



Detailed chemical kinetic mechanism for surrogates of alternative jet fuels

Chitralkumar V. Naik^{a,*}, Karthik V. Puduppakkam^a, Abhijit Modak^a, Ellen Meeks^a, Yang L. Wang^b, Qiyao Feng^c, Theodore T. Tsotsis^c

^a Reaction Design, San Diego, CA 92121, USA

^b Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089, USA

^c Mork Family Department of Chemical Engineering and Material Science, University of Southern California, Los Angeles, CA 90089, USA

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ABSTRACT

Blends of *n*- and *iso*-alkane components are employed as surrogates for Fischer–Tropsch (F–T) and biomass-derived jet fuels. The composition of the blends has been determined based on data available for two F–T fuel samples obtained from different sources, using a systematic optimization approach. A detailed chemical kinetic mechanism for combustion of the surrogate blends has been assembled. The mechanism has been validated against fundamental experimental data. While drawing initially from other studies in the literature, the mechanism has been improved by enforcing self-consistency of the kinetic and thermodynamic data for the various surrogate-fuel components represented by the mechanism. These improvements have led to more accurate predictions of flame propagation, flame extinction, and NO_x emissions. As part of the validation process, simulations were performed for a wide variety of experimental configurations, as well as for a wide range of temperatures and equivalence ratios for fuel/air mixtures. Comparison of the model predictions to the available literature data confirms the accuracy of the mechanism as well as of the approach for selecting the surrogate blends.

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1. Introduction

Fischer–Tropsch (F–T) fuels are of increased interest as alternative jet fuels. They can be appropriately tailored for specific applications. The feedstock for such fuels also varies from natural gas to bio-derived syngas. However, combustion and emissions characteristics of different F–T fuels are not yet understood in sufficient detail. It is critical to understand these characteristics when considering them as potential replacements of or blending components with conventional jet fuels, such as Jet-A. Accurate models will assist in understanding the behavior of these fuels and the effects of fuel variability during combustion.

F–T fuels are less complex in composition than conventional fossil fuels that contain many different fuel classes and hundreds of components. Despite that, F–T fuels contain tens to hundreds of hydrocarbon components and their compositions vary depending on the different manufacturing processes. Accurate combustion and emissions modeling require good surrogate-fuels to represent the fuel chemistry of the practical fuel. This study focuses on gaining a better understanding of F–T fuels by developing accurate surrogate blends to represent the fuels and a detailed chemical kinetic mechanism for these surrogates. In developing the surrogate and its detailed mechanism, we have employed fundamental

experimental data to validate predictions of the combustion and emission characteristics. Measurements of NO_x in laminar flames of various pure components and surrogates have been performed in this work. The rest of the fundamental data used for validation has been obtained from the literature. In this paper, we first discuss appropriate surrogates for specific fuels and then the development of a detailed reaction mechanism for these surrogates. Validation of model predictions of combustion behavior for the pure components and surrogate blends using various fundamental experimental data is then reported. This is followed by a discussion of important reaction pathways.

In addition to F–T fuels, we have also considered applying the model to the biomass-derived jet fuels. Biomass-derived fuels are another form of alternative jet fuel. The composition of biomass-derived jet fuel are expected to have similar composition [1,2] to that of the F–T fuels (discussed in the next section). Therefore, we expect the same models to be useful for both types of alternative jet fuels, although the surrogate blend composition may be different for different sources of fuels. Validation of the model against the limited fundamental experimental data available for a bio-jet fuel sample (R-8) has also been reported.

2. Identification of appropriate surrogate blends for F–T fuels

Two different F–T fuels, namely Syntroleum S-8 and Shell GTL, have been studied in this work. Both were produced from natural

* Corresponding author. Fax: +1 858 550 1925.

E-mail address: cnaik@reactiondesign.com (C.V. Naik).

gas using low temperature hydro cracking and isomerization process using cobalt [3]. Detailed composition of the fuels have been provided by the Air Force Research Laboratory [4]. Detailed analysis for S-8 composition is shown in Table 1 and the overall fuel class distribution in Fig. 1. Shell GTL fuel also includes all saturated long-chain paraffins with up to two methyl side-chain components. The major distinctions between Shell GTL and S-8 fuels are that Shell GTL has a narrower carbon number distribution than that of S-8, as shown in Fig. 2, and the Shell GTL fuel contains higher amounts of *n*-alkanes (approximately 35 mol%) than those found in S-8 (approximately 26 mol%). In general, for both F–T fuel samples, the dominant components consisted of C₇ to C₁₆ *n*- and *iso*-paraffins with a narrower distribution in Shell GTL (C₈ to C₁₂). The F–T fuels contain a high concentration of *iso*-paraffins (65–74 mol%), which consist of only one or two methyl branches (–CH₃) on a straight-chain alkane. In addition, based on the carbon number distribution shown in Fig. 2, more than half of these alkanes have a C₁₀ to C₁₂ chain. Capturing this range of carbon number components in a surrogate helps reproduce the overall variation of components in the fuels. The presence of lower carbon number components (C₈) mainly affects the initial boiling point for the F–T fuel. Including components with C₈, C₁₀, and C₁₂ saturated linear and slightly branched hydrocarbons in a surrogate provides a reasonable approximation of the overall chemical structure of F–T fuels.

In order to generate a general-purpose surrogate to represent the physical and chemical properties, the focus of this study was

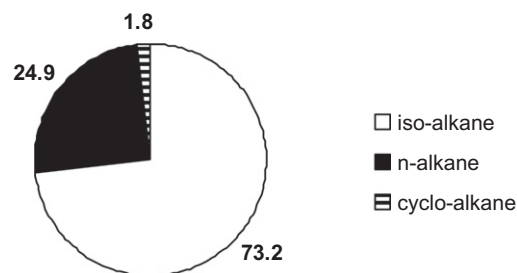


Fig. 1. Hydrocarbon class analysis of the S-8 F–T fuel in mol%.

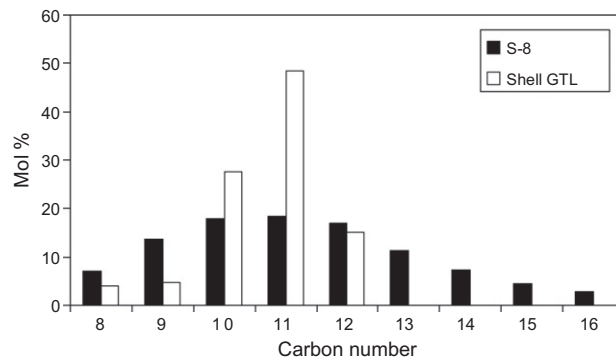


Fig. 2. Carbon number distribution in the S-8 F–T fuel based on Ref. [3].

Table 1

Detailed analysis of fuel composition for S-8 based on the data provided by AFRL [4].

No.	Component name	mol%
1	2-Methyl heptane	0.62
2	3-Methyl heptane	0.84
3	1,2,3-Trimethyl cyclopentane	1.85
4	2,5-Dimethyl heptane	2.17
5	4-Methyl octane	4.80
6	3-Methyl octane	2.53
7	<i>n</i> -Nonane	3.11
8	3,5-Dimethyl octane	1.98
9	2,6-Dimethyl octane	1.45
10	4-Ethyl octane	1.98
11	4-Methyl nonane	3.65
12	2-Methyl nonane	1.95
13	3-Methyl nonane	2.65
14	<i>n</i> -Decane	3.93
15	2-5-Dimethyl nonane	2.25
16	5-Ethyl-2-methyl octane	1.94
17	5-Methyl decane	2.52
18	4-Methyl decane	2.17
19	2-Methyl decane	2.93
20	3-Methyl decane	3.03
21	<i>n</i> -Undecane	4.64
22	<i>x</i> -Methyl undecane	3.05
23	3-Methyl undecane	2.20
24	5-Methyl undecane	3.25
25	4-Methyl undecane	2.00
26	2-Methyl undecane	2.05
27	2,3-Dimethyl undecane	2.32
28	<i>n</i> -Dodecane	4.97
29	4-Methyl dodecane	1.78
30	<i>x</i> -Methyl dodecane	1.43
31	2-Methyl dodecane	2.48
32	<i>x</i> -Methyl dodecane	2.45
33	<i>n</i> -Tridecane	3.33
34	4-Methyl tridecane	1.60
35	6-Propyl tridecane	2.02
36	<i>x</i> -Methyl tridecane	2.04
37	<i>n</i> -Tetradecane	2.99
38	<i>x</i> -Methyl tetradecane	2.30
39	5-Methyl tetradecane	1.38
40	<i>n</i> -Pentadecane	1.98
41	<i>x</i> -Methyl tetradecane	1.39

to propose simple surrogates that not only represent combustion and emission characteristics of F–T fuels but also reflect some of the fuel composition and structural characteristics, as well as some of the physical properties like liquid density. Cetane Number is one important indicator of the combustion characteristics of jet fuels. Fundamental laminar flame properties that are governed by high-temperature chemical kinetics are also relevant for jet-engine combustion. NO_x and soot emissions are additional factors that should be considered when designing the surrogate. Though physical properties are of lesser importance from a pure-combustion modeling point of view, it is desirable to capture also some physical properties. A single component surrogate may be able to describe one or a few combustion characteristics such as laminar flame speeds, but is not likely to be able to accurately capture a broader range of characteristics and certainly cannot reflect effects of differences in fuel composition like carbon number variation and boiling range. Capturing physical properties with surrogate is useful for Computational Fluid Dynamics (CFD) modeling where spray and evaporation are important along with fuel-combustion chemistry.

In this study, we have limited the choice of components to three in order to limit the size of the detailed reaction mechanism and at the same time capture the range of carbon number variation, initial boiling point, and Cetane Number (CN) of F–T fuels. Another constraint in component selection for surrogates was the availability of sufficiently accurate detailed reaction mechanisms. We have selected the components for which there existed detailed reaction mechanisms in the literature that we used to assemble a unified master mechanism for the surrogates discussed in the next section. We selected a three-component blend of *n*-dodecane, *n*-decane, and *iso*-octane for both F–T fuels. The same blend is also tested for biomass-derived jet fuels as. *n*-Dodecane and *n*-decane are selected to represent the peaks in carbon number distribution as seen in Fig. 2. They also represent well the linear alkanes in practical fuels. While *iso*-decane and *iso*-dodecane could be good choices of components for representing the branched alkane class,

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