Large Eddy Simulations of n-heptane and n-dodecane Binary Blends in Swirling Multi-Component Spray Flames

Nikola Sekularac\textsuperscript{a,*}, Thomas Lesaffre\textsuperscript{a}, Davide Laera\textsuperscript{a,b}, Laurent Gicquel\textsuperscript{a}

\textsuperscript{a}CERFACS, 42 Avenue Gaspard Coriolis, 31057, Toulouse, France
\textsuperscript{b}Department of Mechanics, Mathematics and Management, Polytechnic University of Bari, Via Orabona 4, Bari 70125, Italy

Abstract

Well-understanding and mastering Sustainable Aviation Fuels (SAF) mixture composition as well as the potential of their initial component concentrations’ impact on flames is clearly of critical importance in today’s effort and energy transition. In this study, the focus lies on conducting Large Eddy Simulations (LES) to comprehend the impact of species concentration changes in well-controlled multi-component fuel blends on flame structures. The SICCA-spray rig from the EM2C laboratory operated with three blends of n-dodecane and n-heptane in varying proportions, is specifically addressed and investigated in light of the available data. To conduct these simulations, the dynamically thickened flame model and an evaporation multi-component sub-model are coupled with a reduced chemistry mechanism for n-heptane and n-dodecane binary blends. Across all investigated blends, the simulated swirling spray flame predictions align well with the experimental measurements confirming the suitability of the proposed modeling. For this configuration, the alterations in species concentration do not appear to significantly impact the overall flame structures and characteristics when observed from an average perspective. However, localized differences are identified, revealing notable composition effects. The simulation outcomes indicate that the early consumption of n-heptane contributes to stabilizing the flame, whereas the vaporization of n-dodecane is the primary factor responsible for combustion occurring further downstream. These effects are closely tied to the evaporation properties of each fuel compound and their concentration proportions within the blend, as expected. This insight highlights the intricate relationship between fuel properties, their concentrations within blends, and the resulting combustion behavior, shedding light on the complexities of multi-component fuel combustion characteristics.

Keywords: Multi-phase LES; Swirl-spray flame; Multi-component fuel; Thickened flame model
1) Novelty and Significance Statement

The novelty of this research relies on using Large Eddy Simulations (LES) to assess the impact of species concentration changes in three well-controlled multi-component fuel blends on swirling spray flames. It is significant considering that literature about the latter is still limited, in particular within a numerical framework and with associated and dedicated experimental measurements. To the best of the authors’ knowledge, this is one of the few quantitative and numerical studies in open literature adopting three binary blends of n-heptane and n-dodecane, and their corresponding experimental measurements as benchmarks.

2) Author Contributions

- NS: Conceptualization, Investigation, Methodology, Formal analysis, Data curation, Writing – original draft, Writing – review & editing.
- TL: Conceptualization, Methodology, Writing – review & editing.
- DL: Conceptualization, Methodology, Investigation, Writing – review & editing, Supervision.
- LG: Conceptualization, Methodology, Investigation, Writing – review & editing, Supervision, Funding acquisition.

3) Authors’ Preference and Justification for Mode of Presentation at the Symposium

The authors prefer OPP presentation at the Symposium, for the following reasons:

- Presenting to the community a numerical methodology that can be extended to alternative fuels such as SAF.
- The paper focuses on using LES to model three well-controlled multi-component fuel blends. Their associated experimental measurements are used for validation purposes.
- Raising the community’s awareness about the effects of initial species concentration changes on swirl-spray flame structures and/or characteristics.
- The background and theory of multi-component fuel blends in swirl-spray flames can be quickly understood such that the results can be rapidly presented to the audience.
1. Introduction

Alternative fuels have gained considerable attention over the past few years in the aviation de- carbonization road-map by replacing conventional fossil fuels [1]. Among many others, Sustainable Aviation Fuels (SAF) refer to renewable hydrocarbons obtained from a variety of sustainable source materials whose properties match the standard aviation fuels [2]. They have been identified as a viable short-term solution due to their ability to be blended with standard fossil fuels or be used directly in current gas turbine engines, earning them the designation of “drop-in” fuels.

Like typical transportation fuels, SAF are mixtures of several hundreds of compounds belonging to different hydrocarbon classes, each with their own combustion and vaporization characteristics [3]. As such, one can suppose that a first step towards a successful transition relies on gaining a better understanding (experimentally and numerically) of how these multi-component blends influence the combustion process. Dedicated numerical simulations of swirled multi-component spray flames are however still limited due to the difficulty of implementing adequate and validated models. As a consequence, a common approach used within the numerical community consists of adopting a single-component fuel surrogate having chemical properties close to the desired blend [4]. While this approach is arguably accepted and efficient, the difference in volatility and reactivity of the various species in real fuel blends is not explicitly accounted for. This has often led to the use of two classes of multi-component models, the Continuous Multi-Component (CMC) model or the Discrete Multi-Component (DMC) model, for which more information can be found in [4, 5]. Mohd Yasin et al. [6] compared both approach performances in a numerical study involving swirl-stabilized flames of diesel and bio-diesel. Overall, DMC was found to better perform against experimental data, particularly in predicting a longer spray penetration length compared to CMC. Recently, Shastry et al. [7] performed LES of a liquid-fueled gas turbine combustor using the same DMC formalism. The two commercial aviation fuels used were modeled each by a three-component formulation. The predicted results were in good agreement with the set of experimental measurements, where each component’s evaporation process on the spray flame structure was captured/identified. Both of these studies show the importance of considering multi-component models to account for the effects of spray formation and evaporation of practical fuels on the flame characteristics.

However, and to the best of the authors’ knowledge, less attention has so far been devoted to numerical simulations studying the effect of the blend initial species concentration changes on swirl-spray flames, in particular with associated and dedicated experimental measurements.

In view of that, this study proposes to investigate the influence of concentration changes in multi-component fuel blends using LES. To that purpose, the recent experimental measurements [8] of three swirling spray flames with different proportions of n-heptane and n-dodecane were used as benchmarks. First, the experimental rig and the computational setup used within this study are presented before discussing the results, from which physical insights are provided based on the predictions.

2. Numerical setup and modeling

The SICCA-spray experimental rig [8] illustrated in Fig. 1 comprises a plenum feeding an air mass flow rate of \( \dot{m}_{\text{air}} = 2.33 \text{ g/s} \) into a cylindrical combustion chamber equipped with a quartz tube via a radial swirler. Note that the swirler configuration retained here is referred to as S727 in [9]. The chamber’s wall length is fixed at \( l_w = 100 \text{ mm} \) to prevent possible unstable sustained oscillations.

The fuel injector system consists of a typical hollow-cone-shaped atomizer positioned centrally in the swirler body with \( \dot{m}_f = 0.15 \text{ g/s} \). The operating conditions prescribe a global equivalence ratio of \( \phi_{\text{global}} = 1.0 \). Three n-heptane/n-dodecane blends were investigated within the test campaign performed at the EM2C laboratory [8] with increasing proportions of n-heptane, summarized in Table 1. Further information on the measurement techniques, the experimental setup and the burner’s characteristics can be found in [10].
The numerical domain, Fig. 1, and the modeling techniques employed are similar to those utilized in prior research detailed in [10, 12]. Only essential elements are summarized below, with a focus on the modifications and improvements made for the specific multi-component spray investigated here.

2.1. Gaseous phase

The simulations have been conducted using the 3-D fully compressible reactive flow solver AVBP (http://cerfacs.fr/avbp7x/) developed by CERFACS. A second-order Lax-Wendroff convective scheme is used in conjunction with an explicit Runge-Kutta time stepping. The WALE [13] model is employed for turbulent subgrid-scale closure. The Navier-Stokes Characteristic Boundary Condition (NSCBC) treatments [14] are adopted at the inlet by imposing the Characteristic Boundary Condition (NSCBC) treatment. The Navier-Stokes stepping. The W ALE [13] model is employed for use in conjunction with an explicit Runge-Kutta time

The domain is discretized using an unstructured mesh composed of ~ 32 million tetrahedral elements illustrated in Fig. 2. A refined region of Δx = 0.1 mm is fixed in the swirler and the flame root while Δx = 0.2 – 0.3 mm is enforced further downstream the injector’s exit.

The numerical domain showing the SICCA-spray and the atmosphere in the mid-plane. The zoom window shows by means of orange (top) and green (bottom) solid lines the film and slip boundary conditions used for the spray, respectively. Adapted from [12].

The resulting ARC scheme consists of 30 transported species, 17 quasi-steady-state (QSS) species, and 597 irreversible reactions. More information on the reduced chemistry scheme can be found in the supplementary material. Figure 3 compares the Laminar Burning Velocity (LBV) profiles obtained with the ARC chemistry against various experimental data for both n-heptane/n-dodecane neat fuels and blends.

![Fig. 3: Comparison of laminar burning velocities obtained with the ARC mechanism (solid lines) at 400 K and 1 bar for (a) n-heptane/air against experiments (markers) [17, 18] and detailed chemical kinetics simulations (dash-dotted line) [16] – for (b) n-dodecane/air against experiments (markers) [19, 20] and detailed chemical kinetics simulations (dash-dotted line) [16] – for (c) three n-dodecane/n-heptane blends against detailed chemical kinetics simulations (markers) [16].](image)

To the best of the authors’ knowledge, burning velocities have not been studied yet for n-heptane/n-dodecane blends. Regardless of the blend investi-
gated (neat or multi-component), the ARC LBV results are in reasonable agreement with the experimental data and chemical kinetics simulations across the full range of mixture conditions examined.

Turbulent combustion is accounted for using the dynamically thickened flame (TFLES) model coupled with the Charlette et al. efficiency function [21] to include subgrid-scale turbulent interactions. In terms of numerical treatment, the flame surface wrinkling parameter $\beta$ is fixed to 0.5 and the flame is thickened on 7 mesh points to accurately describe the premixed flame front. Considering that two-phase flows are susceptible to exhibiting premixed and non-premixed flame structures, a Takeno index is used within the current study to prevent the thickening of reaction zones dominated by diffusion effects. Note that the study of multi-component fuels requires adapting the definition of the Takeno index initially developed for a single-step global reaction. As such, a Takeno index using both fuels and their corresponding pyrolysis products is adopted [22]. It should be noted that TFLES requires careful attention when dealing with multi-component fuels, in particular those involving different characteristics and/or properties (e.g., hydrogen and ammonia blends) as the local composition can alter the predicted burning velocities and flame thickness, promoting biased results in the thickened regions. However, and perhaps the most significant finding from the results shown in Fig. 3, all fuel blends (including neat) considered in this work yield very similar values of burning velocities for a given equivalence ratio condition, suggesting that composition variation effects are perhaps negligible within the proposed TFLES methodology.

2.2. Liquid phase

A Lagrangian point particle formalism is utilized to simulate the behavior of the liquid spray, distributing mass, momentum, and energy source terms from the liquid phase to the nearest nodes in the Eulerian gas phase. The number of parcels has been fixed to one, indicating that each numerical particle is considered to represent one physical droplet. Evaporation is modeled using the DMC model previously validated by Shastry et al. [7, 23]. This model expands upon the well-known Abramzon-Sirignano evaporation model [24] to handle multi-component fuels by addressing the phase change of each individual component. Droplets are injected at 300 K using the semi-empirical FIM-UR atomization model [25], where a droplet diameter distribution is fixed to correctly reproduce the spray velocity and diameter distribution downstream of the atomizer. An injection half-cone spray angle was fixed to 45° following the previous work conducted in [10, 12] where the impact of the angle on the spray and flame dynamics has been thoroughly studied. The droplets size is prescribed with a Rosin-Rammler probability density function (PDF) fitted from previous experimental measurements with a Sauter Mean Diameter (SMD) of 18 $\mu$m and a shape parameter of $q \approx 1.56$. Injected particles hit the inner surface of the swirler body where slip and film boundary conditions are applied, Fig. 2, elsewhere the elastic rebound formalism is employed. Note that secondary breakup and breakup atomization models have not been used differently from what was done in the study of Treleaven et al. [26] as the latter require to be extended and validated to multi-component liquid fuels, which will be tackled in future investigations.

3. Results and discussion

Within the framework of this study, the experimental data include the swirl number $S$, the pressure drop across the swirler $\Delta p$, the thermal power $P$, and OH* chemiluminescence images.

Table 2: Comparison between LES and experiments of some global quantities. $\Delta p$, $S$, and $P$ denote the pressure drop, the swirl number, and the thermal power, respectively.

<table>
<thead>
<tr>
<th>Experiment [8, 9]</th>
<th>LES</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta p$</td>
<td>5.7 kPa</td>
<td>5.1 kPa</td>
</tr>
<tr>
<td>$S$</td>
<td>0.74</td>
<td>0.8</td>
</tr>
<tr>
<td>$P$</td>
<td>6.9 kW</td>
<td>6.75 kW</td>
</tr>
</tbody>
</table>

Table 2 compares the LES predictions against the set of measurements mentioned above. It should be noted that neither velocity nor particle diameter distribution data are available within the current work.

Fig. 4: Comparison of time-averaged heat release rate [J m$^{-3}$ s$^{-1}$] with experimental OH* snapshots from [8].
Note that $P$-experiment in Table 2 is directly derived from the fuel mass flow rate whereas $P$-LES is calculated using the heat release rate integral. The comparison between experiments and LES results is undertaken by using time-averaged solutions spanning slightly over 40 ms of simulation, after having reached steady-state conditions. The swirl number $S$, the thermal power $P$, and the pressure drop $\Delta p$ seem to closely match the experimental trends with errors not exceeding 10% (the indicative threshold used as a guideline within this study). The comparison between LES and experiments is further extended by means of averaged heat release rates and OH$^*$ chemiluminescence images depicted in Fig. 4. The flame retains an overall slanted M-shape with thin side branches at the injector’s exit and two high-intensity lobes further downstream located at $z \approx 35$ mm.

Overall, the LES results are in good agreement with the set of experimental snapshots presented, in particular for the flame’s anchoring position, the angle of opening at the inlet and within the inner recirculation zone, as well as the positions of maximum heat release rate. Interestingly, and regardless of the framework selected (LES or experiments), $a$-priori no apparent differences can be identified between the three blends with very similar behaviors. This perhaps relates to the quasi-identical LBV profiles found between the three blends and the two neat fuels in Fig. 3. Regardless of the blend investigated, the simulation results seem to over-predict the penetration length of the inner evaporation zone which could be potentially attributed to the spray/atomization sub-model.

Figure 5 illustrates the averaged evaporation rate $\Gamma$ for each fuel compound (left $y$-axis) and the mean temperature (right $y$-axis) downstream the combustion chamber. The temperature is expressed in Kelvin. The blue and green oversized markers illustrate the mean position of evaporation of n-heptane and n-dodecane, respectively.

Fig. 6: Cross-sectional average of the mean evaporation rate $\Gamma$ for each fuel component (left $y$-axis) and the mean temperature (right $y$-axis) downstream the combustion chamber. The temperature is expressed in Kelvin. The blue and green oversized markers illustrate the mean position of evaporation of n-heptane and n-dodecane, respectively.
Regardless of the blend, it can be seen that n-heptane has a much steeper gradient than n-dodecane at the combustion chamber’s inlet with maximum values peaking around $z \approx 15$ mm before progressively decreasing further downstream. In comparison, the evaporation rate of n-dodecane is more sustained and marks further downstream of the injector’s exit with a decrease aligned with the maximum temperature rise location at $z \approx 35$ mm. Further downstream where temperature values reach $\sim 1800$ K, the cross-sectional average of $\Gamma_{n\text{-dodecane}}$ is for all three blends above n-heptane, coinciding with the results depicted previously in Fig. 5. To quantify this difference, the mean position of evaporation of each fuel is calculated as:

$$z_{\text{evap}, f} = \frac{\int_{z_i}^{z_f} \Gamma_f(z) dz}{\int_{z_i}^{z_f} \Gamma_f(z) dz}$$

(1)

with $z_i$ and $z_f$ being the lower and upper bounds of the axial distance integral, respectively. Both quantities are highlighted in Fig. 6 for each blend, where the mean position of evaporation of n-dodecane is found to be $\sim 8$ mm downstream of n-heptane. Overall, the presented results are in good agreement with both fuels’ evaporation characteristics. Consequently, due to changes in fuel concentrations within each blend, which in fine alter the evaporation process, the composition within each flame is expected to vary. Figure 7 illustrates the instantaneous equivalence ratio $\phi$ of all three blends with white solid lines corresponding to a lean iso-contour of $\phi = 0.8$. As the proportion of n-heptane increases (and conversely, the proportion of n-dodecane reduces), the lean zones seem to penetrate less downstream of the injector’s exit. Due to higher proportions of n-dodecane in Blend A, the lean regions propagate further in the inner evaporation zone up until $z \approx 30$ mm, whereas the lean mixtures in Blend C stagnate around values of $z$ equal to $\sim 15$ mm. This is once again due to the different evaporation times of both neat fuels, coinciding with the trends depicted previously.

It should be noted that the averaged evaporation...
rate of n-heptane in Fig. 6 is higher than n-dodecane throughout the downstream positions for Blend B and C. Interestingly, this same behavior occurs as well for Blend A in the first 10–15 mm after the injector’s exit as depicted in Fig. 6a. In view of the above observations, one can suppose that the faster evaporation rates of n-heptane will promote an earlier consumption of n-heptane’s chemical source term in comparison to n-dodecane. Figure 8 shows this in a more detailed way by looking at the cross-sectional average consumption rates of the different fuel components and the mean heat release rate. In the case of n-heptane, consumption is found to be above the one of n-dodecane in the 10 – 15 mm downstream part of the combustion chamber’s inlet for all blends.

![Figure 9: Instantaneous fields of the flame index in the mid-plane for both fuels. The flame index is calculated as the product of the Takeno index and the absolute value of each fuel’s consumption rate. In the colorbar, P and NP denote respectively premixed and non-premixed flame structures.](image)

This behavior can potentially explain the steep rise of n-dodecane’s mean evaporation rate in this region as seen in Fig. 6a and where the heat release induced by n-heptane’s consumption enhances the evaporation of n-dodecane. This leads to believe that n-heptane is perhaps the dominant contributor in the flame’s anchoring and stabilization mechanisms along with swirl effects for this specific configuration. As expected, due to lower proportions of n-dodecane within Blend B and C, the consumption rate of the latter is reduced. Moreover, while both fuels’ mean consumption rates seem to peak at the same location, i.e. $z \approx 35$ mm, suggesting that both n-heptane and n-dodecane participate in the combustion process, further downstream (i.e. $z \geq 40$) n-dodecane’s consumption seems to control the flame. Similarly to Eq. 1, the mean position of consumption, $z_{cons}$, of both fuels is calculated and illustrated in Fig. 8.

While $z_{evap}$ is significantly smaller for n-heptane, $z_{cons}$ is still rather similar for the two fuels, where n-dodecane’s mean position of consumption peaks approximately 3 mm downstream of n-heptane. Indeed, the reactions seem to be activated at the same temperature level for both fuels (similar molecule type and reactivity) whereas this is not the case for the evaporation. The flame index of all three flames is illustrated in Fig. 9 by means of instantaneous snapshots. Throughout the three blends investigated, both fuels’ consumption rates burn mainly in a premixed manner, in particular with n-heptane where almost no diffusion reaction zones can be identified. This can be once again due to the evaporation properties of n-heptane allowing locally to improve mixture homogeneity with the surrounding air. Conversely, due to longer evaporation times, isolated n-dodecane droplets can be seen burning in a non-premixed fashion. This trend is particularly visible in Blend A. It is expected that n-dodecane droplets that have not evaporated yet can penetrate and pass through the premixed flame front before creating a small rich mixture surrounded by air and/or products, increasing locally unburnt hydrocarbon emissions. These trends coincide very well with the staged evaporation results depicted previously.

4. Conclusion

Within this study, Large Eddy Simulations are performed to understand how swirling spray flames are influenced by composition changes within multi-component fuel blends. To do that, the SICCA-spray experimental rig from the EM2C laboratory is used. Three n-heptane/n-dodecane blends were investigated with increasing proportions of n-heptane. The simulations were carried out using the AVBP solver in conjunction with a dynamically thickened flame model and an evaporation multi-component sub-model for the liquid phase. A new analytically reduced chemistry mechanism for n-heptane and n-dodecane binary blends is derived and validated by means of experimental data and chemical kinetics simulations of burning velocities. Regardless of the blend investigated, the predicted swirling spray flames are in good agreement with the set of experimental measurements available. It is found that species concentration changes do not seem to influence the characteristics of the studied flames from an averaged perspective. However, local differences were identified with non-negligible composition effects. The simulation results suggested that n-heptane’s earlier consump-
tion plays a stabilizing role within the three studied flames whereas n-dodecane’s decomposition is solely responsible for combustion occurring further downstream of the maximum heat release location. Ultimately, it is found that these effects are correlated to the evaporation properties of each fuel compound and their concentration proportions within a given blend. Nevertheless, it should be noted that the proposed numerical approach is subject to uncertainties attributed to the wall heat transfer effects in the combustion chamber and the liquid pre-heating in the swirler body that are an approximation of the real experimental setup. Both of these effects require additional analysis that can perhaps be tackled in conjunction with liquid fuel blend composition effects on combustion instabilities that are still limited in the literature to the authors’ knowledge. Finally, one can suppose that different blends’ proportions of fuels possessing radically different evaporation and flame speed properties/characteristics would perhaps make the flames’ structures more susceptible to composition changes.

Declaration of competing interest

The authors declare that co-author Laurent Gicquel is a colloquium co-chair.

Acknowledgments

The authors gratefully acknowledge the financial support from Agence Nationale de la Recherche (ANR) under the project FlySAFe (ANR-22-CE05-0022-01). Substantial thanks are given to the EM2C members, namely Prof. Candel, Dr. Durox, Dr. Renaud, Dr. Rajendram Soundararajan, and Ph.D. candidate Latour, for the high-quality measurements of the SICCA-spray flames and for making them available to the community.

Supplementary materials

A supplementary material is included to provide further details about the reduced chemistry mechanism used in this study.

References

[20] N. Rajesh, C. Prathap, Investigation on the laminar burning velocity and flame stability of premixed n-dodecane-air mixtures at elevated pressures and tem-


