



Experimental and detailed kinetic model for the oxidation of a Gas to Liquid (GtL) jet fuel



Philippe Dagaut^{a,*}, Florent Karsenty^a, Guillaume Dayma^a, Pascal Diévert^a, Kamal Hadj-Ali^a, Amir Mzé-Ahmed^a, Marina Braun-Unkhoff^{b,*}, Jürgen Herzler^b, Trupti Kathrotia^b, Thomas Kick^b, Clemens Naumann^b, Uwe Riedel^b, Levi Thomas^{b,1}

^a Centre National de la Recherche Scientifique, 1C, Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France

^b Institute of Combustion Technology, German Aerospace Center (DLR), Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

ARTICLE INFO

Article history:

Available online 14 September 2013

Keywords:

Jet fuel
Ignition delay
Flame speed
Jet-stirred reactor
Shock tube
Kinetic modeling

ABSTRACT

The kinetics of oxidation, ignition, and combustion of Gas-to-Liquid (GtL) Fischer–Tropsch Synthetic kerosene as well as of a selected GtL-surrogate were studied. New experimental results were obtained using (i) a jet-stirred reactor – species profiles (10 bar, constant mean residence time of 1 s, temperature range 550–1150 K, equivalence ratios $\varphi = 0.5, 1, \text{ and } 2$), (ii) a shock tube – ignition delay time (≈ 16 bar, temperature range 650–1400 K, $\varphi = 0.5$ and 1), and (iii) a burner – laminar burning velocity (atmospheric pressure, preheating temperature = 473 K, $1.0 \leq \varphi \leq 1.5$). The concentrations of the reactants, stable intermediates, and final products were measured as a function of temperature in the jet-stirred reactor (JSR) using probe sampling followed by on-line Fourier Transformed Infra-Red spectrometry, and gas chromatography analyses (on-line and off-line). Ignition delay times behind reflected shock waves were determined by measuring time-dependent CH^* emission at 431 nm. Laminar flame speeds were obtained in a bunsen-type burner by applying the cone angle method. Comparison with the corresponding results for Jet A-1 showed comparable combustion properties. The GtL-fuel oxidation was modeled under these conditions using a detailed chemical kinetic reaction mechanism (8217 reactions vs. 2185 species) and a 3-component model fuel mixture composed of *n*-decane, *iso*-octane (2,2,4-trimethyl pentane), and *n*-propylcyclohexane. The model showed good agreement with concentration profiles obtained in a JSR at 10 bar. In the high temperature regime, the model represents well the ignition delay times for the fuel air mixtures investigated; however, the calculated delays are longer than the measurements. It was observed that the ignition behavior of the surrogate fuel is mainly influenced by *n*-alkanes and not by the addition of *iso*-alkanes and *cyclo*-alkanes. The simulated laminar burning velocities were found in excellent agreement with the measurements. No deviation between burning velocity data for the GtL-surrogate and GtL was seen, within the uncertainty range. The presented data on ignition delay times and burning velocities agree with earlier results obtained for petrol-derived jet fuel. The suitability of both the current detailed reaction model and the selected GtL surrogate was demonstrated. Finally, our results support the use of the GtL fuel as an alternative jet fuel.

© 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

1. Introduction

Fossil fuels are currently the primary energy source worldwide [1]. In the 21st century, alternative energy resources became increasingly used [2] to guarantee security of supply and to mitigate global warming. Correspondingly, the search for alternative aviation fuels has grown rapidly over the last 10 years. In 2011,

the European Advanced Biofuels Flight Path was launched by the European Commission for the purpose of accelerating the commercialization of aviation biofuels [3]. However, this effort is technically challenging due to strict fuel specifications which include: fuel freezing point, energy density, flash point, flammability limit, and amount of aromatics [4,5]. It is important, therefore, to improve our knowledge of synthetic jet fuel properties through experimental characterization and computational fluid dynamics modeling. For optimizing applications of synthetic fuels in aero-engines, their combustion properties must be well characterized and understood. Therefore, ignition delay times and laminar flame speed as well as transient chemical species and combustion products, must be measured over a broad range of conditions

* Corresponding authors. Fax: +33 238 696004 (P. Dagaut), fax: +49 7116862578 (M. Braun-Unkhoff).

E-mail addresses: dagaut@cnr-orleans.fr (P. Dagaut), Marina.Braun-Unkhoff@dlr.de (M. Braun-Unkhoff).

¹ On exchange from Wright Patterson Air Force Base, Ohio, USA.

(temperature, pressure, fuel composition, and equivalence ratio). Nevertheless, only limited data sets exist for the combustion of synthetic jet fuels which are complex mixtures of several chemical classes [6,7].

Measurement of the ignition delay time of kerosene [7–12] and of GtL [8,10–12], has been the subject of a few studies while some data exist for various surrogates [7,9,13–16]. Concerning laminar flame speed measurements of GtL fuels, only a few investigations are published [17–20].

Concerning modeling the oxidation of a jet fuel, it is not possible to incorporate in the reaction model all of the species composing kerosene. Instead, a surrogate is used, with a limited number of compounds with known kinetic sub-models as a means to represent kerosene [4]. 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. Depending on the objective, 3–7 well-selected hydrocarbons might be present in the initial formula of a surrogate, to describe the combustion properties of practical blends. Presently, many proposals concerning the composition of a surrogate fuels exist, see e.g. [4,7,9,14,15].

As part of continuing efforts in our laboratories to improve our knowledge of fuels combustion, the oxidation kinetics of a GtL jet fuel and a selected GtL surrogate were studied in a jet-stirred reactor (JSR) at 10 bar, over a range of temperatures and equivalence ratios. Ignition delays of GtL/synthetic air mixtures diluted in nitrogen and of a GtL-surrogate blend were measured. The experiments were performed at initial pressures of about 16 bar and at two equivalence ratios. Burning velocities of the GtL jet fuel and of a selected surrogate mixed with air were measured at ambient pressures and a preheating temperature of 473 K. A detailed chemical kinetic reaction mechanism was proposed to represent the present data, complementing recent developments on the formulation of alternative jet fuel surrogates and kinetic combustion models [8,9,21].

2. Experimental

To understand a fuel's combustion under aero-turbine operating conditions several aspects have to be considered. These processes occur over a range of temperatures, pressures, and fuel–air ratios and are considered to be among the most important operating parameters for an aero-turbine. The main focus of the current work is the oxidation of the fuel and the formation of pollutants but also major combustion properties, i.e. burning velocity and ignition. To investigate each of these parameters, complementary

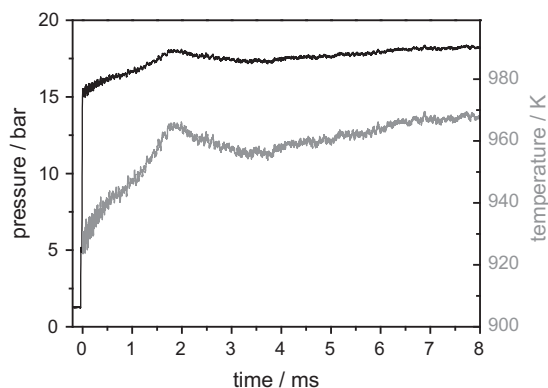


Fig. 2. Typical pressure (black line) and derived temperature (grey line) profile assuming adiabatic isentropic compression obtained for a non-igniting fuel/air mixture (dilution 1:2) at the following conditions: $T_{5,\text{initial}} = 929\text{ K}$ and $p_{5,\text{initial}} = 15.30\text{ bar}$.

experimental systems were used: a jet stirred reactor for studying fuel oxidation and pollutants formation, a shock tube to study self-ignition of the fuel, and a flame test rig to measure laminar flame speeds. Each test rig was used to investigate the combustion of several fuels; the results were used for developing a detailed kinetic reaction scheme. The same GtL fuel was used in all the experiments (JSR, shock tube, and flame): a GtL Fischer–Tropsch synthetic jet fuel provided by Shell ($\text{C}_{10.45}\text{H}_{23.06}$, $M = 148.44\text{ g mol}^{-1}$, density = 737.7 g l^{-1} , composition in mass%: 28.1% *n*-alkanes, 62.8% *iso*-alkanes, 8.8% *cyclo*-alkanes, and 0.2% aromatics). Detailed GC/MS analyses were used to determine the mass composition of the fuel and derive the global chemical formula used here (see Section 3).

2.1. Jet stirred reactor

The experiments were performed in the JSR set-up used previously [22–24]. It consists of a 39 cm^3 fused-silica sphere to avoid wall catalyzed reactions. The reactor has four injectors with nozzles of 1 mm inner diameter (ID) which both admit and stir the gases. A 100 l h^{-1} nitrogen flow was used to dilute the fuel. As presented before [23,24], all gases were preheated to a temperature close to that in the JSR prior to injection in order to reduce temperature gradients. The selected operating temperatures in the reactor were maintained due to a regulated oven. The reactants were mixed just before reaching the injectors. Nitrogen (<50 ppm of O_2 ; <1000 ppm of Ar; <5 ppm of H_2 , Air Liquide) was used as bath

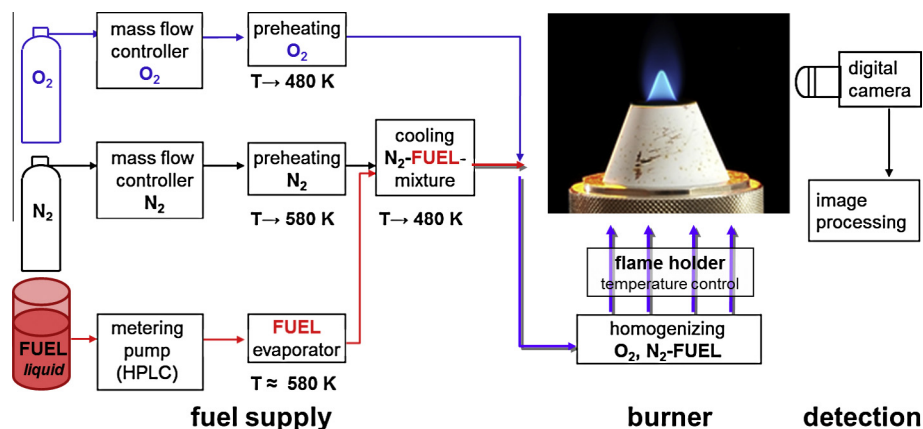


Fig. 1. Experimental set up used for determining burning velocity of a liquid fuel.

Download English Version:

<https://daneshyari.com/en/article/169640>

Download Persian Version:

<https://daneshyari.com/article/169640>

[Daneshyari.com](https://daneshyari.com)