



Combustion of synthetic jet fuels: Naphthenic cut and blend with a gas-to-liquid (GtL) jet fuel

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Received 30 November 2015; accepted 30 May 2016
Available online 15 June 2016

Abstract

There is increasing interest for utilizing synthetic biofuels in blends with conventional oil-derived liquid fuels. In this context, research on the combustion of synthetic jet fuels has lately gained significance because they could help addressing sustainability and security of supply for air transportation. Improving the kinetic modeling of the oxidation of synthetic fuels requires further investigations under well-controlled conditions. The combustion of a 100% naphthenic cut fitting typical chemical composition of biomass or coal liquefaction products and a 50% vol. mixture with Gas to Liquid fuel were studied in a jet-stirred reactor (JSR) under the same conditions (550–1150 K, 10 bar, equivalence ratio of 0.5, 1, and 2, and 1000 ppm of fuel). For simulating the kinetics of oxidation of these fuels, model-fuels were designed to fit fuels chemical composition and properties. They consisted of mixtures of n-decane, 2-methylheptane, 3-methylheptane, n-propylcyclohexane, decahydronaphthalene, and tetrahydronaphthalene. The proposed detailed chemical kinetic reaction scheme was validated using the whole experimental data set acquired in the present work; for the oxidation of pure GtL, we used previous obtained data. For interpreting the results, reaction pathways and sensitivity analyses were used.

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Keywords: Jet fuel; Gas-to-liquid; Naphthenic cut; Jet-stirred reactor; Modeling

1. Introduction

Whereas there is growing importance of electric-powered ground transportation, combustion in aero gas turbines will remain important for years. In this context, reducing carbon foot print and dependence of air transportation on oil represent tremendous challenges that synthetic and bio-derived kerosene could help address-

ing [1–3]. The Fischer–Tropsch (F-T) synthesis produces liquid fuels (n-paraffins) from syngas. After post-processing (isomerization, cyclization) synthetic kerosenes mainly containing n-alkanes, iso-alkanes, and naphthenes [4] are produced. Their chemical properties (e.g., degree of isomerization or aromaticity) are adjusted to comply with specifications for fuels usable in commercial semi-synthetic jet fuels. The very low fraction of aromatic hydrocarbons in GtL kerosene yields to a reduction of unburned hydrocarbons and soot emissions [2,5,6]. The composition of synthetic paraffinic jet fuels allows also lowering fossil

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Table 1
Properties of the fuels studied experimentally.

Properties	GtL	NC ^a	NC/GtL
Formula	C _{10.45} H _{23.06}	C _{12.64} H _{23.64}	C _{11.54} H _{23.35}
M (g/mol)	148.44	175.32	161.83
H/C ratio	2.20	1.87	2.02
DCN ^b	58.0	39.3	45.8
Density (g/l)	737.7	863.1	800.3

^a Naphthenic cut.

^b Derived cetane number measured, ASTM D7668.

carbon dioxide emissions [7]. This fuel is a good alternative to conventional oil-derived jet fuels.

This work intends to provide (i) kinetic data for synthetic jet fuels oxidation and (ii) a representative combustion model. The kinetics of oxidation of substitute jet fuels (GtL, naphthenic cut) were studied in a JSR under the same initial conditions. GtL is produced by converting natural gas into liquid hydrocarbons through partial oxidation, yielding syngas, and F-T synthesis. GtL is almost colorless and odorless. It contains almost none of the impurities found in conventional jet fuels, i.e., sulphur and nitrogen compounds or aromatics. The naphthenic cut used here is a commercial solvent fitting typical chemical composition of products coming from the liquefaction of coal or biomass. This work provides additional information to our earlier experimental and computational results [8,9]. Model-fuels were designed to model the oxidation of a naphthenic cut and its mixture with a GtL jet fuel. A detailed kinetic reaction scheme was validated against the present and previously obtained [9] experimental results.

2. Experimental

The experiments were performed in a jet-stirred reactor (JSR) analogous to that described in previous publications [9–11]. The JSR consisted of a 2 cm radius sphere of 33 cm³ in volume. It is made of fused SiO₂ to reduce catalyzed reactions on inner wall. Four injectors opposite in pairs with 1 mm inner diameter nozzles allowed getting highly homogeneous reaction mixtures. The reactants were highly diluted with N₂ and mixed before admission into the JSR injectors. 99.995% pure oxygen was used in the experiments. The reactants were preheated before being admitted inside the JSR for limiting temperature gradients inside the reactor. Two insulated heating wires (Thermocoax) surrounded the reactor to heat the reaction zone to the working temperature. Before injection into the reactor, the liquid fuels were sent by a Shimadzu LC10 ADVP pump to a temperature regulated in-house atomizer-vaporizer assembly kept at ca. 550 K.

Table 1 gives the main properties of the fuels studied here. The composition of the fuels and

their molecular weight were determined through gas chromatography (<http://www.alfa-bird.eu-vri.eu/>) and used in earlier publications, e.g. [9]. The mass percent composition of the GtL fuel was 62.8% iso-alkanes, 28.1% n-alkanes, 8.8% naphthenes, and 0.2% aromatics. A naphthenic cut was also considered in this work. Its mass percent composition was 4.7% paraffins, 85.2% cyclo-paraffins, 9.6% monoaromatics and 0.5% polyaromatics. The oxidation of a mixture of the naphthenic cut and the GtL jet fuel 50:50 v:v was also studied.

A low-pressure fused-silica sonic probe was used to collect gas samples of the reactive mixture in the JSR at stable residence time and temperature. In order to stop the chemical reactions, sampling was done at low-pressure (≤ 50 mbar). Temperature inside the reacting zone was measured using a 0.1 mm Pt/Pt-Rh thermocouple protected by a thin-wall fused silica tube. The mobility of the probe-thermocouple assembly allows sampling and temperature measurements at various locations inside the reactor. We recorded temperature gradients lower than 3 K/cm along the JSR vertical axis. The working temperature was increased stepwise at constant residence time. In order to get concentration profiles vs. temperature, the samples were analyzed online by gas chromatography (GC) and Fourier Transformed Infrared Spectrometry (FTIR) and offline by GC after collection and storage at low pressure (≤ 50 mbar) in 1 L Pyrex bulbs. The high-boiling point chemicals were analyzed online, whilst low-boiling point species and permanent gases were quantified offline. For the offline analyses we measured the species mole fractions using gas chromatographs equipped with capillary columns (Carboplot-P7, Al₂O₃/KCl, DB-5 ms, DB-624), a flame ionization detector (FID), a mass spectrometer, and a thermal conductivity detector. FTIR analyses (Nicolet Magna 560, 0.5 cm⁻¹ resolution) allowed quantifying online H₂O, CO, CO₂, CH₂O, CH₄, C₂H₂, and C₂H₄. For FTIR analyses, the samples were sent to a temperature controlled gas cell (413 K, 2 m path length, 500 mbar) using a 6.35 mm o.d. deactivated stainless-steel heated tube (473 K). A good repeatability of the measurements and a reasonably good C-balance (on average 100 \pm 15%) were observed. Because many oxygenated intermediates were not quantified, no O-balance could be computed. The experiments were performed at 10.0 \pm 0.1 bar, over the temperature range 550–1150 K, and at a fixed mean residence time of 1.00 \pm 0.05 s. Mole fractions of reactants, stable intermediates, and final products were measured as a function of temperature at three equivalence ratios ($\varphi = 0.5, 1.0, \text{ and } 2.0$).

3. Modeling

The kinetic computations employed the PSR code [15]. The complex fuels were represented by

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