Comparison of the experimental and kinetic study of two aviation surrogate fuels

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1 Introduction

As the major energy source of aircraft engine, aviation fuels are always considered on its combustion efficiency and pollution. In case to study the combustion chemistry mechanism of aviation fuels, surrogate fuels were widely used and efficient on the mechanism establishment in decades. Surrogate components are selected based on the components of jet fuels, which should represent the physical properties, chemical properties, or combustion properties (kinetic, speed or efficiency of combustion) of jet fuels. Some literatures [1-4] shows that the jet fuels mainly consist of alkanes, aromatics and naphthenes.

In 2006, Dagaut et al. present a review of Jet-A, Jet A-1, JP-8, TR0 and their corresponding surrogate combustion [5]. The conclusion said that more data of high pressure and lean condition flame are necessary. After that, more studies of surrogate fuels are performed including flame, low-temperature oxidation and high pressure ignition [1-4, 6-8]. Among these studies, a surrogate fuel presented by Honnet et al. [9] (74% n-decane and 26% 1,2,4-trimethylbenzene) was famous and widely used in the simulation of jet fuels. Wang et al. [10, 11] from our group studied a similar surrogate (74% n-decane and 26% 1,3,5-trimethylbenzene, 2-C surrogate) in 2018 and presented a detail mechanism of oxidation and high pressure ignition.

RP-3 is the most widely used jet fuel in China. Zheng et al. [12] used GC and GC-MS to detect the consistent of RP-3 jet fuel, and released that RP-3 is composed by 53.0% alkanes, 4.6% aromatics 37.7% naphthenes and other species. The surrogate fuels of RP-3 were rarely studied, several groups reported their surrogate studies on RP-3 [12-16]. Xu et al. present a surrogate consists with 66.2% n-dodecane, 18.0% 1,3,5-trumethylcyclohexane, and 15.8% n-propylbenzene (3-C surrogate) to study RP-3 jet fuel. They studied the ignition delay times in a high pressure shock tube and compared with the ignition delay times of RP-3. Based on this study, our group investigate the oxidation, high pressure ignition and flame speed of this surrogate and present a comprehensive kinetic model.

This work compares the two surrogate fuels studied by our groups on both experimental and simulated results, and aim to release the combustion properties and the relationship between the surrogates and jet fuels. Table 1 shows some chemistry properties of the two surrogates and the corresponding jet fuels.

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Table 1: chemistry properties of two surrogates and jet fuels

Surrogate / Jet Fuel	H/C ratio	Mole Weight g/mol
2-C surrogate	2.016	155
3-C surrogate	2.033	148
JP-8	1.919	152
RP-3	2.049	150

2 Experiments

The experiments of 2-C surrogate and 3-C surrogate were performed and presented in previous literatures [11]. The volume of the reactor sphere is 65 cm3 with the diameter of 5cm. The temperature range is 500-1100K and the increasement is 25K between the data points. The inlet concentration of 2-C surrogate and 3-C surrogate are 1.0 vol.% and 0.5 vol.%, respectively. Thus, the mole fraction of 3-C surrogate experiments and simulations shown in the following parts are normalize to 1.0 vol.% inlet concentration. The surrogate fuels are inject into a gasification tank by a high-pressure infusion pump and gasified at 473 K. The gas phase surrogate is carried out by 450 sccm gas flow of Ar. The flow rates are controlled by MKS mass-flow controllers. The pipes were preheated to 473K before and after JSR to avoid condensation. The JSR is heated by a furnace. The reaction temperature was measured by a K-type thermocouple located at the center of the sphere. Online GC and GC-MS are equipped after furnace to qualify and quantify the mole fraction of reactants, products, and intermediates in the experiments. Two different detectors are used on GC; TCD is used to analyze H_2, CO, CO_2 and CH_4, and FID is used to analyze light hydrocarbons and aromatics. Light hydrocarbons and aromatics are quantified by chromatographic columns of Al2O3-KCl and HP-INNOWax, respectively. The calibration was performed by injecting known amounts of the standard gas. The detection threshold of GC was about 0.1 ppm for FID and 10 ppm for TCD. The estimated uncertainty was about ±5% for major species and ±15% for intermediates. A list of the species profiles measured is included in the Supplements.

3 Modeling

The simulation work is performed by using CHEMKIN II software [17]. PSR code is used to calculate the results of oxidation, and the SENKIN code is used for ignition simulation. The mechanisms come from our previous work; 2-C surrogate mechanism is presented by Wang et al. [11], and 3-C surrogate mechanism is presented by Liu et al. [18]. The 2-C surrogate mechanism is established based on the acetylene mechanism presented by Wang et al. [19], the n-decane mechanism presented by Biet et al.[20], and the 1,3,5-trimethylbenzene mechanism from Diévart et al. [21] with the modification by Wang et al. [10]. The 3-C surrogate mechanism consists of acetylene mechanism (Wang et al. [19]), n-propylbenzene sub-mechanism (Liu et al. [22]), n-dodecane sub-mechanism (Banerjee et al. [23]), and 1,3,5-trimethylcyclohexane sub-mechanism which is estimated from methylcyclohexane (Wang et al.[24]). The coupled reactions in two surrogate mechanisms are estimated mostly based on Biet et al. [20], Zeng et al. [25] and Sivaramakrishnan et al. [26].

4 Results and discussion

Figure 1 shows the comparison of the mole fractions of the surrogate components in the oxidation experiments. The negative temperature coefficient (NTC) effect is obviously observed in the experiments, and correctly predicted by mechanism. The NTC region of 2-C surrogate starts from 500 K and ends at 775

K, the lowest point is 600 K with about 80% n-decane and 50% 1,3,5-trimethylbenzene (T135MB) consumed. The NTC region of 3-C surrogate is shorter than the region of 2-C surrogate, the onset temperature is 625 K but the end point is as same as the previous one (775 K). The 3-C surrogate NTC region reach the bottom at 675 K. The appearance of the NCT regions are led by long chain alkanes, which are the major component of these two surrogate fuels. The alkane concentration in 2-C surrogate (74% n-decane) is higher than the 3-C surrogate (66.2% n-dodecane), so the onset temperature of 2-C surrogate NTC region is lower than the NTC region of 3-C surrogate. At the meantime, T135MB and n-propylbenzene (NPB) are also affected by NTC effect from alkanes. The alkanes react with O_2 under low temperature and generate HO_2 radical, then the HO_2 radical react with T135MB or NPB lead the consumption of these aromatics at NTC region. The mechanisms give good predictions over the temperature range of 500-1100 K. The two surrogate kinetic models reasonably predict the start and end temperature and the concentrations for all components, especially for aromatics. In the 3-C surrogate oxidation, 1,3,5-trimethylcyclohexane (T135MCH) exhibits stronger NTC influence than NPB. The reason is that NPB is more stable than T135MCH lead by the existence of benzene ring.

Figure 2 exhibits experimental and simulated results of the major products of the oxidation experiments. The two surrogate fuels produce CO and CO_2 and H_2 in a similar tendency when they are oxidizing, both of them show the significant NTC effect under low temperature. The peak temperatures in NCT region are close to the bottom temperatures of the surrogate components mole fraction. The final mole fractions of CO, CO_2, and H_2 in 3-C surrogate are higher than 2-C surrogate, because the average molecular formula of 3-C surrogate ($C_{11.0}H_{22.3}$) is larger than 2-C surrogate ($C_{9.8}H_{19.7}$) and lead more production of CO, CO_2, and H2 under the same inlet concentration. The mechanisms could successfully predict the mole fractions of these major products, besides the CO_2 production under low temperature. The low speed conversion pathways from CO to CO_2 of 3-C surrogate mechanism in NTC region lead this regional under-prediction.

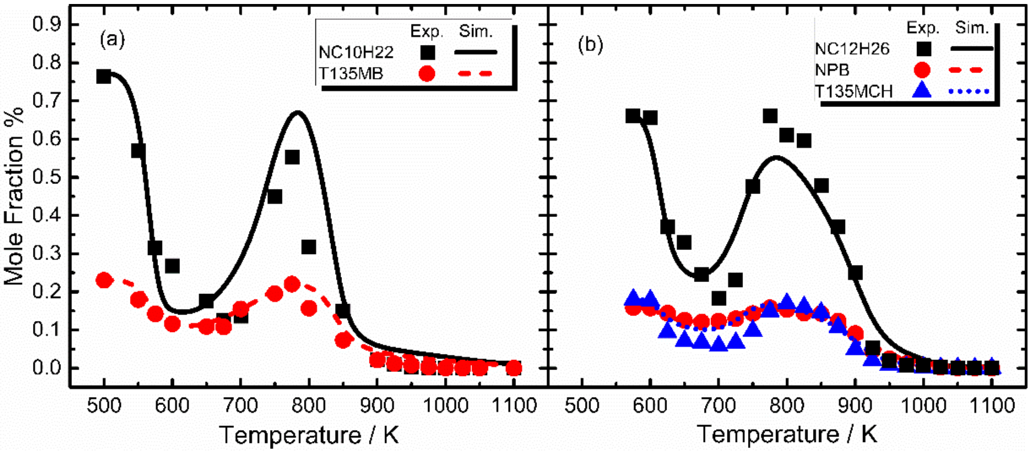

Figure 1. Mole fractions of the components in two surrogate fuels, (a) 2-C surrogate fuel, and (b) 3-C surrogate fuel

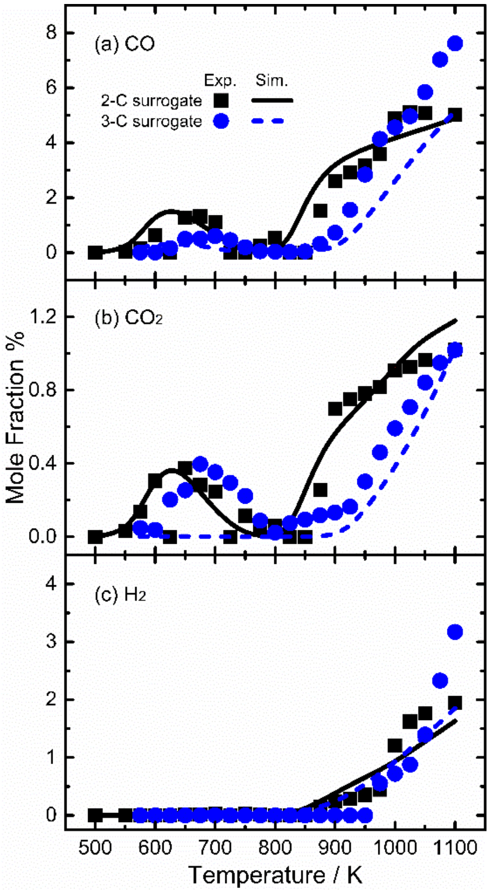

Figure 2. Mole fractions of the major products of the two surrogate fuel oxidation experiments, (black) 2-C surrogate fuel, and (blue) 3-C surrogate fuel

5 Conclusions

This work compare the experimental and simulated results of two surrogate fuels; 2-C surrogate and 3-C surrogate. The chemistry properties reveal that 2-C surrogate is similar to JP-8 jet fuel, and 3-C surrogate is more suitable for RP-3 jet fuel research. Both of the two surrogate oxidation experimental results show significant NTC effect, while the NTC region of 2-C surrogate appears at lower temperature with more consumption of fuel. The comparison of pollutants reveals that 3-C surrogate is a cleaner surrogate fuel which could generate less aromatic and aldehyde pollution than 2-C surrogate. The mechanisms of two surrogate fuel are considered in this work. The mechanisms predict the oxidation and ignition experimental results reasonably, and successfully predict the NTC region in these results. The comparison of ignition delay times indicates that 2-C surrogate mechanism could well predict under low temperature and 3-C surrogate mechanism gives better simulated result at high temperature, and reveals the focus area for further modification of mechanisms. These conclusions will be benefit for the understanding of combustion kinetic of jet fuel and the further studies of surrogate and jet fuels combustion.

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