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Brief Communication

Ignition characteristics of cracked JP-7 fuel

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1. Introduction

High-speed air-breathing propulsion systems often use the endothermic properties of fuels to create an extra heat sink. This involves cracking of the fuel into a mixture of smaller hydrocarbons in a heat exchanger/reactor prior to combustion [1]. Design and development of such endothermic fueled engines require an understanding of the autoignition characteristics of cracked product mixtures. The present work attempts to develop correlations for the ignition delay time of cracked JP-7 fuel. It is also motivated by the development of combustion wave ignition (CWI) systems [2]. These devices provide simultaneous ignition in multiple combustion chambers by delivering detonation or deflagration waves of cracked JP-7/oxygen mixtures through the flame tubes. Investigation of ignition characteristics of cracked JP-7/oxygen mixtures as a function of various initial parameters is a crucial component of this study [2].

JP-7 is a low-volatility endothermic fuel developed specifically for the Mach 3.5 SR-71 aircraft, and has a thermal stability limit of 560 K [3]. It is a highly refined kerosene with low sulfur and aromatics, consisting mainly of alkanes with an average carbon number of 12. The aromatic content is limited to 5%. JP-7 is a blend of several hydrocarbons and additives. Additives such as corrosion inhibitors, icing inhibitors, static dissipators, metal deactivators, and antioxidants are included in limited quantities to improve the fuel performance [4].

There has been significant research on ignition characteristics of several JP fuels. Results for JP-8 and JP-10 are given in Refs. [1,5,6] and [7–9], respectively. Compared with other JP fuels, the study of JP-7, however, is still in a nascent stage. Mawid et al. [9] treated the ignition characteristics of a lean JP-7/air mixture at atmospheric pressure conditions for the temperature range 900–1050 K. A surrogate blend consisting of 30% n-$C_{10}H_{22}$, 30% n-$C_{12}H_{26}$, 30% n-$C_{10}H_{20}$, 5% i-C_8H_{18}, and 5% C_7H_8 by weight was employed. Owing to the lack of experimental data on JP-7, the predicted ignition delays were compared with those of Jet-A obtained by injecting liquid fuel into the air stream in a shock tube apparatus. The predicted ignition delays were found to be shorter than the measured values, especially at lower temperatures. Maurice et al. [10] experimentally investigated the effects of additives like 2-ethylhexyl nitrate (EHN) and a proprietary additive (PA-1) on the ignition characteristics of JP-7 and JP-8. The experiments involved injection of liquid fuels in air behind reflected shocks over the temperature range 1200–1800 K at a pressure of 2 atm. A reduction in ignition delay of up to 25% was achieved through the inclusion of additives.

In the following, the ignition characteristics of cracked JP-7 fuel with both oxygen and air is studied over a wide range of pressures (1–20 atm), temperatures (1200–2000 K), and equivalence ratios (0.5–1.5). Correlations of ignition delay times, of the form $\tau = A\exp(E/RT)[\mathrm{F}]^a[\mathrm{O}_2]^b$, are established using the Chemkin-II package and least-squares analysis. The effect of C_3 hydrocarbons in cracked JP-7 fuel is

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Table 1
Molar composition of cracked JP-7 fuel

Compound	Ref. [11]	B. Bullard (private communication)
Hydrogen (H_2)	–	0.0523
Methane (CH_4)	0.281	0.5029
Ethane (C_2H_6)	0.215	0.2053
Ethene (C_2H_4)	0.159	0.2395
Propane (C_3H_8)	0.135	–
Propene (C_3H_6)	0.210	–

examined by comparing ignition delay times for two different cracked compositions.

2. Methodology

Two different compositions of cracked JP-7 fuel are considered in the present work, as summarized in Table 1. The composition obtained by Edwards and Anderson [11] contains such species as methane, ethane, ethene, propane, and propene. It was obtained for a residence time of 1.1 s with a flow rate of 10 ml/min in a 0.125-in.-o.d. 304 stainless-steel tube. Temperatures above 850 K and pressures above 68 atm were applied for an 80% conversion. The other composition, adopted from B. Bullard (private communication), consists of hydrogen, methane, ethane, and ethene and shows an absence of C_3 hydrocarbons. The exact cracking conditions are not available.

The chemical kinetic mechanisms used in the present study were acquired from three different sources. The first one, taken from GRI-Mech-3.0 [12], involves 53 species and 325 reactions. The second scheme, developed by Williams [13], includes detailed reactions for C_3 species like C_3H_6 and C_3H_8. The third scheme was developed by Marinov et al. [14] to model aromatic and polycyclic aromatic hydrocarbon (PAH) formation in fuel-rich, *n*-butane/oxygen/argon, propane/oxygen flames at atmospheric pressure. This mechanism was previously validated against experimental data for modeling ethane, ethylene, and methane flames under fuel-rich conditions. GRI-Mech is the basic mechanism employed herein, and the other two were selected due to the lack of C_3 kinetics in GRI-Mech.

The chemical kinetic schemes were incorporated into the Chemkin II Package [15] to study the ignition characteristics of cracked JP-7 with both air and oxygen. The resultant linear differential equations were solved using the LSODE solver, and correlations for ignition delay times were established using the least-squares-fit technique. As will be shown later, there is little difference in ignition delay times between the cracked compositions given in Edwards and Anderson [11] and B. Bullard (private communication), under most of the conditions. The composition in B. Bullard was thus selected as the baseline due to its comparative simplicity.

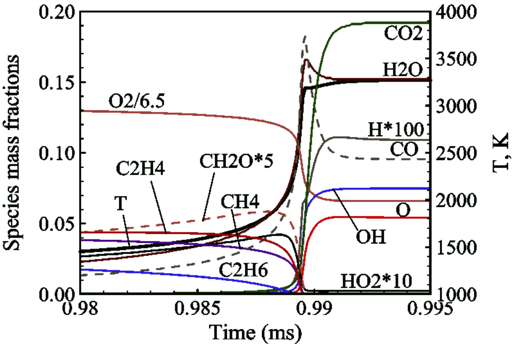

Fig. 1. Temporal evolution of species mass fractions for stoichiometric cracked JP-7/oxygen mixture at $p = 1$ atm with initial temperature of 1200 K.

Fig. 1 shows the temporal evolution of temperature for a stoichiometric cracked JP-7/oxygen mixture at 1 atm and an initial temperature of 1200 K for the baseline composition. The ignition delay time is characterized by a sharp increase in the temperature profile resulting from highly exothermic reactions with large activation energies. An ignition process of this kind is normally driven by free radical chain reactions, comprising the initiation, propagation, branching, and termination stages. The initial horizontal portion of the profile represents the induction time associated with various chain initiation reactions. The figure also shows the evolution of various species. Formaldehyde (CH_2O) is prominent in hydrocarbon reactions and is involved at the final stage of conversion to carbon oxides. Water is formed at each stage, principally by an H-atom abstraction in a propagation process of the form $RH + OH \rightarrow R + H_2O$, where RH represents any intermediate molecule. Formation of H_2O and CO_2 and reactions involving radicals like H, O, HO_2, OH in the terminating processes are the main sources of heat release and result in a rapid increase in temperature.

The ignition delay time represents the time for fractional completion of the reaction at given temperature and pressure. For premixed fuel and oxygen, it can be written mathematically as

$$\tau = A \exp(E/R_u T)[F]^a[O_2]^b, \qquad (1)$$

where τ is the ignition delay time (in s), E the global activation energy (in kcal/kmol), T the initial temperature (in K), R_u the universal gas constant (in kcal/kmol K), [F] and $[O_2]$ the fuel and oxygen concentrations (in mol/m^3), and A the preexponential factor. Equation (1) can be further expressed in terms

Table 2
Activation energies for ignition delay time of cracked JP-7, hydrogen, and hydrocarbons with oxygen

Fuel	*E* (kcal/kmol)
Hydrogen	19,700[a]
Methane	45,000[a]
Ethylene	35,000[a]
Heptane	40,160[a]
JP-10	43,855[a]
JP-7 (cracked)	39,167

[a] Obtained from Ref. [1].

of pressure, temperature, and equivalence ratio, Φ, as

$$\tau = A[0.405\Phi]^{a}\left[\frac{p}{R_{\mathrm{u}}T(1+0.405\Phi)}\right]^{a+b} \times \exp(E/R_{\mathrm{u}}T), \quad (2)$$

where p is the pressure in Pa.

3. Results

A least-squares fit on the data obtained for the cracked JP-7 (B. Bullard, private communication) with oxygen using GRI-Mech kinetic results in the expression

$$\tau = 8.32 \times 10^{-10}\exp(39{,}166/R_{\mathrm{u}}T) \times [\mathrm{F}]^{-0.3455}[\mathrm{O_2}]^{-0.3573}. \quad (3)$$

The ignition delay time decreases with an increase in the concentrations of fuel and oxidizer and varies exponentially with temperature. In Table 2, the activation energies for hydrogen and several hydrocarbon fuels, taken from the study by Colket and Spadaccini [1], are compared. The value of 39,166 kcal/kmol for cracked JP-7 is found to be comparable with most hydrocarbon fuels. Equation (3) can also be used to show the explicit dependence of ignition delay time on pressure, temperature, and equivalence ratio as

$$\tau \propto p^{-0.7028}, \quad (4)$$

$$\tau \propto T^{0.7028}\exp(39{,}166/R_{\mathrm{u}}T), \quad (5)$$

$$\tau \propto (0.405\Phi)^{-0.3455}/(1+0.405\Phi)^{-0.7028}. \quad (6)$$

Following the same approach for the case with oxygen, the ignition delay time for a cracked JP-7/air mixture can be correlated using

$$\tau = 4.21 \times 10^{-9}\exp(36{,}396/R_{\mathrm{u}}T) \times [\mathrm{F}]^{-0.1788}[\mathrm{air}]^{-0.4978}. \quad (7)$$

The ignition delay decreases with an increase in the fuel and air concentrations, with the latter exerting a much stronger influence. The explicit dependence on pressure, temperature, and equivalence ratio for a cracked JP-7-in-air mixture can be written as

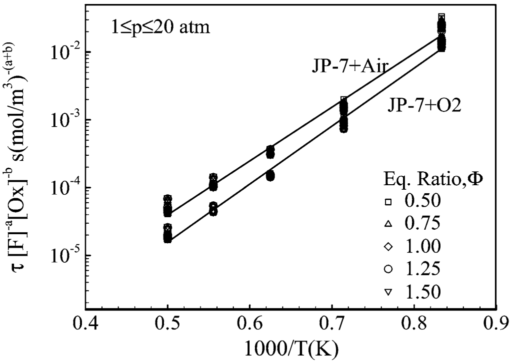

Fig. 2. Ignition delay times of cracked JP-7 with oxygen and air.

$$\tau \propto p^{-0.6766}, \quad (8)$$

$$\tau \propto T^{0.6766}\exp(36{,}396/R_{\mathrm{u}}T), \quad (9)$$

$$\tau \propto (0.0851\Phi)^{-0.1788}/(1+0.0851\Phi)^{-0.6766}. \quad (10)$$

Fig. 2 shows the correlations for the ignition delay times of cracked JP-7 mixtures with oxygen and air. τ varies strongly with pressure, but weakly with stoichiometric ratio. As expected, the ignition delay for JP-7 in air is greater than that in oxygen for the same initial condition. The difference between the two cases increases with increasing pressure and temperature.

The influence of fuel composition on ignition delay is examined by considering the different cracking products acquired from Edwards and Anderson [11] and B. Bullard (private communication). The chemical kinetics associated with C_3 hydrocarbons are treated by means of the scheme proposed by Williams [13]. For the composition given in Ref. [11], which includes C_3 hydrocarbons, the correlation for a cracked JP-7/oxygen mixture is found to be

$$\tau = 3.47 \times 10^{-9}\exp(37{,}388/R_{\mathrm{u}}T) \times [\mathrm{F}]^{0.1886}[\mathrm{O_2}]^{-0.9087}. \quad (11)$$

A similar analysis for the composition from Bullard yields the expression

$$\tau = 4.69 \times 10^{-9}\exp(34{,}775/R_{\mathrm{u}}T) \times [\mathrm{F}]^{0.1357}[\mathrm{O_2}]^{-0.7607}. \quad (12)$$

There is a 7.5% increase in the activation energy and a limited decrease in the preexponential factor for the case with C_3 hydrocarbons, thereby leading to a longer ignition delay.

The ignition delay for cracked fuel in oxygen is also studied using a different kinetic scheme given in

Ref. [14]. For the composition including C_3 species [11],

$$\tau = 7.48 \times 10^{-11} \exp(46{,}129/R_u T) \times [F]^{-0.1018}[O_2]^{-0.5867}. \quad (13)$$

For the composition given in by Bullard (private communication), the expression for ignition delay time can be written as

$$\tau = 2.61 \times 10^{-10} \exp(42{,}463/R_u T) \times [F]^{-0.1873}[O_2]^{-0.5130}. \quad (14)$$

This kinetic scheme also shows an 8.9% increase in activation energy and a negligible decrease in the pre-exponential factor for the C_3 composition. In general, the scheme of Williams [13] results in an ignition delay time longer than that predicted based on the mechanism of Marinov et al. [14], especially at higher temperatures.

4. Conclusions

The ignition delay of cracked JP-7 fuel in both air and oxygen has been studied using three different chemical kinetic schemes. The work covers a broad range of pressures (1–20 atm), temperatures (1200–2000 K), and equivalence ratios (0.5–1.5). The effect of cracked-fuel composition was also examined. The presence of C_3 species tends to reduce the ignition delay time over the temperatures of concern, but the difference appears to be limited.

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