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

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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

Information for Colloquium Chairs and Cochairs, Editors, and Reviewers

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 1. Introduction

Alternative fuels have gained considerable atten-2 tion over the past few years in the aviation decar-3 bonization road-map by replacing conventional fos-4 5 sil fuels [1]. Among many others, Sustainable Aviation Fuels (SAF) refer to renewable hydrocarbons 6 obtained from a variety of sustainable source materi-7 als whose properties match the standard aviation fuels 8 [2]. They have been identified as a viable short-term 9 solution due to their ability to be blended with stan-10 dard fossil fuels or be used directly in current gas tur-11 bine engines, earning them the designation of "drop-12 in" fuels. 13

14 Like typical transportation fuels, SAF are mixtures of several hundreds of compounds belonging to dif-15 ferent hydrocarbon classes, each with their own com-16 bustion and vaporization characteristics [3]. As such, 17 one can suppose that a first step towards a success-18 ful transition relies on gaining a better understanding 19 (experimentally and numerically) of how these multi-20 component blends influence the combustion process. 21 Dedicated numerical simulations of swirled multi-22 component spray flames are however still limited due 23 to the difficulty of implementing adequate and val-24 idated models. As a consequence, a common ap-25 proach used within the numerical community con-26 sists of adopting a single-component fuel surrogate 27 having chemical properties close to the desired blend 28 [4]. While this approach is arguably accepted and ef-29 ficient, the difference in volatility and reactivity of 30 the various species in real fuel blends is not explic-31 itly accounted for. This has often led to the use of 32 two classes of multi-component models, the Contin-33 uous Multi-Component (CMC) model or the Discrete 34 Multi-Component (DMC) model, for which more in-35 formation can be found in [4, 5]. Mohd Yasin et 36 al. [6] compared both approach performances in 37 a numerical study involving swirl-stabilized flames 38 of diesel and bio-diesel. Overall, DMC was found 39 to better perform against experimental data, particu-40 41 larly in predicting a longer spray penetration length compared to CMC. Recently, Shastry et al. [7] per-42 formed LES of a liquid-fueled gas turbine combustor 43 using the same DMC formalism. The two commer-44 cial aviation fuels used were modeled each by a three-45 46 component formulation. The predicted results were in good agreement with the set of experimental measure-47 ments, where each component's evaporation process 48 on the spray flame structure was captured/identified. 49 Both of these studies show the importance of consid-50 ering multi-component models to account for the ef-51 fects of spray formation and evaporation of practical 52 fuels on the flame characteristics. 53 However, and to the best of the authors' knowl-54

edge, 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 ex-

*Corresponding author *Email address*: sekularac@cerfacs.fr perimental measurements.

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In view of that, this study proposes to investigate the influence of concentration changes in multicomponent 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 are 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 $\dot{m}_{air} = 2.33$ 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 $l_c = 100$ mm to prevent possible unstable self-sustained oscillations.



Fig. 1: Schematic view of the SICCA-spray setup [8]. The dotted parts colored in yellow illustrate the LES domain. Taken from [10].

The fuel injector system consists of a typical hollow-cone-shaped atomizer positioned centrally in the swirler body with $\dot{m}_f = 0.15$ 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 [11].

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Table 1: Fuel blends mass fractions and (volume fractions) in percentage.

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Fuel	n-heptane	n-dodecane
Blend A	37 (50)	63 (50)
Blend B	64 (75)	36(25)
Blend C	80 (87)	20 (13)

1 The numerical domain, Fig. 1, and the modeling 2 techniques employed are similar to those utilized in

³ prior research detailed in [10, 12]. Only essential el-

⁴ ements are summarized below, with a focus on the

⁵ modifications and improvements made for the specific

6 multi-component spray investigated here.



Fig. 2: The meshed numerical domain showing the SICCAspray 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 domain is discretized using an unstructured mesh composed of ~ 32 million tetrahedral elements illustrated in Fig. 2. A refined region of $\Delta x = 0.1$ mm is fixed in the swirler and the flame root while $\Delta x = 0.2 - 0.3$ mm is enforced further downstream the injector's exit.

13 2.1. Gaseous phase

The simulations have been conducted using the 14 3-D fully compressible reactive flow solver AVBP 15 (http://cerfacs.fr/avbp7x/) developed by CERFACS. 16 A second-order Lax-Wendroff convective scheme is 17 used in conjunction with an explicit Runge-Kutta time 18 stepping. The WALE [13] model is employed for 19 turbulent subgrid-scale closure. The Navier-Stokes 20 Characteristic Boundary Condition (NSCBC) treat-21 ments [14] are adopted at the inlet by imposing the 22 air mass flow rate at 300 K, and at the outlet by fix-23 ing the pressure. Adiabatic non-slip walls are applied 24 across the domain except for the chamber backplane 25 and the combustion chamber quartz tube where heat 26 losses are taken into account [10]. Within the frame-27 work of this study, an Analytically Reduced Chem-28 istry (ARC) scheme for n-heptane and n-dodecane 29 binary blends was derived using the code ARCANE 30 [15]. To do so, the POLIMI chemical kinetics mech-31 anism [16] with high-temperature pathways consist-32 33 ing of 368 species and 14462 reactions was used. 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.



(c) n-dodecane/n-heptane 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 (dashdotted line) [16] – for (c) three n-dodecane,n-heptane/air blends against detailed chemical kinetics simulations (markers) [16].

To the best of the authors' knowledge, burning velocities have not been studied yet for n-heptane/ndodecane blends. Regardless of the blend investi-

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1 gated (neat or multi-component), the ARC LBV re-

2 sults are in reasonable agreement with the experimen-

3 tal data and chemical kinetics simulations across the

⁴ full range of mixture conditions examined.

Turbulent combustion is accounted for using the 5 dynamically thickened flame (TFLES) model coupled 6 with the Charlette et al. efficiency function [21] to in-7 clude subgrid-scale turbulent interactions. In terms of 8 numerical treatment, the flame surface wrinkling pa-9 rameter β is fixed to 0.5 and the flame is thickened 10 on 7 mesh points to accurately describe the premixed 11 flame front. Considering that two-phase flows are 12 13 susceptible to exhibiting premixed and non-premixed flame structures, a Takeno index is used within the 14 current study to prevent the thickening of reaction 15 zones dominated by diffusion effects. Note that the 16 study of multi-component fuels requires adapting the 17 definition of the Takeno index initially developed for 18 a single-step global reaction. As such, a Takeno in-19 dex using both fuels and their corresponding pyroly-20 sis products is adopted [22]. It should be noted that 21 22 TFLES requires careful attention when dealing with multi-component fuels, in particular those involving 23 different characteristics and/or properties (e.g., hy-24 drogen and ammonia blends) as the local composition 25 can alter the predicted burning velocities and flame 26 thickness, promoting biased results in the thickened 27 regions. However, and perhaps the most significant 28 finding from the results shown in Fig. 3, all fuel 29 blends (including neat) considered in this work yield 30 very similar values of burning velocities for a given 31 equivalence ratio condition, suggesting that composi-32 tion variation effects are perhaps negligible within the 33 proposed TFLES methodology. 34

35 2.2. Liquid phase

A Lagrangian point particle formalism is utilized 36 to simulate the behavior of the liquid spray, distribut-37 ing mass, momentum, and energy source terms from 38 the liquid phase to the nearest nodes in the Eulerian 39 gas phase. The number of parcels has been fixed to 40 one, indicating that each numerical particle is con-41 sidered to represent one physical droplet. Evapora-42 tion is modeled using the DMC model previously val-43 idated by Shastry et al. [7, 23]. This model expands 44 upon the well-known Abramzon-Sirignano evapora-45 tion model [24] to handle multi-component fuels by 46 47 addressing the phase change of each individual component. Droplets are injected at 300 K using the semi-48 empirical FIM-UR atomization model [25], where a 49 droplet diameter distribution is fixed to correctly re-50 produce the spray velocity and diameter distribution 51 downstream of the atomizer. An injection half-cone 52 spray angle was fixed to 45° following the previous 53 work conducted in [10, 12] where the impact of the 54 angle on the spray and flame dynamics has been thor-55 oughly studied. The droplets size is prescribed with 56 a Rosin-Rammler probability density function (PDF) 57 fitted from previous experimental measurements with 58 a Sauter Mean Diameter (SMD) of $18 \,\mu\text{m}$ and a shape 59 60 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

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Within the framework of this study, the experimental data include the swirl number S, the pressure drop across the swirler Δp , the thermal power P, and OH^{*} chemiluminescence images.

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

	· · · · · · · · · · · · · · · · · · ·	1 / 1	2
	Experiment [8, 9]	LES	Error
Δp	5.7 kPa	5.1 kPa	$\sim 10\%$
S	0.74	0.8	$\sim 8\%$
P	6.9 kW	6.75 kW	$\sim 2\%$

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.

Experimental

LES



Fig. 4: Comparison of time-averaged heat release rate $[J \cdot m^{-3} \cdot s^{-1}]$ with experimental OH* snapshots from [8].

Note that P-experiment in Table 2 is directly de-1 rived from the fuel mass flow rate whereas P-LES is 2 calculated using the heat release rate integral. The 3 comparison between experiments and LES results is 4 undertaken by using time-averaged solutions span-5 ning slightly over 40 ms of simulation, after having 6 reached steady-state conditions. The swirl number S, 7 8 the thermal power P, and the pressure drop Δp seem to closely match the experimental trends with errors 9 not exceeding 10% (the indicative threshold used as a 10 guideline within this study). The comparison between 11 LES and experiments is further extended by means of 12 13 averaged heat release rates and OH* chemiluminescence images depicted in Fig. 4. The flame retains 14 an overall slanted M-shape with thin side branches at 15 the injector's exit and two high-intensity lobes further 16 downstream located at $z \approx 35$ mm. 17



Fig. 5: Time-averaged field of the evaporation rate Γ [kg·m⁻³·s⁻¹] in the mid-plane for each fuel component.

Overall, the LES results are in good agreement 18 with the set of experimental snapshots presented, in 19 particular for the flame's anchoring position, the an-20 gle of opening at the inlet and within the inner recir-21 22 culation zone, as well as the positions of maximum heat release rate. Interestingly, and regardless of the 23 framework selected (LES or experiments), a-priori 24 no apparent differences can be identified between the 25 26 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.

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(c) Blend C

Fig. 6: Cross-sectional average of the mean evaporation rate $\overline{\Gamma}$ 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.

Figure 5 illustrates the averaged evaporation rate Γ of each fuel compound in the mid-plane. The gradual increase of n-heptane concentrations within Blend B and C is clearly visible in comparison to Blend A which contains a majority of n-dodecane (by mass fraction). More importantly and somewhat expected, staged vaporization is emphasized by the proportion changes, n-heptane being the first fuel to evaporate with a much narrower evaporation region compared to n-dodecane which appears later on. This trend is depicted in a more quantitative way in Fig. 6 where the cross-sectional average of $\overline{\Gamma}$ is plotted as a function of the axial distance from the chamber backplane. The mean temperature has also been added along the cross-sectional averaged plane for clarity purposes.

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Fig. 7: Instantaneous fields of the equivalence ratio ϕ in the mid-plane. The white (thin) and black (thick) solid lines illustrate the lean and stoichiometric equivalence ratio iso-contours corresponding to $\phi = 0.8$ and $\phi = 1.0$, respectively.

Regardless of the blend, it can be seen that n-heptane has a much steeper gradient than n-dodecane at the 2 combustion chamber's inlet with maximum values 3 peaking around $z \approx 15$ mm before progressively 4 decreasing further downstream. In comparison, the 5 evaporation rate of n-dodecane is more sustained and 6 marks further downstream of the injector's exit with a decrease aligned with the maximum temperature 8 rise location at $z \approx 35$ mm. Further downstream 9 where temperature values reach ~ 1800 K, the cross-10 sectional average of $\overline{\Gamma}_{n-dodecane}$ is for all three blends 11 above n-heptane, coinciding with the results depicted 12 previously in Fig. 5. To quantify this difference, the 13 mean position of evaporation of each fuel is calcu-14 lated as: 15

$$z_{evap,f} = \frac{\int_{z_i}^{z_f} \Gamma_f(z) z dz}{\int_{z_i}^{z_f} \overline{\Gamma}_f(z) dz}$$
(1)

with z_i and z_f being the lower and upper bounds of 16 the axial distance integral, respectively. Both quanti-17 ties are highlighted in Fig. 6 for each blend, where the 18 mean position of evaporation of n-dodecane is found 19 to be $\sim 8 \text{ mm}$ downstream of n-heptane. Overall, 20 the presented results are in good agreement with both 21 22 fuels' evaporation characteristics. Consequently, due to changes in fuel concentrations within each blend, 23 which in fine alter the evaporation process, the com-24 25 position within each flame is expected to vary. Figure 7 illustrates the instantaneous equivalence ratio ϕ of 26 all three blends with white solid lines corresponding 27 to a lean iso-contour of $\phi = 0.8$. As the proportion of 28 n-heptane increases (and conversely, the proportion of 29 n-dodecane reduces), the lean zones seem to penetrate 30 less downstream of the injector's exit. Due to higher 31 proportions of n-dodecane in Blend A, the lean re-32 gions propagate further in the inner evaporation zone 33 34 up until $z \approx 30$ mm, whereas the lean mixtures in Blend C stagnate around values of z equal to ~ 15 35 mm. This is once again due to the different evapo-36 ration times of both neat fuels, coinciding with the 37 38 trends depicted previously.



(c) Blend C

Fig. 8: Cross-sectional average of the mean consumption rate of each fuel component (left *y*-axis) and the mean heat release rate (right *y*-axis) downstream the combustion chamber. The heat release rate is expressed in $J \cdot m^{-3} \cdot s^{-1}$. The blue and green oversized markers illustrate the mean position of consumption of n-heptane and n-dodecane, respectively.

It should be noted that the averaged evaporation

rate of n-heptane in Fig. 6 is higher than n-dodecane 1 throughout the downstream positions for Blend B and 2 C. Interestingly, this same behavior occurs as well for 3 Blend A in the first 10-15 mm after the injector's exit as depicted in Fig. 6a. In view of the above observa-5 tions, one can suppose that the faster evaporation rates 6 7 of n-heptane will promote an earlier consumption of 8 n-heptane's chemical source term in comparison to ndodecane. Figure 8 shows this in a more detailed way 9 by looking at the cross-sectional average consumption 10 rates of the different fuel components and the mean 11 heat release rate. In the case of n-heptane, consump-12 13 tion is found to be above the one of n-dodecane in the 10 - 15 mm downstream part of the combustion 14 chamber's inlet for all blends. 15



Fig. 9: Instantaneous fields of the flame index in the midplane 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.

This behavior can potentially explain the steep rise 16 of n-dodecane's mean evaporation rate in this region 17 as seen in Fig. 6a and where the heat release induced 18 19 by n-heptane's consumption enhances the evaporation of n-dodecane. This leads to believe that n-heptane 20 is perhaps the dominant contributor in the flame's 21 anchoring and stabilization mechanisms along with 22 23 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 ndodecane participate in the combustion process, further downstream (i.e. $z \ge 40$) 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 ndodecane'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

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Within this study, Large Eddy Simulations are performed to understand how swirling spray flames are influenced by composition changes within multicomponent 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 1 flames whereas n-dodecane's decomposition is solely 2 responsible for combustion occurring further down-3 stream of the maximum heat release location. Ultimately, it is found that these effects are correlated to 5 the evaporation properties of each fuel compound and 6 their concentration proportions within a given blend. 7 Nevertheless, it should be noted that the proposed nu-8 merical approach is subject to uncertainties attributed 9 to the wall heat transfer effects in the combustion 10 chamber and the liquid pre-heating in the swirler body 11 that are an approximation of the real experimental 12 13 setup. Both of these effects require additional analysis that can perhaps be tackled in conjunction with 14 liquid fuel blend composition effects on combustion 15 instabilities that are still limited in the literature to 16 the authors' knowledge. Finally, one can suppose that 17 different blends' proportions of fuels possessing rad-18 19 ically different evaporation and flame speed properties/characteristics would perhaps make the flames' 20 structures more susceptible to composition changes. 21

22 Declaration of competing interest

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

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35 Supplementary materials

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

39 References

- [1] S. Blakey, L. Rye, C. W. Wilson, Aviation gas turbine
 alternative fuels: A review, Proceedings of the Com bustion Institute 33 (2) (2011) 2863–2885.
- [2] J. Heyne, B. Rauch, P. Le Clercq, M. Colket, Sustain able aviation fuel prescreening tools and procedures,
 Fuel 290 (2021) 120004.
- I. Zhou, W. Zhao, K. H. Luo, M. jia, H. Wei, M. Xie, Spray–turbulence–chemistry interactions under engine-like conditions, Progress in Energy and Combustion Science 86 (2021) 100939.
- Combustion Science 86 (2021) 100939.
 [4] G. Eckel, J. Grohmann, L. Cantu, N. Slavinskaya, T. Kathrotia, M. Rachner, P. Le Clercq, W. Meier, M. Aigner, LES of a swirl-stabilized kerosene spray flame with a multi-component vaporization model and detailed chemistry, Combustion and Flame 207 (2019)
- detailed chemistry, Combustion and Flame 207 (2019)
 134–152.

[5] J. Hinrichs, V. Shastry, M. Junk, Y. Hemberger, H. Pitsch, An experimental and computational study on multicomponent evaporation of diesel fuel droplets, Fuel 275 (2020) 117727.

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- [6] M. Mohd Yasin, R. Cant, C. Chong, S. Hochgreb, Discrete multicomponent model for biodiesel spray combustion simulation, Fuel 126 (2014) 44–54.
- [7] V. Shastry, E. Riber, L. Gicquel, B. Cuenot, V. Bodoc, Large Eddy Simulations of complex multicomponent swirling spray flames in a realistic gas turbine combustor, Proceedings of the Combustion Institute 39 (2) (2023) 2693–2702.
- [8] V. Latour, D. Durox, P. Rajendram Soundararajan, A. Renaud, S. Candel, Effects of Fuel Composition on Azimuthal Combustion Instabilities in an Annular Combustor Equipped With Spray Injectors, Proceedings of the ASME Turbo Expo 2023 Volume 3A: Combustion, Fuels, and Emissions (2023) V03AT04A023.
- [9] P. Rajendram Soundararajan, D. Durox, A. Renaud, S. Candel, Azimuthal Instabilities of an Annular Combustor With Different Swirling Injectors, Journal of Engineering for Gas Turbines and Power 144 (11) (2022) 111018.
- [10] E. Lo Schiavo, D. Laera, E. Riber, L. Gicquel, T. Poinsot, Effects of liquid fuel/wall interaction on thermoacoustic instabilities in swirling spray flames, Combustion and Flame 219 (2020) 86–101.
- [11] P. Rajendram Soundararajan, D. Durox, A. Renaud, G. Vignat, S. Candel, Swirler effects on combustion instabilities analyzed with measured FDFs, injector impedances and damping rates, Combustion and Flame 238 (2022) 111947.
- [12] E. Lo Schiavo, D. Laera, E. Riber, L. Gicquel, T. Poinsot, On the impact of fuel injection angle in euler-lagrange large eddy simulations of swirling spray flames exhibiting thermoacoustic instabilities, Combustion and Flame 227 (2021) 359–370.
- [13] F. Nicoud, F. Ducros, Subgrid-Scale Stress Modelling Based on the Square of the Velocity Gradient Tensor, Flow, Turbulence and Combustion 62 (1999) 183–200.
- [14] T. Poinsot, S. Lelef, Boundary conditions for direct simulations of compressible viscous flows, Journal of Computational Physics 101 (1) (1992) 104–129.
- [15] Q. Cazères, P. Pepiot, E. Riber, B. Cuenot, A fully automatic procedure for the analytical reduction of chemical kinetics mechanisms for Computational Fluid Dynamics applications, Fuel 303 (2021) 121247.
- [16] E. Ranzi, A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A. Kelley, C. Law, Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels, Progress in Energy and Combustion Science 38 (4) (2012) 468–501.
- [17] K. Kumar, J. E. Freeh, C. J. Sung, Y. Huang, Laminar Flame Speeds of Preheated iso-Octane/O2/N2 and n-Heptane/O2/N2 Mixtures, Journal of Propulsion and Power 23 (2) (2007) 428–436.
- [18] P. Dirrenberger, P. Glaude, R. Bounaceur, H. Le Gall, A. P. da Cruz, A. Konnov, F. Battin-Leclerc, Laminar burning velocity of gasolines with addition of ethanol, Fuel 115 (2014) 162–169.
- [19] K. Kumar, C.-J. Sung, Laminar flame speeds and extinction limits of preheated n-decane/O2/N2 and n-dodecane/O2/N2 mixtures, Combustion and Flame 151 (1) (2007) 209–224.
- [20] N. Rajesh, C. Prathap, Investigation on the laminar burning velocity and flame stability of premixed ndodecane-air mixtures at elevated pressures and tem-

- peratures, Fuel 318 (2022) 123347.
- [21] F. Charlette, C. Meneveau, D. Veynante, A power-law
 flame wrinkling model for LES of premixed turbulent
 combustion Part I: non-dynamic formulation and initial tests, Combustion and Flame 131 (1) (2002) 159–
 180.
- 7 [22] A. Felden, L. Esclapez, E. Riber, B. Cuenot, H. Wang,
 8 Including real fuel chemistry in LES of turbulent spray
 9 combustion, Combustion and Flame 193 (2018) 397–
 10 416.
- [23] V. Shastry, Q. Cazeres, B. Rochette, E. Riber,
 B. Cuenot, Numerical study of multicomponent spray
 flame propagation, Proceedings of the Combustion In stitute 38 (2) (2021) 3201–3211.
- [24] W. A. Sirignano, Fluid Dynamics and Transport of
 Droplets and Sprays, Cambridge University Press,
 17 1999.
- [25] M. Sanjosé, J. Senoner, F. Jaegle, B. Cuenot,
 S. Moreau, T. Poinsot, Fuel injection model for Euler-Euler and Euler-Lagrange large-eddy simulations
 of an evaporating spray inside an aeronautical combustor, International Journal of Multiphase Flow 37 (5)
 (2011) 514–529.
- 24 [26] N. C. W. Treleaven, D. Laera, J. Carmona, N. Odier,
- 25 Y. Gentil, J. Dombard, G. Daviller, L. Gicquel, T. Bringer, Complete of Combustion Simulation with
- T. Poinsot, Coupling of Combustion Simulation with
 Atomisation and Filming Models for LES in Swirled
- Atomisation and Filming Models for LES in Swiried
 Spray Flames, Flow Turbulence Combustion 109
 (2022) 759–789.