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AN EXPERIMENTAL AND MODELING STUDY OF LAMINAR FLAME SPEEDS OF ALTERNATIVE AVIATION FUELS

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ABSTRACT

The present work reports on measurements of burning velocities of synthetic fuel air mixtures exploiting the coneangle method, as part of the EU project ALFA-BIRD. The GtL (Gas-to-Liquid)-air mixtures - (i) 100% GtL and (ii) GtL+20% hexanol, respectively - were studied at atmospheric pressure, with values of the equivalence ratio φ ranging between $\varphi \sim$ 1.0 and $\varphi \sim 1.3$, at preheat temperatures $T_0 = 423$ K (GtL+20% hexanol) as well as $T_0 = 473$ K (for 100% GtL and GtL+20% hexanol). A comparison between experimentally obtained burning velocities and predicted values of laminar flame speed is presented, too. In general, good agreement was found between predicted and measured data for the range of conditions considered in the present study. The predictive capability of the detailed reaction model consisting of 3479 reactions involving 490 species will be discussed focusing on the laminar flame speed and the combustion of the components (n-decane, iso-octane, and 1-hexanol) of the surrogate used.

[Keywords: reaction model, synthetic jet fuel, flame speed, heat release, burner]

NOMENCLATURE

р	pressure
Т	temperature
Su	burning velocity
v	gas velocity

Greek letters

φ	equivalence ratio		
α	angle		
ρ	density		
Subscripts			

0	initial
u	unburned

INTRODUCTION

In the last decade, alternative and renewable energy resources became increasingly important for several reasons such as costs, greenhouse emissions, reduction of fuel import dependency, and security of supply. Sustainability in energy supplies requires new concepts as well as improvements in overall efficiency and fuel flexibility. Therefore, initiatives are ongoing to enable substitution of noble fuels (gas, crude oil) through, for example, long-term available coal, low-grade fuels (waste as well as by- and side- products), or biomass [1].

Presently, the largest part of worldwide electric power generation is by far based on fossil fuels [2]. For the transportation sector, similar activities are ongoing leading to the operation of cars with natural or biogas, ethanol or biodiesel, and to the development of fuel flexible and hybrid cars [3].

Recently, the European Commission agreed on proposals for a new energy policy for Europe. These included a renewable energy roadmap proposing, among other measures, a binding 20% target for the overall share of renewable energy by 2020. The aviation sector is also included in the EU policy package concerning renewable energy and CO₂-emissions (Emission Trading Scheme, ETS), although jet fuels constitute presently only about 6% of the global oil consumption and about 2% of the overall CO₂-emissions [4]. However, the air traffic is expected to increase further by about 5% per year, see[5].

As a consequence, to ensure sustainability in energy supplies, new concepts as well as improvements in overall efficiency and fuel flexibility are required. At present, on a worldwide scale, by far the largest part for transportation and aviation is based on fossil fuels. Thus, alternative fuels and renewable energy resources are expected to become more prominent in the future.

For the aviation sector, the only worldwide available jet fuel is nearly exclusively based on kerosene stemming from crude oil. However, synthetic liquid fuels obtained via various processes using a variety of feedstock could be used in the future, see[5]. Research activities on synthetic jet fuels have increased significantly over the last years [6-12]. Despite these activities, no detailed kinetic model is proposed for their combustion over a wide range of conditions, *i.e.*, covering both cool-flame and high-temperature oxidation regimes. The usefulness of existing kerosene combustion models to simulate the oxidation of synthetic jet fuels is not obvious, and must be investigated as the composition of synthetic jet fuels differs from that of conventional Jet A-1 (see [6]).

BACKGROUND

For these reasons, the commercial aviation sector is looking into alternative solutions, such as blends or full substitution to kerosene, with a priority given to renewable fuels [13-14]. However, using alternative fuels in aeronautics is a great challenge. Aircraft needs are much more specific and very strict, with more severe constraints (e.g. freezing point of the fuel, energy density etc.) than any other transport means [15]. Hence, a profound knowledge on jet fuels properties such as heat release or ignition delay time is inevitable, with respect to its technical specification. Also, a newly developed alternative aviation fuel must be compatible with Jet A-1 due to the long lifetime cycle of up to about 40 years ("drop-in fuel"). Hence, any synthetic jet fuel must be characterized and certified, with respect to physical and chemical properties, to ensure a safe and reliable operation for the whole flight envelope [15].

Alternative aviation fuels

Presently, a large number of feedstock, processes, and resulting products are discussed, see e.g. [7, 16].

The first alternative jet fuel having been approved for commercial aviation was CtL (Coal-to Liquid, developed by SASOL), see [6]. It was followed by a GtL fuel. Regarding BtL-fuels (biomass-to-liquid), potential feedstock can be biomass or biomass byproducts, waste, algae and yeast.

Synthetically manufactured fuels (*synthetic kerosenes* or *Fischer-Tropsch fuels*) are considered as the only alternative jet fuels. For the midterm range, synthetic paraffinic kerosenes (SPK) from FT process or hydro treatment blended in Jet A-1 seem to be the most promising alternative. In that case BtL, HRJ (hydrogenated renewable jet), or HEFA (hydroprocessed

esters and fatty acids) are the only ones to provide substantial progress regarding sustainability and emissions. Further alternative candidates to jet fuel could be new plant (or vegetable) oils or fatty acids, blended with kerosene.

Need for characterization of alternative aviation fuels

Any aviation fuel must be characterized and certified[15]. Hence, it is of utmost importance to expand our knowledge on renewable jet fuels not only with respect to the experimental characterization of the fuel properties but also with respect to modeling capabilities enabling predictive computational fluid dynamics simulations.

To best optimize synthetic jet fuel mixture applications in practical combustors, the combustion characteristics of these fuels must be well understood. One of the most important fundamental combustion characteristics of any fuel is the laminar flame speed, as a measure for describing the heat release, besides the ignition delay time. This knowledge enables to avoid conditions where self ignition or flashback may occur. These data must be known reliably over a wide range of parameters, such as temperature, pressure, fuel composition, and fuel-air ratio.

Till now, very limited data exist for synthetic jet fuels. Kerosene, as any practical fuel, e.g. natural gas, biogenic gas mixtures and syngases, and gasoline, is a complex mixture of numerous components, belonging to different chemical families; see e.g.[17-18]. This is true also for fuels which may serve as alternatives (as blends or full substitution) to kerosene.

However, for smaller hydrocarbons (methane [19], propene [20]), synthetic gas mixtures (methane/CO [21] and CO/H₂ [22]), higher hydrocarbons (*n*-decane [23]), kerosene [24-25], as well as small alcohols [26]), values of the laminar flame speed are reported in literature. These data are needed for validation of sub-models which are incorporated in detailed chemical kinetic mechanisms for describing the combustion of kerosene (from crude oil) and synthetic kerosenes as well.

SCOPE OF THE PRESENT WORK

The laminar flame speed has a direct impact on the flame length: depending on, the flame will stabilize at a certain height above the burner surface (HAB). If the laminar flame speed of an alternative fuel would differ from the one of kerosene (from crude oil), the heat load of the walls or the recirculation zone might change. Such findings might have some impact on the design of a burner and the burner chamber.

Therefore, in the present work, burning velocities S_u of two GtL-fuels – GtL and GtL+20% hexanol, their potential as possible alternative aviation fuels to be investigated within the EU-project ALFA-BIRD [16] – were determined at ambient pressure, for different fuel-air mixing ratios. For this purpose, an existing test rig [27] was modified and built up to allow the use of evaporated liquid fuels.

The experimental data were used to validate the predictive capability of a detailed reaction model, see e.g. [25] and references therein. Some aspects of the reaction model will be discussed, focusing on the laminar flame speed and on the combustion of the components of the used surrogate (*n*-decane, *iso*-octane, and *1*-hexanol).

It should be mentioned that the presented reaction model was – and will be further - developed with the ultimate goal to predict the combustion behaviour of different synthetic jet fuels – in particular CtL and GtL – for different parameters, focusing on the laminar flame speed and ignition delay time [28], species profiles including stable intermediates, aromates [29] and particles [30], as a joint initiative within ALFA-BIRD [16].

Thus, the reaction model will be validated for several parameters, such as temperature, pressure, time scale, and fuelair mixtures. Once a detailed reaction model will be established, then its reduction potential will be investigated. This is a necessary precondition for establishing numerical tools in order to verify a proper design of the burner and the combustion chamber already at early development stages.

METHODOLOGY

First, measurements of the burning velocities of synthetic fuel air mixtures exploiting the cone-angle method will be presented, for atmospheric pressure and different fuel-air mixtures, at high preheat temperatures.

Then, a detailed reaction model will be used to predict the measured laminar flame speed data. However, as discussed later, it is not possible to use a reaction model for all of the hundreds of different species a kerosene from crude-oil is composed of. Instead of, a surrogate was used: with *n*-decane and *iso*-octane for GtL, and with *I*-hexanol included for GtL+20% hexanol [16, 31]. To justify this choice of a surrogate, a detailed analysis of the used GtL fuel was conducted [32], to determine the chemical composition, see Fig. 1.

Note that – in order to use the same reaction model for all of the targets mentioned above - no attempt was made to modify the used reaction model, in order improve its predictive capability with respect to laminar flame speed data.



Fig. 1: The composition of a GtL [32], depicting the chemical families. i-P: iso-paraffins; n-P: n-paraffins; N: napthenes; DiN: di-naphthenes; MoAr: mono aromates; NmoAr: mono-aromates, with n-paraffins as side chain; DiAr: di-aromates.

INVESTIGATED FUEL MIXTURES

Two synthetic fuel mixtures were used for the experiments, a pure GtL fuel [33] and a fuel consisting of GtL+20% hexanol [34]. Some fundamental properties of the two GtL-mixtures coming from physical and chemical analysis [32] and of Jet A-1 such as density, elementary composition, flashpoint, viscosity, and heating value are given in Table 1.

Table 1. 1 Toperties of typical a viation rules			
Fuel	GtL	GtL+20%hex	Jet-A1
Property	[32]	[32]	[15]
Density /kgm ⁻³	738	754	775 - 840
@ 15°C			
C / % mass	85.8	82.5	> 99
H / % mass	14.8	14.1	
O/% mass	0.0	3.6	0.0
Flashpoint / °C	48.5	46.5	38 minimum
Heating value /	43242	42559	42800
/ kJ kg ⁻¹			(minimum)
Viscosity / cSto	0.8296	1.026	0.80 - 0.88
@ 40°C			@ 20°C

Table 1: Properties of typical aviation fuels

Table 2: Chemical sum formula for the experimentally
investigated fuel-air mixtures [16, 29]

Fuel	Formula	M/gmol ⁻¹	O ₂ /Fuel
Gas to Liquid (GtL)	$C_{9.81}H_{21.62}$	139.3	15.215
Gas to Liquid (GtL)	C _{8.76} H _{19.53} O _{0.275}	129.1	13.505
+ 20% hexanol			

Table 3: Experimentally studied fuel-air mixtures

Fuel	Fuel-air ratio	Preheat
		temperature / K
Gas to Liquid (GtL)	0.95 - 1.4	473
Gas to Liquid (GtL) +	0.95 - 1.4	473
20% hexanol		423
For comparison:		
Jet-A1 [35]	0.9 – 1.4	473

Fuel	Fuel-air	Preheat	
	ratio	temperature / K	
Gas to Liquid (GtL)	0.9 – 1.4	473	
Gas to Liquid (GtL) + 20%	0.9 – 1.4	473	
hexanol		423	
Neat components of surrogate:			
<i>iso</i> -octane	0.9 – 1.4	473	
<i>n</i> -decane	0.9 – 1.4	473	
1-hexanol	0.9 - 1.4	473	

The chemical composition of the used GtL fuel was determined by GC-MS analysis [32], see Table 2. For this purpose, a DB5-MS column (low bleeding) was used, with a length of 60 m and an internal diameter of 0.25 mm. Such a chromatogram can be considered as a finger print for a specific fuel mixture. A GtL typically does not contain any aromatics, in contrast to Jet A-1, but alkanes, both long chained (*n*-alkanes)

and branched (iso-alkanes) as well as cyclic components (naphthenics), see Fig. 1. Tables 3 and 4 summarize important parameters of the experimentally and numerically investigated fuel-air mixtures.

EXPERIMENTAL

In order to determine burning velocities of vaporized liquid fuels, the commonly known cone angle method [36] was applied (see Fig. 2). For this purpose, an existing burner system used previously for measuring the burning velocity of biogenic and synthetic gas mixtures [27] was modified.

The experimental setup

The experimental setup used in the present work is shown schematically in Fig. 3. The main technical data of the burner are given in Table 5.

The facility consists of the burner housing with the flame holder, mass flow controllers (MFC from Bronckhorst) for regulating oxygen and nitrogen flows, the fuel metering pump (HPLC pump, Shimadzu, Prominence LC-20AD), the fuel evaporator (delivered and produced by Institut für Chemische Verfahrenstechnik, University of Stuttgart [37]), and the homogenizing and cooling sections. The evaporator's main features are: mass flow up to 250 g/h (water), maximum vaporizing temperature of 670 K, and pressure up to 10 bar; volume of heated capillary system: few cubic centimetres [37].



Fig. 2: Determination of the burning velocity by applying the angle method.



Fig. 3: The experimental setup.

In order to avoid thermal-oxidative degradation, the fuel is deoxygenated by sparging with helium for displacement of the dissolved oxygen. The fuel is vaporized at about 580 K and mixed with the preheated nitrogen flow. Thermal degradation or cracking of the fuel is negligible at temperatures up to 570 K according to the study of Edwards and Atria [38]. They observed pyrolytic deposition from deoxygenated kerosenes starting at temperatures above ~ 770 K. This type of deposition appeared directly related to thermal cracking.

Table 5: Technical data of burner		
Maximum pressure	Up to 40 bar	
Optical access	25 mm	
Highest preheat	520 K	
temperature		
Nozzles' material	Inconel (coated)	
	Copper (uncoated)	
Nozzles' orifice	1.5 - 10 mm	

To avoid premature ignition, the mixture is cooled down to 480 K, before adding the oxygen flow. The ratio of nitrogen to oxygen flow is set to 79:21 (volume %) in order to mimic fuelair-mixtures. In two chambers - for homogenizing and mixing - the nitrogen and the air flow are homogenized. All parts containing vaporized fuel have to be heated to avoid condensation. By controlling temperature of the flame holder, the unburnt air fuel mixture is preheated to the desired value.

Method of determining the burning velocity

Premixed conical shaped flames are stabilized above nozzle flame holders. By changing the nozzle's diameter, flames with different air fuel ratios are realized. Digital images of the flames were captured by a CCD camera (La Vision, Imager Pro Plus 2M, 1200x1600 Pixel); from these images, contours and cone angles are calculated. The values of S_u were derived from the cone angles α and the velocities v_u of the unburnt gas based on the nozzle diameter and the volumetric flow rate (Fig. 2):

 $S_u = v_u \cdot \sin \alpha$.





Fig. 4: Premixed conical flame: GtL/air, $\varphi = 1.2$; suitable for obtaining S_u.

Fig. 5: Premixed conical flame: GtL/air, $\varphi = 1.55$; not suitable for obtaining S_u

Currently, conical flames can be stabilized at equivalence ratios from $\varphi = 0.95$ up to $\varphi = 1.4$ using nozzle diameters of 4 mm and 6 mm. Figures 4 and 5 show typical flames suitable and not suitable to determine burning velocities. At $\varphi < 1.0$, flames are extinguished. At $\varphi > 1.5$, the flame tip is opened (see Fig. 5), or the contour is wrinkled; thus, measurements of burning velocities are impossible.

The accuracy of the cone angle method is especially affected by flame strain and curvature [39], and by deviation of the flow pattern from an ideal plug flow [35, 40]. In [41], flame speeds of methane and hydrogen obtained by various methods were compared, including nozzle burners with conical flames and button shaped flames, closed vessel combustors, and counterflow burners. Depending on heat conductivity and diffusivities of the components of the gas mixtures, flame speeds determined from the cone angle method might differ from those values obtained by more exact stretch corrected measurements. Markstein [42] proposed a relation between burning velocity and flame stretch; for details see also [43]. Vukadinovic et al. [44] have determined Markstein numbers of kerosene Jet A-1/air mixtures by means of spherical expanding flames for equivalence ratios between $\varphi = 0.8$ and $\varphi = 1.4$. The Markstein numbers are strongly depending on the equivalence ratio. Based on this work, our measurements might deviate up to -15% compared to stretched corrected measurements, in the fuel rich regime ($\varphi = 1.4$). At stoichiometric conditions, the corrected values might be up to 5% lower than our measured values of the burning velocities.

MODELING

In the present work, a chemical kinetic model consisting of 3479 reactions involving 490 species is used, elaborated within the frame of ALFA-BIRD [16], mainly from the work of Dagaut et al. [31]. The predictive capability of this reaction model with respect to the laminar flame speed of the two synthetic fuel–air mixtures will be discussed below. Note: for the simulations, a surrogate will be used for representing the GtL fuels.

Computer simulations of the structure of a laminar premixed flame were performed with the SANDIA code PREMIX [45] including thermal diffusion, for the assumption of a free flame. Transport data for the species involved in the reaction model were taken from the CHEMKIN transport database [46], thermodynamical data from [47] or evaluated with group additives rules [48]. Typically, more than 100 grid points were computed to ensure having a grid independent solution (no further change in the flame speed with increasing number of grid points).

<u>Surrogate</u>

Aviation jet fuels may consist of blends of numerous species, up to over a thousand belonging to different chemical families. Among them, kerosene is used as a base of most jet fuels. The annual U.S. usage of jet fuel was about 80 billion liters in 2006 [49]. On the other hand, kerosene is the only fuel produced under very strict physical standards (boiling point, freezing point, viscosity, polarity, minimum ignition temperature etc.) in order to cope with the demands of aviation.

The chemical kinetic modeling of the combustion of a kerosene is a challenging task. Its complex composition does not allow developing a detailed reaction model which consists of all of the hundreds of different species and of all of the reactions that may occur between these species. Instead of; a surrogate is used, with a limited number of compounds with known kinetic sub models as a means to represent kerosene with its numerous species with different chemical behavior [50]. Surrogates should show a behavior similar to that of commercial jet fuels, ideally for predicting both chemical and physical properties. Such surrogates are of high interest since they can be utilized to study the effect of chemical composition and fuel properties on the combustion process. Presently, many proposals concerning the composition of a surrogate fuels exist, see e.g. [51-57].

The GtL-mixtures investigated are composed of alkanes, long-chained and branched; no aromates are present [29] (see Fig. 1). Therefore, in the present work, a surrogate was used consisting of two (for GtL) or three (for GtL+20% hexanol) initial species: *n*-decane, *iso*-octane, and *1*-hexanol (Table 6).

 Table 6: Used Surrogates for GtL and GtL+20% hexanol

Fuel	Surrogate	
	Species	Percentage / mol%
Gas to Liquid (GtL)	<i>n</i> -decane <i>iso</i> -octane	90.6 9.4
Gas to Liquid (GtL) +20% hexanol	<i>n</i> -decane <i>iso</i> -octane	65.7 6.8
	1-hexanol	27.5

Combustion of kerosene

First studies dealing with the combustion mechanism of practical fuels focused on simple hydrocarbon fuels as practical fuels were too complex and completely undefined in terms of chemical composition. Over the years, first, small hydrocarbons and aromatics were investigated and modeled, then, higher fuels such as *n*-decane [23], [58-61], dodecane [62], and hexadecane [63]. Measurement of the ignition delay time of kerosene has been the subject of a few studies [24-25], while some data exist for surrogates [18, 50, 54-57, 64-65].

Detailed reaction kinetics model

In the present work, the underlying reaction model is based on previous chemical mechanisms elaborated for the oxidation of e.g. *n*-decane, gasoline, and kerosene, see e.g. [25, 31]. It should be emphasized that the key principle of the reaction model is the application of extensively validated and evaluated chemical kinetic and elementary kinetic data. Thus, no modifications concerning for example rate coefficients of a particular elementary reaction was done.

Higher alkanes, such as *n*-heptane $(n-C_7H_{16})$, *iso*-octane $(i-C_8H_{18})_{,}$ and *n*-decane $(n-C_{10}H_{22})$ are important constituent of practical hydrocarbons fuels [16, 18]. Reaction mechanisms of $n-C_7H_{16}$ and *iso*-C_8H_{18} combustion are key parts in any kinetic model of reference fuels combustion [18, 25, 64-65].

RESULTS AND DISCUSSION

The burning velocities of the GtL-air mixture are represented in Fig. 6, the ones of the (GtL+20% hexanol)-air mixture in Fig. 13. Also, a comparison between measured burning velocities of the two investigated synthetic fuels and predicted laminar flame speed data of the two surrogates is shown. Results of a sensitivity (normalized local sensitivity) and rate of production analysis will be presented, too. The calculations were performed with a detailed reaction model (3479 reactions and 490 species). In general, the calculations of the laminar flame speed data of the two surrogates are in good agreement with the measured burning velocities of the two studied GtL-air mixtures.

The burning velocity of GtL-air mixtures

In Fig. 6, the measured burning velocity data of the GtL fuel are plotted, with their uncertainty limits; for comparison, the predicted data (of the surrogate) are also shown. The values are given for a fuel equivalence ratio φ between 0.9 and 1.4, for a preheat temperature $T_0 = 473$ K, at ambient pressure. The simulations show a very good agreement with the experimental results. The trends and the main features are well captured by the calculations.



Figure 7 depicts the most dominant reactions determining the laminar flame speed of the studied GtL fuel, for a stoichiometric (upper bars) and a fuel rich mixture (lower bars), as the result of a sensitivity analysis. The burning velocities are mostly sensitive to the kinetics of the chain branching reaction $H + O_2 = OH + O$ followed by reactions pertaining to the H / O- and CO-sub-system and methyl. In particular, the competition between the chain branching reaction and the chain terminating reaction (H + O₂ + H₂O = HO₂ + H₂O) is of great importance. With a higher value for the equivalence ratio ϕ , reactions of C₂H_x and C₃H_x species resulting from the combustion of the large alkanes, become more important.

Calculated temperature and species profiles are depicted in Fig. 8, for a stoichiometric GtL-air mixture. The hydrocarbons (*n*-decane and *iso*-octane) are consumed very rapidly in the flame zone. The major stable product, besides CO, CO_2 , H_2 , and H_2O , is ethene (C_2H_4). The predicted formation of hydrogen - although in very low concentrations – even at a

HAB value around zero - is caused by the high thermal diffusion of hydrogen (see also Fig. 14).



Fig. 7: GtL-air-mixture: Sensitivity analysis of burning velocity, p = 1 bar, $T_0 = 473$ K, $\varphi = 1.0$ and $\varphi = 1.2$. Calculations with detailed reaction model [16, 31].



Fig. 8: Combustion of a stoichiometric GtL / air mixture for p = 1 bar and $T_0 = 473$ K: selected species profiles. Calculations with detailed reaction model [16, 31].

In order to get more insight into the combustion chemistry of the initial species of the surrogate used, sensitivity analysis as well as rate-of-production analysis were carried out for the two constituents of the surrogate, *n*-decane (Figs. 9 and 11) and *iso*-octane (Figs. 10 and 12), for two different heights above the burner surface (HAB). The patterns are quite similar for the two species considered.

For the sensitivity analysis (Figs. 9-10), close to the flame front, at a low HAB value, the combustion is dominated by reactions pertaining to the H / O- and CO-sub-system as well as by reactions with methyl, C_2H_x and C_3H_x species involved (only given for *n*-decane). At a larger HAB value, reactions of the initial species (fuel specific) are the most important, besides the chain branching reaction (H + O₂ + H₂O = HO₂ + H₂O).



Fig. 11: GtL / air mixture: Rate of production analysis of *n*-decane for p = 1 bar, $\varphi = 1.0$, and $T_0 = 473$ K. Top: *HAB* = 2 cm; Bottom: *HAB* = 0.1 cm. Calculations with detailed reaction model [16, 31].



Fig. 12: GtL / air mixture: Rate of production analysis of *iso*-octane for p = 1 bar, $\varphi = 1.0$, and $T_0 = 473$ K at HAB = 2 cm. Calculations with detailed reaction model [16, 31].

The burning velocity of GtL+20% hexanol-air mixtures

Values of the burning velocities of the GtL-20% hexanolair mixture measured under ambient pressure (open symbols) are shown in Fig. 13. The data are given for equivalence ratios φ between 1.0 and 1.35, at two preheat temperatures, $T_0 = 423$ K and $T_0 = 473$ K. As expected and clearly to be seen from the values obtained at the lower preheat temperature, the maximum of the burning velocities is observed in the slightly fuel-rich regime, between $\varphi = 1.00$ and $\varphi = 1.05$. The same behavior is considered to be valid for the burning velocities obtained at $T_0 = 473$ K (triangles), taking into account the experimental uncertainty ranges of the measured data points and the failure



Fig. 9: GtL / air mixture: Sensitivity analysis of *n*-decane for p = 1 bar, $\varphi = 1.0$, and $T_0 = 473$ K. Top: HAB = 2 cm; Bottom: HAB = 0.1 cm. Calculations with detailed reaction model [16, 31].





Looking at the rate-of-production analysis (Figs. 11-12), *n*-decane and *iso*-octane react quite similar. The differences in the pattern plotted for different heights above the burner surface are small, as nearly the same reactions were found to have the largest influence (see e.g. Fig. 11). Only reactions leading to a depletion of the species – thermal decomposition and abstraction by H or O atoms – are identified for a small HAB value, whereas at higher HAB values, reactions leading to a production of these species – by recombination of H atoms with the species radicals (decyl and octyl, respectively) or of C_4H_9 radicals – are seen to be of major influence. in stabilizing conical flames for fuel-air ratios lower than $\varphi = 1.0$. The predictions (full symbols) show a reasonable agreement with the experimental results. The trends and the main features are well captured by the calculations. However, for lower φ values, the experimental data are underpredicted, whereas at larger φ values, the predicted data are slightly larger.



Fig. 13: GtL-20% hexanol-air mixtures: Comparison between predicted (solid curve) and measured (open symbols) burning velocity for p = 1 bar.

Calculated temperature and species profiles are depicted in Fig. 14, for a stoichiometric GtL-air mixture. The three components of the surrogate (*n*-decane, *iso*-octane, and *l*-hexanol) are consumed very rapidly in the flame zone. The major stable (hydrocarbon) product is ethene (C_2H_4).



Fig. 14: Combustion of a stoichiometric GtL-20% hexanol-air mixture for p = 1 bar and $T_0 = 473$ K: selected species profiles. Calculations with detailed reaction model [16, 31].

Figure 15 depicts the most dominant reactions determining the burning velocity of the GtL-20% hexanol fuel, for a stoichiometric and a fuel rich mixture. The chain branching reaction (H + O₂ = OH + O) competing with the chain terminating reaction (H + O₂ + H₂O = HO₂ + H₂O), and reactions pertaining to the H / O- and CO-sub-system and C₂H₃ are of great importance. This pattern is very similar to the one of the GtL fuel, without *1*-hexanol added (see Fig. 7).



Fig. 15: GtL-20% hexanol-air-mixture: Sensitivity analysis of burning velocity, p = 1 bar, $T_0 = 473$ K, $\varphi = 1.0$ and $\varphi = 1.2$. Calculations with detailed reaction model [16, 31].



Fig. 16: GtL-20% hexanol-air mixture: Sensitivity analysis of 1-hexanol, p = 1 bar, $\varphi = 1.0$, and $T_0 =$ 473 K. Top: HAB = 2.0 cm; Bottom: HAB = 0.1 cm. Calculations with detailed reaction model [16, 31].

To get more insight of the overall combustion, sensitivity as well as rate-of-production analysis were carried out for the three constituents of the surrogate, *n*-decane, *iso*-octane, and *l*-hexanol for two different heights above the burner surface (HAB). The patterns found for the sensitivity analysis as well as for the rate-of-production analysis with respect to *n*-decane and *iso*-octane mixtures are quite similar to those of the pure GtL fuel (Figs. 9-12). Therefore, only the results with respect to *l*-hexanol are shown (Figs. 16-17).



Fig. 17: GtL-20% hexanol-air mixture: *1*-hexanol rate of production analysis, p = 1 bar, $\varphi = 1.0$ and $T_0 =$ 473 K. Top: HAB = 2.0 cm; Bottom: HAB = 0.1 cm. Calculations with detailed reaction model [16, 31].

Comparison between the two GtL fuels and Jet-A1

Figure 18 shows the comparison between measured burning velocities and predicted values of the laminar flame speed for the studied GtL-air-mixtures (triangles, squares), as a function of the equivalence ratio φ , together with experimental data of a Jet-A1 fuel (diamonds) measured previously [35]. Such information is needed as part of characterization studies of alternative fuels to ensure their suitability with respect to the properties of Jet A-1 ("drop-in fuel").



Fig. 18: Comparison between predicted (solid curve) and measured (symbols) burning velocity for Jet-A1air [35], GtL-air and GtL-20% hexanol-air mixtures.

The shape of the three curves is very similar. Within the range of the equivalence ratio φ between 0.9 and ~ 1.2, the

data of Jet-A1 are higher than those of the two GtL fuels, by up to about 10 - 15%. For the more fuel-rich mixtures, no significant differences can be derived.

The simulations with a two or three surrogate respectively show a good agreement with the results obtained for the GtL mixtures. For clarity, the laminar flame speed data of the three components were calculated also, for the same experimental conditions. From Fig. 19 it can be seen that *n*-decane and *l*-hexanol have very similar burning velocities whereas those of *iso*-octane are significantly lower.



Fig. 19: Predicted burning velocity for the three components of the surrogate; $T_0 = 473$ K, p = 1 bar Calculations with detailed reaction model [16, 31].

CONCLUSIONS

Measurements of the burning velocities of two synthetic fuels – 100% GtL and GtL+20% hexanol, respectively – were presented. The GtL-air mixtures were studied for atmospheric pressure, and at different preheat temperatures ($T_0 = 423$ K and 473 K), for equivalence ratios φ between 0.9 and 1.35. The predictive capability of the used detailed reaction mechanism was demonstrated. Good agreement was found between measured and calculated data. Also, the trends and main features were captured by the predictions.

In the future, further alternative aviation fuels, with CtL (Coal to Liquid) and a blend of GtL and naphthenic cut among them, will be investigated in detail within ALFA-BIRD [16]. Also, experiments are planned for elevated pressure. In addition, measurements of the ignition delay times of the alternative jet fuels will be conducted.

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