Combustion of a Gas-to-Liquid-Based Alternative Jet Fuel: Experimental and Detailed Kinetic Modeling

Philippe Dagaut, Guillaume Dayma, Pascal Diévart, Kamal Hadj-Ali, Amir Mzé-Ahmed Centre National de la Recherche Scientifique

1-C Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France

1 Introduction

Energy used worldwide is still mainly provided by fossil fuels. Since the end of the 20th century, alternative energy resources have increasingly been used for guaranteeing security of supply and with hope to mitigate global warming. Recently, the European Advanced Biofuels Flight Path was launched by the European Commission to accelerate the commercialization of bio-jet fuels for aviation. However, this is technically very challenging due to very strict fuel specifications (e.g., fuel freezing point, energy density, flash point, flammability limit, amount of aromatics)[1]. Therefore, it is crucial to improve our knowledge with respect to the experimental characterization of synthetic jet fuels properties and combustion behavior. Global combustion parameters alone (ignition delay times and laminar flame speed) are not sufficient and combustion products must be measured over a broad range of conditions (temperature, pressure, fuel composition, and equivalence ratio). But, only a limited set of combustion data is available for of synthetic jet fuels which are complex mixtures of different chemical classes (n-alkanes, iso-alkanes, cyclo-alkanes, and aromatics). Blending of such synthetic fuels with large alcohols such as 1-hexanol could be of interest, although the combustion of this alcohol has received little attention even if bio-hexanol production has already been reported. As part of continuing efforts in this laboratory for increasing our knowledge of combustion, the kinetics of oxidation of a GtL-hexanol (80/20 in vol.) jet fuel was studied experimentally in a jet-stirred reactor (JSR) at 10 bar, over a range of temperatures and equivalence ratios. A detailed chemical kinetic reaction mechanism was proposed to represent the present data and literature flame speeds[2], complementing recent studies on the combustion of synthetic/alternative jet fuels and surrogates [3-6].

2 Experimental

To understand the combustion of a fuel within an aero-turbine one has to take into account many aspects. Within the current work, we primarily focus on the oxidation of the fuel and the formation of pollutants whereas burning velocities have been determined earlier[2]. These processes occur over a range of temperatures, pressures, and equivalence ratios being among the most important parameters for operating an aero-turbine. In the present experimental work we used a fuel mixture of 1-hexanol and a GtL (Fischer-Tropsch synthetic jet fuel, FSJF) provided by Shell ($C_{10.45}H_{23.06}$, M=148.44g·mol⁻¹, density= 0.7377 g·L⁻¹). The GtL mass composition was determined via multi-dimensional gas chromatography analyses (28.1% *n*-alkanes, 62.8% *iso*-alkanes, 8.8% *cyclo*-alkanes, and 0.2%

Dagaut, P.

aromatics). The experiments were performed using a JSR set-up presented earlier[7]. The reactor consists of a 39 cm³ fused-silica sphere (4 cm diameter). Fused-silica is used to minimize wall catalytic reactions. It is equipped with 4 nozzles of 1 mm i.d. to admit the gases which are achieving the stirring. A 100 L \cdot .h⁻¹ nitrogen flow was used to dilute the fuel. As before [8-9] all the gases were preheated at a temperature close to the JSR operating temperature to minimize temperature gradients. A regulated heating wire of ~1.5 kW (Thermocoax) maintained the reactor temperature at the selected working temperature. The reactants were mixed just before the entrance of the injectors. Nitrogen (<50 ppm of O₂; <1000 ppm of Ar; <5 ppm of H₂, all supplied by Air Liquide) was used as diluent and high purity oxygen (99.995% pure, Air Liquide) was the oxidizer. All the gases were delivered using mass flow controllers (Brooks 5850TR). A HPLC pump with on-line degasser (Shimadzu LC10 AD VP and DGU-20 A3) was used to deliver the fuel to a temperature-controlled atomizer-vaporizer assembly maintained at 523 K. The reactants were continually flowing into the reactor while its temperature of was varied stepwise. Thermal homogeneity along the vertical axis of the reactor was measured for each experiment using a 0.1mm Pt-Pt/Rh 10% thermocouple located inside a thin-wall silica tube. A high degree of dilution was used, reducing heat release, temperature gradients (gradients of $\sim 1 \text{ K.cm}^{-1}$) in the reactor, and preventing flame occurrence in the JSR. A high precision gage was used to manometrically measure the operating pressure at the exhaust. The reacting mixtures were probe sampled using a fused-silica low pressure sonic probe. The fused-silica sampling probe was connected to a temperature controlled (413 K) gas cell via a 6.35 mm o.d. deactivated stainless steal heated line (413 K). The samples (~4-6 kPa) were taken at steady temperature and constant residence time. They were analyzed on-line by gas chromatography- flame ionization detector (FID)/ mass spectrometry (GC-MS Saturn 2000, Varian) and Fourier Transformed Infra-Red spectrometry (FTIR, Magna 550, Nicolet; 2 m path length, 1 cm⁻¹ resolution), and off-line, after collection and storage in 1 l Pyrex bulbs, by GC. Permanent gases and high vapor-pressure compounds were analyzed off-line by GC whereas low vapor-pressure compounds were analyzed on-line by GC. GCs equipped with capillary columns (DB-5ms: 30m and 0.32mm i.d., DB-624: 60m and 0.32mm i.d., Plot Al₂O₃/KCl: 50m and 0.32mm i.d., Carboplot-P7: 25m and 0.53mm i.d.), thermal conductivity detector, and FID were used for quantifying stable species. A quadrupole mass spectrometer (GC/MS Varian 1200) operating in electron impact ionization mode (70 eV) was used for compounds identifications. On-line FTIR analyses allowed measuring H₂O, CO, CO₂, CH₂O, CH₄, and C₂H₄. Good repeatability of the measurements and good carbon balance $(100\pm15\%)$ were obtained.

3 Modeling

The kinetic modeling was performed using the CHEMKIN II package[10-11]. The reverse reactions rate constants were computed from the corresponding equilibrium constants, $K_c = k_{forward} / k_{reverse}$ calculated from thermochemistry[5] and the forward rate constants. The kinetic reaction mechanism used in this work derives from previous modeling efforts for describing the oxidation of 1-hexanol[12] and conventional and synthetic jet fuels with simple surrogates [2, 5, 13].

I able	1: Fuels properties	
Property	GtL-hexanol fuel	Model fuel
Formula	$C_{9.17}H_{20.45}O_{0.29}$	$C_{9.17}H_{20.38}O_{0.29}*$
H/C	2.23	2.22
Molar weight (g·mole ⁻¹)	135.134	135.04*
Density $(g \cdot L^{-1})$	753.9	765.8
Derived Cetane Number*	47.3	47.6

Г	able	1:	Fuels	pro	perties
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* $1.093 \times C_{8.39}H_{18.65}O_{0.264}$ since we used 1093 ppm of model fuel to represent 1000 ppm of GtL-hexanol. [†] Derived Cetane Number (ASTM D7668) measured using a Herzog Cetane ID 510 by PAC.

Dagaut, P.

The surrogate was defined based on the chemical composition of the fuel (determined by GC analyses). Representative hydrocarbons were selected in accordance with previous work on jet fuels combustion [14]. In the computations, the fuel was represented by a mixture of *n*-decane, *iso*-octane, *n*-propylcyclohexane, and 1-hexanol. To represent 1000 ppm of fuel, we used the following mole fractions for the model-fuel: $n-C_{10}H_{22}$: 0.000465, *iso-C*₈H₁₈: 0.000267, *n*-propylcyclohexane: 0.000073, and 1-hexanol: 0.000288. The model-fuel and the GtL-hexanol fuel properties are compared in Table 1. The model fuel composition was chosen on the basis of multidimensional GC and GC/MS analyses (62.8% iso-alkanes -mainly C10 to C12, 28.1% n-alkanes -mainly C9 to C11, 0.6% mononaphthenes -mainly C₉ to C₁₁, 8.2% di-naphthenes -mainly C₁₀ to C₁₁, 0.2% mono-aromatics -mainly C₉ to C₁₀, all in mass %) and previous studies on SPK (synthetic paraffinic kerosene) and SPK/Jet A-1 oxidation [14]. Iso-octane is more branched than iso-alkanes present in the GtL fuel (mostly mono methyl-alkanes). Therefore, less iso-octane is needed to represent the iso-alkane fraction of the fuel[14]. To take this parameter into account, the fraction of *n*-alkanes must be increased significantly while reducing that of *iso*-alkanes. Therefore, the model fuels compares reasonably well with the GtL for paraffins (91% vs. 91% in the model) and for naphthenes (8.8% vs. 8.75% in the model). The proposed kinetic reaction mechanism (8217 reactions vs. 2185 species) is available from the authors.

4 **Results and Discussion**

The kinetic of oxidation of 1000 ppm of a GtL-hexanol fuel mixture was studied at 10 bars in a JSR, over the temperature range 550 to 1150 K, and at a constant mean residence time of 1 s. The experiments were performed at three equivalence ratios $\varphi = 0.5$, 1.0, and 2.0 (Fig. 1).



Figure 1. GtL-hexanol oxidation in a JSR at $\varphi = 1.0$, p = 10 bar, and t = 1 s (Data: large symbols, simulations: lines and small symbols).

Under these conditions, the fuel oxidized rapidly, yielding hydrocarbon intermediates (mostly methane and C_2 - C_3 olefins) and oxygenates (mainly formaldehyde and CO). A cool flame occurred over the temperature range 550-730 K. Mole fractions were measured for reactants (O₂, 1-hexanol), main stable intermediates, and products: hydrogen, water, carbon monoxide, carbon dioxide, formaldehyde, methane, ethane, ethylene, acetylene, propane, propene, 1-butene, 2-butenes, isobutene, 1,3-butadiene, isoprene, 1,3-pentadiene, benzene, and cyclohexene. A good repeatability of the measurements was observed. The accuracy of mole fractions derived from repeated experiments and analyses, was typically $\pm 10\%$ and better than 15\%. The uncertainty on temperature measurements was ± 5 K. As can be seen from Table 2, the main products were CO₂, CO, H₂O, CH₂O, CH₄, C₂H₄, and C₃H₆. Their mole fractions were larger under high-temperature oxidation regime than under cool-flame conditions. The experimental results were compared to previously obtained data for the oxidation of a typical Jet A-1. As can be seen from Figure 2, the two fuels oxidize similarly. However, it was observed that under cool flame conditions (550-750 K) the oxidation of Jet A-1 is slower than that of the GtL-hexanol blend (smaller formation of stable intermediates and products with Jet A-1, e.g., CH₂O, CO, H₂O, and CO_2). At higher temperature both fuels seem to oxidize at nearly the same rate if we consider the formation of CO_2 and H_2O . The main difference in terms of intermediates formation concerns ethylene

Dagaut, P.

that accumulates at higher concentration with the GtL-hexanol blend. This results from the higher concentration of alkanes in the synthetic fuel. However, with the blend, ethylene formation is reduced from the GtL base case (Table 2)

Measured	Maximum Mole Fraction			
Products	at low temperature		at high temperature	
	Blend‡	GtL	Blend‡	GtL
H_2	1.9 x10 ⁻⁵	1.3 x10 ⁻⁵	$4.3 \text{ x} 10^{-4}$	$4.3 \text{ x}10^{-4}$
CO	$1.0 \text{ x} 10^{-3}$	$1.3 \text{ x} 10^{-3}$	$4.5 \text{ x} 10^{-3}$	$5.9 \text{ x} 10^{-3}$
CH_2O	2.7 x10 ⁻⁴	3.1 x10 ⁻⁴	2.8×10^{-4}	3.1×10^{-4}
CH_4	6.4 x10 ⁻⁶	+	3.4×10^{-4}	4.0×10^{-4}
C_2H_6	$6 \text{ x} 10^{-7}$	+	2.5×10^{-5}	3.0×10^{-5}
C_2H_4	6.5 x10 ⁻⁵	+	8.2×10^{-4}	9.9x10 ⁻⁴
C_3H_6	3.4 x10 ⁻⁵	+	2.3×10^{-4}	2.4×10^{-4}
$1-C_4H_8$	2.7 x10 ⁻⁴	+	4.8x10 ⁻⁵	5.2x10 ⁻⁵
$1 - C_5 H_{10}$	÷	+	2.5×10^{-5}	2.3×10^{-5}
$1 - C_6 H_{12}$	÷	+	1.9×10^{-5}	1.8×10^{-5}
trans-2-C ₄ H ₈	÷	+	5.2×10^{-6}	6.5x10 ⁻⁶
cis-2-C ₄ H ₈	÷	*	4.0×10^{-6}	4.7×10^{-6}
$trans-2-C_5H_{10}$	÷	*	1.6×10^{-6}	1.4×10^{-6}
$cis-2-C_5H_{10}$	÷	+	4.5×10^{-6}	6.0x10 ⁻⁶
iso-C ₄ H ₈	÷	+	1.7×10^{-5}	2.2×10^{-5}
isoprene	÷	+	4.1×10^{-6}	4.2×10^{-6}
C_2H_2	÷	+	1.1×10^{-5}	1.1×10^{-5}
$1,3-C_5H_8$	÷	*	1.5×10^{-5}	1.7×10^{-5}
$1,3-C_5H_8$	Ť		4.0×10^{-6}	4.6×10^{-6}

Table 2. Products from the oxidation of GtL-hexanol/ O_2/N_2 in a JSR at 10 bars and $\varphi=1$.

‡ GtL-hexanol 80/20 in volume. † Maximum not detected or not reached

We found that 1-hexanol blending reduces the fuel reactivity under cool flame conditions whereas at higher temperature, the rates of oxidation of GtL and blended-GtL fuels are very close.



Figure 2. Comparison of experimental data obtained in a JSR for the oxidation of Jet A-1 (closed symbols) and GtL-hexanol (open symbols) at $\varphi = 1.0$, p = 10 bar, and t = 1 s. The initial fuel concentration was 1000 ppm.

On Figure 1, where the concentrations of the most important intermediates and products (cf. Table 2) are reported, one can see that the proposed kinetic model represents fairly well the data. Improvements in the modeling could likely be achievable by using a more complex model fuel composition that would raise the complexity of the kinetic scheme. Also, a variation of the composition of the model-fuel could help improving the modeling. Reaction paths analyses, where normalized rates of reaction (*R*) were computed, showed that the model-fuel's components are primarily oxidized by H-atom abstraction with OH radicals (φ =1, 900 K, 1 s). 1-Hexanol reacts via reactions 5826: 1-hexanol + OH =H₂O+C₆H₁₃O; (*R*=-0.012), 5827: 1-hexanol+OH=H₂O+1-C₆H₁₂OH; (*R*=-0.224), 5828: 1-hexanol +

 $OH \Rightarrow H_2O+6-C_6H_{12}OH$; (*R*=-0.08), 5829: 1-hexanol+OH \Rightarrow H_2O+5-C_6H_{12}OH; (*R*=-0.137), 5830: 1hexanol+OH= $H_2O+4-C_6H_{12}OH$; (*R*=-0.137), 5831: 1-hexanol+OH= $H_2O+3-C_6H_{12}OH$; (*R*=-0.137), and 5832: 1-hexanol+OH= $H_2O+2-C_6H_{12}OH$; (*R*=-0.137). *n*-Decane reacts through reactions 1914: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 1 - C_{10}H_{21}$; (*R*=-0.1), 1915: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{22} + OH \Rightarrow H_2O + 2 - C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{21} + C_{10}H_{21} + C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{21} + C_{10}H_{21} + C_{10}H_{21}$; (*R*=-0.2), 1916: $n-C_{10}H_{21} + C_{10}H_{21} + C_{10}$ $C_{10}H_{22} + OH \Rightarrow H_2O + 3 - C_{10}H_{21}$; (*R*=-0.2), 1917: n- $C_{10}H_{22} + OH \Rightarrow H_2O + 4 - C_{10}H_{21}$; (*R*=-0.2), and 1918: n- $C_{10}H_{22} + OH \Rightarrow H_2O + 5 - C_{10}H_{21}$; (*R*=-0.2). *iso*-Octane reacts via reactions 5502: iC_8H_{18} + OH \Rightarrow 2,2,4-trimethyl-1-pentene + H_2O; (*R*=-0.4), 5503: iC_8H_{18} + OH \Rightarrow 2,2,4-trimethyl-3-pentene + H_2O; (*R*=-0.17), 5504: iC₈H₁₈+OH \approx 2,4,4-trimethyl-2-pentene +H₂O; (*R*=-0.13), and iC₈H₁₈+OH \approx 2,4,4-trimethyl-1pentene +H₂O; (R=-0.14). *n*-Propylcyclohexane (pch) reacts through reactions 2992: pch+OH=1pch+H₂O; (*R*=-0.11), 2993: pch+OH \Rightarrow 2-pch+H₂O; (*R*=-0.07), 2994: pch+OH \Rightarrow 3-pch+H₂O; (*R*=-0.11), 3-pch+OH \Rightarrow 3-pch+H₂O; (*R*=-0.11), 3-pch+OH \Rightarrow 3-pch+H₂O; (*R*=-0.11), 3-pch+OH \Rightarrow 0.07), 2995: pch+OH=4-pch+H₂O; (*R*=-0.1), 2996: pch+OH=5-pch+H₂O; (*R*=-0.2), 2997: pch + OH \Rightarrow 6-pch+H₂O; (*R*=-0.2), and 2998: pch+OH \Rightarrow 8-pch+H₂O; (*R*=-0.1). Methane is among the main products. It is mostly produced by reactions of methyl radicals with HO₂, formaldehyde, and ethylene, i.e. via reactions 75: $CH_3+HO_2 \Rightarrow CH_4+O_2$; (R=0.18), 199: $CH_2O+CH_3 \Rightarrow HCO+CH_4$; (R=0.38), and 238: $C_2H_4+CH_3 \Rightarrow C_2H_3+CH_4$; (*R*=0.09). Ethylene is produced by ethyl radical's oxidation and betascissions, i.e. through reactions 217: $C_2H_5 + HO_2 \Rightarrow C_2H_4 + H_2O_2$; (*R*=0.04), 231: $C_2H_4 + HO_2 \Rightarrow C_2H_4O_2H$; $(R=0.28), 325: C_2H_3O_2 = C_2H_4 + HO_2; (R=0.19), and 463: n-C_3H_7(+M) = C_2H_4 + CH_3(+M); (R=0.09).$ Formaldehyde is formed by oxidation of vinyl and hydroxymethyl radicals and by the decomposition of methoxy radicals in reactions 2: $C_2H_3+O_2 \Rightarrow CH_2O+HCO$; (*R*=0.37), 161: CH₂OH+O₂ \Rightarrow CH₂O+O₂ CH₂O+HO₂; (R=0.08), and 165: CH₃O+M=CH₂O+H+M; (R=0.2). Reactions pertaining to the oxidation sub-scheme of *iso*-octane are responsible for the formation of *iso*-butene. The main important are reactions 5395: $tC_4H_9+O_2 \Rightarrow iC_4H_8+HO_2$; (*R*=0.4), 5476: $iC_4H_8+CH_3 \Rightarrow 2$ -methyl-1-butene +H₁ (R=0.075), and 5592: 2,4,4-trimethyl-2-pentene \Rightarrow tC₄H₉+iC₄H₈: (R=0.3).

5 Conclusion

The kinetics of oxidation of a Gas-to-Liquid Jet fuel blended with hexanol was studied in a JSR (p = 10 bar, constant mean residence time of 1 s, 550 < T/K < 1150, $0.5 < \varphi < 2$. Concentration profiles of reactants, stable intermediates, and final products were obtained by probe sampling followed by online Fourier Transformed Infra-Red spectrometry and on-line and off-line gas chromatography analyses. The oxidation of this GtL-jet fuel under these conditions was modeled using a detailed kinetic reaction mechanism and a 4-component model fuel (*n*-decane, *iso*-octane, *n*-propylcyclohexane, and 1-hexanol). A reasonable representation of the kinetics of oxidation of the fuel was obtained. Modeling improvements might be obtained by using a more complex model fuel involving more realistic *iso*-alkanes for which the kinetics has recently been proposed [15-18].

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