (1.5E-12 mole fraction) and its width at half maximum is 0.2 mm. The MD flame front is located at \( z = 11.8 \) mm. The maximum \( CH^* \) mole fraction is 2.53E-13 and its width at half maximum is 0.5 mm.

The stagnation point (axial velocity \( v = 0 \)) is located at \( z = 12.3 \) mm. The equivalence ratio of the MD/air flame is 0.26 and the corresponding flame speed is too small (about 5 cm s\(^{-1}\)), that is why the MD flame front is very close to the stagnation point. The ratio between the \( CH^* \) mole fraction (respectively \( OH^* \)) at the MD flame front to the \( CH^* \) mole fraction (respectively \( OH^* \)) at the methane flame front will be called \( R_{CH^*} \) (respectively \( R_{OH^*} \)). These ratios will be used to analyze the \( CH^* \) and \( OH^* \) submechanisms in Section 3.3. The value of \( R_{CH^*} \) for MD Flame A is 0.17.

The temperature variation at the MD side is essentially due to heat diffusion across the stagnation point. The heat released by the MD flame front has small influence at this region. The droplet diameter decreases progressively until \( z = 7 \) mm and then very rapidly vanishes at \( z = 8 \) mm. Consequently the MD mass fraction increases from 1.03E-02 to 2.13E-02 due to droplet evaporation and then diminishes very rapidly at \( z = 11 \) mm due to thermal dissociation. The droplet number density increases progressively from 820 to 854 droplets per cm\(^3\) due to the decrease of the flow velocity and then diminishes very rapidly at \( z = 8 \) mm.

### 3 RESULTS AND DISCUSSION

#### 3.1 Typical Flame Structure

Figure 5 (top) presents a typical spray flame structure. The boundary conditions correspond to the flame A (see Tab. 1). The initial droplet diameter is 30 \( \mu m \). In this figure \( z = 0 \) corresponds to the upper burner edge and \( z = 40 \) to the lower burner edge. The premixed methane/air flame front is located at about \( z = 20.2 \) mm. At this point, the gas temperature increases very rapidly from 300 K to 1600 K within 1 mm. The \( CH^* \) profile at this point passes through a maximum (1.5E-12 mole fraction) and its width at half maximum is 0.2 mm. The MD flame front is located at \( z = 11.8 \) mm. The maximum \( CH^* \) mole fraction is 2.53E-13 and its width at half maximum is 0.5 mm.

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#### 3.1.1 Gas and two phase simulations comparison

Figure 5 (bottom) gives a comparison between a gaseous and a two-phase (30 \( \mu m \) droplets diameter) simulation for Flame A. The MD mass fraction in the gaseous simulation has a constant

### TABLE 3. BOUNDARY CONDITIONS

<table>
<thead>
<tr>
<th></th>
<th>Upper ((z = 0))</th>
<th>Lower ((z = H))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas temperature</td>
<td>(T_g = T_g^{up})</td>
<td>(T_g = T_g^{low})</td>
</tr>
<tr>
<td>Species mass fractions</td>
<td>(Y_k = Y_k^{up})</td>
<td>(Y_k = Y_k^{low})</td>
</tr>
<tr>
<td>Gas axial velocity</td>
<td>(v_g = v_g^{up})</td>
<td>(v_g = v_g^{low})</td>
</tr>
<tr>
<td>Gas radial velocity</td>
<td>(u_g = 0)</td>
<td>(u_g = 0)</td>
</tr>
<tr>
<td>Droplet temperature</td>
<td>(T_l = T_l^{up})</td>
<td>NA</td>
</tr>
<tr>
<td>Spray axial velocity</td>
<td>(v_l = v_l^{up})</td>
<td>NA</td>
</tr>
<tr>
<td>Spray radial velocity</td>
<td>(u_l = 0)</td>
<td>NA</td>
</tr>
<tr>
<td>Droplet radius</td>
<td>(R_l = R_l^0)</td>
<td>NA</td>
</tr>
<tr>
<td>Droplet number density</td>
<td>(n_l = n_l^0)</td>
<td>NA</td>
</tr>
</tbody>
</table>

The literature data for different kinetics of formation, quenching and chemiluminescence of \( CH^* \) and \( OH^* \) in flames were recently summarized by [8], where the authors have given 6 submechanisms that account for the formation and destruction of the species \( CH^* \) and \( OH^* \). We have employed the different submechanisms to evaluate the results against our experimental data and the ones with the best agreement were selected. This point will be developed in details in Section 3.3.
value of 2.13E-02 up to 9 mm far from the upper injector, while as explained before in the two-phase simulation it increases from 1.03E-02 to 2.13E-02 due to droplet evaporation, it reaches a plateau, and then, they both decrease very rapidly at 11 mm from the upper injector, about 0.8 mm before the MD flame front. It is also shown that in the temperature profiles there is a very small difference in the zone between the upper burner and the MD Flame, because in the two-phase simulation the temperature decreases slightly due to the heat transfer to the droplets.

**FIGURE 5.** TYPICAL FLAME STRUCTURE - FLAME A: $D_l = 30\mu m$ (TOP), GAS AND TWO PHASE SIMULATION OF FLAME A (BOTTOM)

**FIGURE 6.** COMPARISON BETWEEN THE EXPERIMENTAL AND NUMERICAL OH PROFILE OF FLAME A AND TEMPERATURE PROFILE OF FLAME G

### 3.2 Experimental and Numerical Profiles of the Temperature and OH Radical

Figure 6 gives a comparison between experimental and numerical profiles of the OH radical (top) obtained by PLIF and the temperature (bottom) for the MD/air flames A and G, respectively.

As the OH measurements are only qualitative, the experimental profiles were normalized by the maximum values of this radical, corresponding to the methane/air flame.

The position of the increase in the OH mole fraction due to the MD and methane flames are well predicted by the simulation. Furthermore, the relative OH mole fraction of the MD/air flame, compared to that of methane/air flame, is well predicted by the
simulation. Moreover, in the hot zone between flame fronts, OH is underestimated by the simulation. This may also be due to the experimental poorer spatial resolution.

3.3 Experimental and Numerical Profiles of $CH^*$ and $OH^*$ Radicals

Figure 7 gives a comparison between experimental and numerical mole fraction profiles of $CH^*$ (top) and $OH^*$ (bottom) radicals for the MD/air flame A.

As the measurements do not give absolute values, in order to make comparisons with the numerical results, the experimental profiles of $CH^*$ and $OH^*$ were normalized by their maximum values, corresponding to the methane/air flame front. Also, it was chosen to present the curves of $OH^*$ in logarithmic scale, because the maximum peak mole fraction of MD/air flames is considerably lower than that of the methane/air flame.

Among the 6 studied submechanisms describing the production, quenching and chemiluminescence of $CH^*$ and $OH^*$ [8], the one suggested by Elsamra et al. [9], who studied the temperature dependence of reaction $C_2H + O_2 \rightleftharpoons CO_2 + CH^*$ using pulsed laser photolysis techniques, gives the best prediction of $R_{CH^*}$ ratio, which is equal to 0.17 in the case of the MD Flame A, to be compared to the experimental value ($R_{CH^*}^{exp}$ = 0.14). But the value of $R_{OH^*}$ obtained by this submechanism is equal to 0.0007, which is too small compared to the experimental value ($R_{OH^*}^{exp} = 0.01$). Using the submechanism of Smith et al. [10], who proposed a rate constant for $OH^*$ formation by measuring absolute concentrations of $OH^*$ in a flat premixed low-pressure methane-air flame, one obtains $R_{CH^*} = 0.25$ which is far from $R_{CH^*}^{exp} = 0.14$, and $R_{OH^*} = 0.0022$ which is closer to $R_{OH^*}^{exp} = 0.01$.

We should note that both submechanisms have the same elementary reactions and corresponding rate constants for quenching and chemiluminescence of $CH^*$ and $OH^*$. For $OH^*$ they are $OH^* + M \rightleftharpoons OH + M$ and $OH^* \Rightarrow OH + h\nu$, respectively, where $h$ is Planck constant and $\nu$ is the wavelength of chemiluminescent emission. The main difference between the two submechanisms concerns the $CH^*$ (Reaction 2) and $OH^*$ (Reaction 4) formation reactions (see Tab. 4).

We have studied in this work a submechanism containing the $CH^*$ reactions and rate constants of Elsamra et al. [9], and the $OH^*$ reactions and rate constants of Smith et al. [10]. In this case, the methane flame $OH^*$ absolute mole fraction remains constant, while $R_{OH^*} = 0.0014$. This decrease of $R_{OH^*}$ is due to a competition between $CH^*$ and $OH^*$ formation reactions. Considering the $OH^*$ profile comparison in Fig. 7 (bottom), the relative maximum $OH^*$ mole fraction is not very well predicted. Numerically, the $OH^*$ local maximum mole fraction for Flame A are 1.30E-14 and 9.52E-12 for MD and methane flames, respectively. Concerning $CH^*$ mole fraction, the MD and methane flames $CH^*$ absolute mole fraction are doubled, but $R_{CH^*}^{exp}$ remains unchanged (0.17). Considering the very small mole fractions of the measured species (2.53E-13 and 1.5E-12 for MD and methane flames, respectively) and the uncertainties in the chemical excitation modeling, the predictions quality with the skeletal MD kinetic model is very good.

As we can see in Fig. 7, the numerical predictions of $CH^*$
and OH* mole fractions are very similar to the experimental profiles along the axis. The positions of the peaks match almost perfectly. The experimental profiles are slightly thicker than the simulated ones, however this can be explained by the poorer spatial resolution in the experiments.

The agreement is notable when comparing $R_{CH^*}$ and $R_{CH^*}^{exp}$, considering that the production of CH* is inherently sensitive to the predicted mole fraction of species $C_2H$ through reactions (R1) and (R2) (see Table 2), which are responsible for about 5% and 95% respectively of the CH* formation in MD flames. Therefore, reaction (R2) clearly dominates reaction (R1) under these MD flame conditions of equivalence ratio and strain rate. Then, as it was mentioned before, it must be noted that there is a competition between CH* and OH* formation reactions, which gives still more uncertainty to the CH* chemical excitation modelling.

In reaction (R3) it is shown that the formation of OH* is inherently sensitive to the predicted mole fraction of species CH. Therefore, the relative CH mole fraction at MD flame front with respect to that of methane flame front is only 0.1%, which is due to the very small production of the precursors of CH in MD flames. This might be the reason of the underestimation of the OH* mole fraction. By contrast, in the combustion of n-alkane fuels, the CH precursors are produced in large quantities. This reaction accounts however for about 33% of the OH* formation in MD Flame A.

Another chemical reaction leading to the formation of OH* radical is the one presented in reaction (R4), which accounts for about 57% of the OH* formation in MD Flame A. The remainder 10% comes from reverse quenching Reaction $OH^* + M = OH + M$, where OH* radical is formed by thermal excitation within the flame. However, there might be other reactions that could be very important in the OH* formation path in MD flames, and that would be in part responsible for the considerable difference between the numerical and experimental results (even if the absolute values are very small).

### 3.3.1 Influence of Strain Rate $\varepsilon$

Experimental and numerical CH* mole fraction profiles of flames A, B and I (constant $\phi$) are presented in Fig. 7 top, Fig. 8 top, and Fig. 8 bottom respectively. $\varepsilon$ increases by increasing the MD/air injection velocity while methane/air velocity remains constant (see Tab. 1). The MD flame fronts are very close to the stagnation plane, because of the very low flame velocity due to the very low equivalence ratio. The numerical positions of the flame fronts are coherent with the experimental results. In this situation by increasing $\varepsilon$ the methane flame front is slightly displaced towards the lower burner and the distance between simulation peak and experimental peak slightly increases. But as the MD flame front is very close to the stagnation point, species maximum values are slightly modified by strain rate.

### 3.3.2 Influence of Equivalence Ratio $\phi$

Experimental and numerical CH* mole fraction profiles of flames B, E and H (constant $\varepsilon$) are presented in Fig. 8 top, Fig. 9 top, and Fig. 9 bottom respectively. The MD and methane flames positions are very well predicted for all cases. As the MD equivalence ratio does not vary much, the MD flames position does not either.

### 4 CONCLUSION

This work presents an experimental and numerical study of methyl decanoate combustion. We have studied MD flames CH* and OH* emission profiles, as well as temperature and OH species profiles.

The first step of this work was to design a setup that permits to study the behavior of such flames. For that, a counterflow configuration was chosen with, on the lower part of the burner, stabilization of a lean premixed flame of methane and air, and on the upper part, stabilization of MD spray and air flame. Measurements of CH* and OH* emissions, OH LIF and temperature profiles have been realized for several MD equivalence ratio and strain rate conditions.

A convenient way to experimentally study the flame behavior is to analyze space and time resolved emission of CH* and

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**TABLE 4. CH* AND OH* FORMATION REACTIONS**

<table>
<thead>
<tr>
<th>#</th>
<th>Reactions</th>
<th>Elsamra et al. [9]</th>
<th>Smith et al. [10]</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>$C_2H + O \leftrightarrow CO + CH^*$</td>
<td>$6.02 \times 10^{12}$</td>
<td>$6.2 \times 10^{12}$</td>
</tr>
<tr>
<td>R2</td>
<td>$C_2H + O_2 \Rightarrow CO_2 + CH^*$</td>
<td>$6.02 \times 10^{-04}$</td>
<td>$4.1 \times 10^{13}$</td>
</tr>
<tr>
<td>R3</td>
<td>$CH + O_2 \leftrightarrow CO + OH^*$</td>
<td>$6.0 \times 10^{10}$</td>
<td>$6.0 \times 10^{10}$</td>
</tr>
<tr>
<td>R4</td>
<td>$O + H + M \leftrightarrow OH^* + M$</td>
<td>-</td>
<td>$3.63 \times 10^{13}$</td>
</tr>
</tbody>
</table>

Reaction rate coefficients given in the form $k = AT^n \exp(-E/RT)$. Units are mol cm s$^{-1}$.
FIGURE 8. COMPARISON OF THE CH* EXPERIMENTAL AND NUMERICAL PROFILES FOR DIFFERENT STRAIN RATES: FLAMES B ($\phi = 0.26, \varepsilon = 45.1 s^{-1}$) AND I ($\phi = 0.26, \varepsilon = 49.2 s^{-1}$). THE EXPERIMENTAL PROFILES ARE NORMALIZED.

FIGURE 9. COMPARISON OF THE CH* EXPERIMENTAL AND NUMERICAL PROFILES FOR DIFFERENT EQUIVALENCE RATIO: FLAMES E ($\phi = 0.28, \varepsilon = 45.1 s^{-1}$) AND H ($\phi = 0.31, \varepsilon = 45.1 s^{-1}$). THE EXPERIMENTAL PROFILES ARE NORMALIZED.

In the chosen reduced MD kinetic scheme consisting of 125 species and 713 elementary reactions [5], CH* and OH* are not taken into account, and comparison with experimental data are consequently not done. For this reason, CH* and OH* reactions were added to the reduced MD kinetic scheme.

By comparing experimental and numerical OH and temperature profiles, we have verified that the counterflow burner permits to reproduce similar combustion as the one simulated with the chosen reduced mechanism.

Concerning the CH* profile comparison, the predictions quality with the skeletal MD kinetic model is very good. In particular, the relative value of the local maximum $\text{CH}^*$ mole fraction at the MD flame front with respect to that of methane flame front ($R_{\text{CH}^*}$) is very well predicted.

Considering the OH* profile comparison, the relative maximum OH* mole fraction ($R_{\text{OH}^*}$) is not very well predicted. A competition exists between OH* and CH* formation reactions for these MD flames conditions of strain rate and equivalence ratio. Reaction (R3) shows that the formation of OH* is inherently sensitive to the predicted mole fraction of species CH. Therefore, the relative CH mole fraction at MD flame front with respect to that of methane flame front is only 0.1%, which is due to the very little production of the precursors of CH in MD flames. This might be the reason of the underestimation of the OH* mole fraction at the MD flame front with respect to that of methane flame front ($R_{\text{CH}^*}$) is very well predicted.
fraction. By contrast, in the combustion of n-alkane fuels, the CH precursors are produced in large quantities. Reaction (R4) is also important in the OH\(^*\) formation in MD flames, while the remainder percentage comes from reverse quenching Reaction \(\textit{OH}^* + M \rightarrow \textit{OH} + M\). However, there might be other reactions that could be very important in the \(\textit{OH}^*\) formation path in MD flames, and that would be in part responsible for the considerable difference between the numerical and experimental results.

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