SYNTHETIC JET FUEL COMBUSTION: EXPERIMENTAL AND KINETIC MODELING STUDY

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ABSTRACT

Fischer-Tropsch liquid fuels synthesized from syngas, also called synthetic paraffinic jet fuel (SPK), can be used to replace conventional petroleum-derived fuels in jet engines. Whereas currently syngas is mostly produced from coal of natural gas, its production from biomass has been reported. These synthetic liquid fuels contain a very high fraction of iso-alkanes, while conventional jet fuels contain large fractions of n-alkanes, cycloalkanes (naphtenes), and aromatics. In that contest, a jetstirred reactor (JSR) was used to study the kinetics of oxidation of a 100% SPK and a 50/50 SPK/Jet A-1mixture over a broad range of experimental conditions (10 atm, 560 to 1030K, equivalence ratios of 0.5 to 2, 1000 ppm of fuel). The temperature was varied step-wise, keeping the mean residence time in the JSR constant and equal to 1s. Three combustion regimes were observed over this temperature range: the coolflame oxidation regime (560-740K), the negative temperature coefficient (NTC) regime (660-740K), and the hightemperature oxidation regime (>740K). More than 15 species were identified and measured by Fourier transform infrared spectrometry (FTIR), gas chromatography/ mass spectrometry (CG/MS), flame ionization detection (FID), and thermal conductivity detection (TCD). The results consisting of concentration profiles of reactants, stable intermediates and products as a function of temperature showed similar kinetics of oxidation for the fuels considered, although the 100% SPK was more reactive. A surrogate detailed chemical kinetic reaction mechanism was used to model these experiments and ignition experiments taken from the literature. The kinetic modeling showed reasonable agreement between the data and the computations whereas model improvements could be achieved using more appropriate surrogate model fuels. Kinetic computations involving reaction paths analyses and sensitivity analyses were used to interpret the results.

INTRODUCTION

Synthetic liquid fuels obtained via various processes (Fischer-Tropsch synthesis, hydro-treatment of organic liquids) using a variety of feedstock could be used in the future to replace petroleum-derived liquid fuels. In that contest, research activities on the synthesis[1-3] and testing of synthetic jet fuels have increased significantly over the last years[1, 4-13] whereas until now no kinetic model was proposed for their ignition and combustion over a wide range of conditions, i.e. for both cool-flame and high temperature oxidation regimes. Since the composition of synthetic paraffinic jet fuels (SPK) differs significantly from that of usual jet fuels (Jet A-1, JP-8), the applicability of existing kerosene combustion models for simulating the oxidation of SPK is not obvious.

In fact, usual aviation fuels consist of complex mixtures of hundreds of medium molecular weight hydrocarbons that participate in thousands of chemical reactions [14-16]. Synthetic paraffinic kerosenes obtained from non-petroleum feedstocks (coal, natural gas, and biomass) are chemically different: the main chemical classes present are *iso*-alkanes (*iso*-paraffins), and *n*-alkanes (*n*-paraffins) whereas a small fraction of aromatics is usually introduced to avoid issues with O-rings leakage [17-18].

To overcome the complexity of computing the kinetics of oxidation of such multi-components fuels, surrogates with a limited number of components must be used. In addition to the simplification of the computations, the use of surrogates allows a molecular-level understanding of oxidation processes.

For usual jet fuels, a surrogate consisting of *n*-decane, *n*-propylcyclohexane, and *n*-propylbenzene was used previously [14-16] to represent Jet A-1 which consists predominantly of *n*-alkanes, cyclic paraffins (naphtenics), and mono-aromatics. No *iso*-alkane oxidation sub-scheme was considered in these

computations. However, the inclusion of an iso-alkane oxidation sub-scheme is required with SPK since iso-alkanes represent the main SPK components. Also, our previous model was limited to the high-temperature oxidation regime while low-temperature oxidation kinetics can play a role until ca. 900 K. Recently, the ignition of SPK/air mixtures was investigated over a range of conditions (1 atm, 900-1200K)[6]. A kinetic model involving the oxidation sub-schemes for *n*-decane, *n*propylcyclohexane, n-propylbenzene, and iso-octane was used to simulate the data. Nevertheless, no kinetic data were available below 900 K where cool flame can develop, and where flashback can occur in lean premixed pre-vaporized (LPP) combustion. In that contest, experimental results were needed for the oxidation of a synthetic paraffinic jet fuel over an extended range of conditions and the previously proposed kerosene oxidation kinetic mechanism [14-15] needed to be extended by including low-temperature oxidation chemistry and an iso-alkane sub-scheme.

In the present study, the kinetics of oxidation of a synthetic paraffinic jet fuel and mixtures of SPK with a commercial jet fuel (Jet A-1) were measured. These experiments were carried out in a pressurized jet-stirred reactor to: (i) supply new data for the kinetics of oxidation of a synthetic paraffinic jet fuel over a wide range of conditions, and (ii) propose and validate a detailed kinetic reaction mechanism for the oxidation of SPK and a semi-synthetic jet fuel from low to high temperatures.

NOMENCLATURE

φ: Equivalence ratio
FID: Flame ionization detector
FTIR: Fast Fourier Transform Infrared
GC: Gas chromatography
JSR: Jet-stirred reactor
MS: mass spectrometry
Su: Laminar burning velocity
SPK: synthetic paraffinic kerosene
TCD: Thermal conductivity detector
τ: residence time in the JSR

EXPERIMENTAL

The jet-stirred reactor (JSR) used here is similar to that used in previous kinetic studies of the oxidation of a range of fuels [19-21]. A schematic overview of the experimental set-up is presented in Figure 1. The JSR consists of a fused silica (to minimize wall catalytic reactions) sphere of 33 cm³ in volume. It is equipped with four nozzles of 1 mm inner diameter for the injection of the gases achieving the stirring. A nitrogen flow of 100 L/h was used to dilute the fuel and avoid its pyrolysis before admission into the reactor. All gases were preheated before injection to minimize temperature gradients inside the JSR. The liquid fuel was atomized and vaporized before injection into the reactor using an in-house atomize-vaporizer assembly maintained at ca. 550 K. The SPK fuel had a density of 0.757 g/cm³ and a global chemical formula of $C_{11.5}H_{24.41}$ (H/C=2.1). Its composition was determined to be ca. 79.9% *iso*-alkanes, 19.6% *n*-alkanes, and 0.5% aromatics in mass. The second fuel considered in the present study is a 50/50 mixture of this SPK with Jet A-1. That fuel mixture had a density of 0.78 g/cm³ and a global formula of $C_{11.24}H_{23.17}$ (Table 1).

Table 1. Composition of the fuels.

Chemical class	% mass SPK	% mass Jet A-1
<i>n</i> -paraffins	19.63	12.19
iso-paraffins	79.88	26.30
aromatics	0.49	33.22
naphtenics		24.28

The fuel and oxygen were diluted by a flow of nitrogen (<50 ppm of O₂; <1000 ppm of Ar; <5 ppm of H₂), and mixed at the entrance of the injectors. The experiments were performed at steady state, at a constant mean residence time of 1 s, the reactants flowing continuously in the reactor. The temperature of the gases inside the JSR ranged from 560 to 1030 K. A high level of dilution was used (11240–11500 ppm of carbon in the fuel), minimizing temperature gradients in the JSR and heat release. Thermocouple measurements, using 0.1 mm Pt/Pt–Rh 10% wires located inside a thin-wall silica tube, showed a good thermal homogeneity along the vertical axis of the JSR (gradient \leq 3 K/cm).



Figure 1: The JSR experimental set-up

The reacting mixtures were sampled using a low-pressure fused-silica sonic probe movable along the vertical axis of the JSR. The samples (≤ 0.06 bar), were taken at steady temperature and residence time. They were analyzed on-line by Fourier Transformed Infra-Red spectrometry (FTIR) and gas chromatography-mass spectrometry (GC-MS), and off-line, after collection and storage at low-pressure (ca. 0.04 bar) in 1 L Pyrex bulbs, by GC. The high vapor-pressure species and permanent gases were analyzed off-line and low vapor-pressure compounds were analyzed on-line. A heated (70 °C) glass piston chamber was used to pressurize the samples to 1 bar in the GC injection loop. Gas chromatographs equipped with capillary columns (DB-5ms, DB-624, Plot Al₂O₃/KCl,

Carboplot-P7), thermal conductivity detector (TCD), and flame ionization detector (FID), were used for species measurements. Compound identification was made via GC/MS analyses using an ion trap detector (Saturn 2000, Varian) and a quadrupole (V1200, Varian) operating in electron impact ionization mode (70 eV). On-line FTIR analyses (Nicolet Magna 550; 1 cm⁻¹ resolution) were used to quantify H₂O, CO, CO₂, CH₂O, CH₄, C₂H₂, and C₂H₄. For these measurements, the sampling probe was connected to a temperature controlled (140 °C) gas cell (2 m path length; 0.5 bar) via a 6.35 mm O.D. deactivated stainless steal heated line (140-200°C). A good repeatability of the measurements and a reasonably good carbon balance (100 ± 10%) were obtained in the present series of experiments. Since many oxygenated intermediates could not be quantified, no oxygen balance could be calculated.

COMPUTATIONS

The Senkin code [22] was used for the ignition simulations. The constant volume approximation was used and the ignition delays were defined as the time at which the computed temperature reaches 200 K above the initial temperature. The PSR computer code [23] was used for the kinetic modeling of the JSR experiments. It computes species concentrations from the balance between the net rate of production of each species by chemical reaction and the difference between the input and output flow rates of species.

The detailed chemical kinetic scheme used here derives from previous studies on the oxidation of liquid fuels, i.e. ndecane, gasoline, diesel, and kerosene surrogates [14, 24-25]. For the kinetic modeling, surrogate model fuels were used. In the computations, the SPK was represented by a mixture of *n*-(2,2,4-trimethylpentane), decane. *iso*-octane and npropylbenzene whereas, as previously [25], a mixture of ndecane, n-propylcyclohexane, and n-propylbenzene was used for representing Jet A-1. The SPK surrogate composition was chosen on the basis of a previous study on SPK ignition[6]. Iso-octane was used to represent the iso-paraffins since a kinetic model was available for the oxidation of this fuel [26-27]. The SPK fuel was represented by a 60/40 n-decane/isooctane mixture. This composition was chosen in order to represent the amount of branched methyl in the SPK. Since isooctane has 3 branched methyl and SPK has \geq 1 branched methyl, the fraction of *iso*-octane should be > 80/3=26.7%.

The proposed kinetic reaction mechanism consisting of 6228 reactions involving 2006 species is available from the authors upon request. Cross-reactions between the fuel components sub-schemes were included [27]. The rate constants for the reverse reactions were computed from the forward rate constants and the equilibrium constants calculated using the appropriate thermochemical data [14, 24-25]. The pressure dependencies of the unimolecular reactions and of pressure-dependent reactions were taken into account when information was available (i.e., k(P,T)). For interpreting the computational results, we performed local first-order sensitivity analyses and reaction rate analyses were done by computing the

rates of consumption (ROC) and production (ROP) for every species.

RESULTS AND DISCUSSION

In this study, the kinetics of oxidation of a SPK and of a 50/50 mixture of this SPK with Jet A-1 were studied under the same conditions. The surrogate model fuels used for the kinetic modeling consist of mixtures of: *n*-decane, *iso*-octane, *n*-propylbenzene, and *n*-propylcyclohexane.

In the present experiments, the temperature was varied step-wise in the range 560–1030 K, keeping the mean residence time constant and equal to 1s. This temperature range allowed the observation of the cool-flame oxidation regime (560–740 K), the negative temperature coefficient (NTC) regime (660–740 K), and the high-temperature oxidation regime (\geq 750K). The experiments were performed for several equivalence ratios, from fuel-lean to fuel-rich condition (i.e. over the range 0.5-2). More than 15 species were identified and measured by CG/MS, FID, and TCD. Experimental concentration profiles were measured for H₂, H₂O, O₂, CO, CO₂, CH₂O, CH₄, C₂H₆, C₂H₄, C₂H₂, C₃H₆, i-C₄H₈, 1-C₄H₈, 1,3-C₄H₆, 1-C₅H₁₀, and benzene. Uncertainties for the measured concentrations based on analytical and systematic error were estimated to be ca. 10%.



Figure 2: (a) Concentration profiles obtained from the oxidation of SPK (open symbols) and Jet A-1 (closed symbols). Initial JSR conditions: 10 atm, τ = 1s, ϕ = 1, 1000 ppm of fuel, (b) Rates of production under the same conditions.

Many minor species were detected at ppm levels but they were not quantified nor used in the modeling. The concentration profiles measured from the oxidation of SPK and Jet A-1 fuels were compared. Figure 2a presents an example of the present results. As can be seen from this figure, the concentration profiles are very similar. However, the concentrations of major stable intermediates, i.e. H_2 , CH_2O and CO, on that Figure tend to be higher when the fuel is SPK. As seen from Figure 2b, SPK is oxidized faster than Jet A-1, as reported previously [6]..

The concentration profiles measured during the oxidation of the SPK and SPK-Jet A-1 fuels were compared to the present model predictions. The mechanisms used previously for modeling the oxidation of Diesel and surrogate Diesel fuels and that of *n*-propylcyclohexane, *iso*-octane, and a surrogate gasoline under similar conditions were merged. The resulting scheme included both low- and high-temperature oxidation processes. The present model was also successfully tested for the oxidation of pure fuels (*n*-decane, *n*-propylcyclohexane, *iso*-octane) under similar JSR conditions.

Since *n*-decane was chosen as one of the surrogate SPK fuel component, and since we wanted to simulate the ignition of SPK fuel, we initially compared the ignition delays of *n*-decane [28] with our computations. As can be seen from Figure 3, the present model represents reasonably well the ignition of *n*-decane/air mixtures under shock-tube conditions.



Figure 3: Ignition of *n*-decane/air (model vs. literature data [28]) and SPK/air (model) at 13 atm.



Figure 4: Ignition of a stoichiometric SPK ($C_{11}H_{22}$)/air mixture at atmospheric pressure. The data (symbols) [6] are compared to the modeling (line; model fuel: 8738 ppm of *n*-decane and 5855 ppm of *iso*-octane).

The ignition delays of SPK $(C_{11}H_{22})/air$ mixtures were computed. An example is given in Figure 3 showing that SPK ignition is similar to that of n-decane above 900 K while SPK is less reactive at lower temperatures due to the presence of isooctane that is less ignitable than *n*-decane under these conditions. Since the model seemed to perform well, it was used to model the SPK ignition experiments available from the literature[6]. Figures 4 and 5 present a comparison between the literature data and the present modeling. As can be seen from Figure 4, the proposed kinetic model well predicts the literature ignition data under stoichiometric conditions. Also the presently predicted ignition delays are very similar to those predicted earlier [6]. The effect of the variation of the equivalence ratio on the ignition of SPK was also modeled, based on previous experiments [6]. The model confirms the increase of ignition delays from fuel-rich to fuel-lean conditions below 1000 K.



Figure 5: Ignition of SPK ($C_{11}H_{22}$) at atmospheric pressure and 3 equivalence ratios (model vs. literature data [6]): $\varphi=0.5$ (dotted line; model fuel: 4396 ppm of *n*-decane and 2946 ppm of *iso*-octane); $\varphi=1$ (dashed line); $\varphi=1.5$ (continuous line; model fuel: 13028 ppm of *n*-decane and 8729 ppm of *iso*-octane).



Figure 6: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 0.5. The initial mole fractions were: fuel, 0.1%; O₂, 3.52%; N₂, 96.38%. The experimental data (large symbols) are compared to the computations (lines and small symbols).



Figure 6 Cont'd: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 0.5. The initial mole fractions were: fuel, 0.1%; O₂, 3.52%; N₂, 96.38%. The experimental data (large symbols) are compared to the computations (lines and small symbols).

Again, the model seems to behave reasonably well and mostly matches previous modeling results [6].

Figures 6–9 show examples of the JSR results obtained at 10 atm for the oxidation of SPK and SPK/Jet A-1 fuels. In the computations, the 1000 ppm of SPK were represented by a mixture of 745 ppm of *n*-decane, 500 ppm of *iso*-octane, and 6 ppm of *n*-propylbenzene (H/C=2.2 for the surrogate SPK). As can be seen from these figures, a cool-flame is observed in the temperature range 560–740K.



Figure 7: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 1. The initial mole fractions were: fuel, 0.1%; O₂, 1.76%; N₂, 98.14%. The experimental data (large symbols) are compared to the computations (lines and small symbols).

Above that temperature range, a high-temperature oxidation regime is observed with large conversion of the fuel to intermediates and final products (CO₂ and H₂O). These figures also show that the present model represents reasonably well the measured concentration profiles obtained for O₂, H₂, CO, CO₂, H₂O, C₂H₂, and 1,3-C₄H₆.



Figure 7 Cont'd: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 1. The initial mole fractions were: fuel, 0.1%; O₂, 1.76%; N₂, 98.14%. The experimental data (large symbols) are compared to the computations (lines and small symbols).



Figure 8: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 2. The initial mole fractions were: fuel, 0.1%; O₂, 0.88%; N₂, 99.02%. The experimental data (large symbols) are compared to the computations (lines and small symbols).



Figure 8 Cont'd: Oxidation of SPK in a JSR at 10 atm, τ = 1s and ϕ = 2. The initial mole fractions were: fuel, 0.1%; O₂, 0.88%; N₂, 99.02%. The experimental data (large symbols) are compared to the computations (lines and small symbols).

The model generally over predicts the concentrations of CH₂O, methane, ethane, and isobutene. In fuel lean conditions ethylene and propene are also over-predicted while in fuel-rich conditions, the model represents well the data. Nevertheless, the different oxidation regimes of SPK, i.e. cool-flame, negative temperature coefficient, and high-temperature are well predicted by the proposed model.

The overestimation of methane and ethane mole fractions is indicative of an overestimation of the concentration of methyl radicals that produce these species via H-atom abstraction and recombination reaction:

$$CH_3 + RH \rightarrow CH_4 + R$$

 $CH_3 + H \rightarrow CH_4$
 $CH_3 + CH_3 \rightarrow C_2H_6.$

The over-production of methyl radicals is due to the too highly branched character of *iso*-octane which has 3 branched methyl groups while most of the *iso*-alkanes present in SPK have only one. Therefore, the *iso*-paraffinic fraction of the fuel is not well-represented by *iso*-octane. Less branched *iso*alkanes such as 2-methyl-heptane or 2-methyl-decane, as proposed earlier[29], should be better surrogate components. However, to date there is no data and no validated model available for their kinetics of oxidation.



Figure 9: Oxidation of a 50/50 SPK/Jet A-1mixture in a JSR at 10 atm, τ = 1s and φ = 1. The initial mole fractions were: fuel, 0.1%; O₂, 1.7%; N₂, 98.2%. The experimental data (large symbols) are compared to the computations (lines and small symbols).

Similar agreement between the JSR data and the modeling was observed for the oxidation of the SPK/Jet A-1 mixtures as exemplified in Figure 9. In these computations, the 1000 ppm of fuel were represented by a mixture of 756 ppm of *n*-decane, 246 ppm of *iso*-octane, 116 ppm of *n*-propylbenzene, and 76 ppm of *n*-propylcyclohexane.

Kinetic computations were used to interpret the results. For the oxidation of SPK at 10 atm, 640 K, and in stoichiometric conditions (Figure 10), OH radicals are responsible for most of the oxidation of the fuel components (*n*-decane 98%, *iso*-octane 96%). Under these conditions, the formation of OH radicals is mainly due to the decomposition of alkylhydroperoxy (O₂QOOH and OQ'OOH) produced through the oxidation of *n*-decane (R + O₂ \Rightarrow RO₂; RO₂ \Rightarrow QOOH; QOOH + O₂ \Rightarrow O₂QOOH). As a result, under these conditions, the overall kinetics of oxidation of the fuel is driven by the oxidation of *n*-decane which has a higher reactivity than *iso*octane and feeds the radical pool.



Figure 10: Sensitivity spectrum for CO_2 during the oxidation of SPK in a JSR at 640 K. Only the main sensitive reactions are shown.

Thus, the main oxidation channels of *n*-decane show large positive influence on CO₂ formation. The oxidation of *iso*-octane consumes OH radicals to produce radicals (2,2,4-trimethyl-pent-1-yl and 2,2,4-trimethyl-pent-3-yl) that do not contribute efficiently to chain branching but form stable intermediates. These processes reduce the overall rate of oxidation of the fuel mixture and CO₂ production rate.

Above ca. 750 K, the negative temperature coefficient regime ends and a transition to the high-temperature oxidation regime occurs. At 1100 K, the oxidation of the fuel components

is still mostly due to reactions with OH radicals (i.e. ca. 88% for *n*-decane and 90% for *iso*-octane). The reactions of *n*-decane and *iso*-octane with O (ca. 5%) also contribute to their consumption. The present sensitivity analyses (Figure 11) showed that CO_2 formation is mostly influenced by the main chain branching reaction, i.e. $H + O_2 \rightleftharpoons OH + O$ and to the kinetics of oxidation of CO by OH and CH₃ by HO₂.



Figure 11: Sensitivity spectrum for CO_2 during the oxidation of SPK in a JSR at 1100 K. Only the main sensitive reactions are shown.

CONCLUSION

The kinetics of oxidation of a synthetic paraffinic jet fuel and a 50/50 mixture with a commercial Jet A-1 were studied in a pressurized jet-stirred reactor under the same initial conditions, i.e. over the temperature range 560–1030K, at 10 atm, for equivalence ratios of 0.5, 1, and 2, and using 1000 ppm of fuel. The JSR results consisting of concentration profiles versus temperature for reactants, stable intermediates, and products obtained by GC and FTIR were used for kinetic modeling.

A detailed kinetic scheme consisting of 6228 reversible reactions involving 2006 species was used for the chemical kinetic modeling of the JSR experiments and of literature ignition experiments. The SPK fuel was represented by a 2-component surrogate mixture: *n*-decane and *iso*-octane were used. The small aromatic fraction (0.5%) in one of the synthetic kerosenes was represented by *n*-propylbenzene. The kinetic modeling showed reasonable agreement between the data and the computations. The SPK was determined to be more reactive than conventional Jet A-1 under JSR conditions but, according to the proposed model, less ignitable than *n*-decane,

particularly below 900 K. The main reaction paths involved in the oxidation of SPK were delineated through kinetic modeling. The great importance of reactions producing and consuming OH radicals was highlighted.

Improvements to the proposed kinetic model are still necessary. SPK flame speeds would be useful to further assess the validity of the proposed kinetic model. The use of an *iso*-alkane less branched than *iso*-octane should help improving the kinetic modeling.

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