Jet Fuel Ignition Delay Times: Shock Tube Investigations at High Pressures

Subith S. Vasu, David F. Davidson and Ronald K. Hanson

Mechanical Engineering, Stanford University, Stanford, CA, 94305, USA

1 Introduction

Ignition delay time (τ_{ign}) is an important parameter in the combustor design of most engines, including ram-jets, scramjets, pulsed detonation engines, and advanced combustor concepts for low NOx emissions. Dependence of ignition delay time on temperature, pressure and composition is critical in describing the combustion of liquid fuels in diesel engines and combustion chambers of various types, as well as in optimizing external combustion. Distillate fuels such as kerosenes are defined by broad composition guidelines, hence ignition delay times vary with fuel composition, among other variables, and this provides a challenge in dealing with most practical fuels. Jet fuels (e.g. JP-4, JP-5, JP-7, Jet-A, JP-8, T-6, TS-1, RG-1, and RP-1) often contain thousands of compounds (Violi et al. [1]). JP-8 fuel is a military equivalent of the commercial fuel Jet-A, and differs primarily by the addition of trace amounts of additives such as lubricity improvers, corrosion inhibitors, icing inhibitors, and antistatic additives (Edwards and Maurice [2]).

Although the ignition characteristics of aviation fuel mixtures have been a subject of investigation for many years, there remains a critical need for experimental data on ignition delay times of Jet-A and JP-8 fuels in air. Recently, ignition delay times of gas-phase Jet-A/Air mixtures at Φ =0.5 to 1.0 were studied behind reflected shock waves by Dean et al. [3] in a heated shock tube. The Jet-A ignition delay time data from Dean et al. [3] range over temperatures of 1000 to 1800 K and fall into two pressure groups: 10 and 20 atm. Two different heated shock tubes and optical arrangements were used in that study. A comparison of the ignition delay times of Dean et al. [3] and the current study is shown later. Due to the high boiling points of large hydrocarbon components of Jet-A and JP-8 fuels, heating of the shock tube and associated mixing facilities is necessary to prepare a homogeneous gas phase mixture for ignition delay time studies, and this largely explains why so few studies have been conducted with gas-phase jet fuel using the shock tube method. This method, however, is generally preferred over other methods as it can provide reliable, reproducible measurements of gas-phase ignition delay times, amenable to a simple constant-volume modeling constraint, over a wide range of temperatures, pressures and fuel mixtures.

In our laboratory we are continuing to build a reference database of combustion-related ignition delay times, species time-histories and critical reaction rates. As part of this effort, we are developing methods to improve the accuracy, reliability, and understanding of shock tube methods in areas such as ignition delay time definition, mixture formation, available test time, diagnostics and kinetic modeling. Shock tubes are nearly ideal devices for studying high temperature ignition phenomena as they provide well-controlled step changes in temperature and pressure, well-defined time zero and ignition delay times, and are not affected by surface or transport problems. Also, shock tubes can reproduce nearly identical pressures and temperatures from shock experiment to experiment. Shock tube ignition delay data thus can provide important validation targets for detailed gas-phase kinetics modeling of fuels. Recent modeling efforts have been focused on developing reduced mechanisms and finding suitable surrogate mixtures for jet fuels. However, challenges still remain in modeling real jet fuel behavior and in finding a suitable physical surrogate (a mixture that has generally the same physical properties as the jet fuel) and a chemical surrogate (a mixture that has generally the same chemical-class composition and average molecular weight as the jet fuel) that can accurately depict the real fuel behavior and ignition times for a wide range of conditions.

In this study, we present new ignition delay time measurements in stoichiometric Jet-A/air and JP-8/air at high pressures using a heated high-pressure shock tube facility. Initial reflected shock conditions spanned the following wide ranges: temperatures of 715-1220 K, and pressures of 18-51 atm in synthetic air. We compare these new data to

previous gas-phase shock tube data (Dean et al. [3]), and to the predictions of a detailed Ranzi et al. [4] kinetic mechanism (280 species, 7800 reactions). One of the simple and most widely known surrogates (Violi et al. [1]) was used for these model calculations and had the following composition: benzene (1%), iso-octane (5.5%), methylcyclohexane (10%), toluene (10%), n-dodecane (73.5%).

2 Experimental Method

All ignition delay time experiments were performed in a high-purity, heated (100 C), helium-driven, turbomolecular-pumped, high-pressure shock tube (HPST) facility at Stanford University. The HPST test section has a 5 cm inside diameter. Uniform temperature along the length of the shock tube is achieved through a series of heaters wrapped around the driven section of the shock tube, with power output to the heaters controlled using WatlowTM controls. Jet fuel can vary widely in its chemical properties. Throughout our study we have assumed a chemical formula of $C_{11}H_{21}$ and a density of 0.81 gm/cm³ for all the jet fuels tested (Edwards and Maurice [2], Dean et al. [3]). It is very important to vaporize the fuels as completely as possible to avoid any errors in the fuel-air mixture calculations. In all the current experiments, research grade liquid Jet-A (JET-A Composite Blend #04POSF4658 supplied by T. Edwards, AFRL-WP) and JP-8 (supplied by P. Schihl, ARL) were measured and added volumetrically into the mixing tank. For jet fuels, the mixing tank had to be heated to 125 C to ensure that there was no further significant change in the fuel evaporation. Shock tailoring methods with different driver gas mixtures (mixtures of He and N₂) was utilized to enable measurement of ignition delay times in the NTC region near 700 K.

Ignition pressure was monitored using a shielded PZT (Kistler model 603B1) located 10 mm from the endwall. The emission from OH* (using a Schott Glass UG-5 filter with >95% transmission at 306 nm) was monitored at an observation window located at the same axial location. The ignition delay time is defined in this study as the time interval between the arrival of the reflected shock wave and the onset of ignition at the sidewall observation location (see Fig. 1). The arrival of the reflected shock wave was determined by the step rise in pressure, and the onset of ignition was determined by monitoring either the pressure history or the emitted light corresponding to OH* emission. The onset of ignition from the pressure history and OH* emission were defined by locating the time of steepest rise and linearly extrapolating back in time to the pre-ignition baseline. The two methods give very similar results and ignition delay times were readily identifiable with both diagnostics. More details about the HPST facility and experimental procedure are given in Petersen et al. [5] and Vasu et al. [6], respectively.

3 Results & Discussion

The ignition delay time data for Jet-A/air over a range of temperatures for reflected shock pressures (P₅) from 18 to 36 atm have been normalized to 20 atm assuming $\tau_{ign} \sim 1/P$ and are presented in Fig. 2. These measurements show relatively good agreement with the earlier (Dean et al. [3], 10-20 atm) data for Jet-A. Sources for jet fuels of current experiments and for Dean et al. [3] are mentioned in an earlier section of the current paper. Over the temperature and pressure range (10-36 atm) of the current and the Dean et al. [3] data, a normalizing pressure scaling of 1/P correlates the data very well.

As a further point of comparison, there does not appear to be a significant difference in the ignition delay time measurements when the shock tube was heated to $T_1 = 80$ C or 150 C (both were employed in Dean et al. [3]) or $T_1=100$ C (current work). This similarity may be attributed to the fact that the initial steps of the ignition process, presumably controlled by decomposition of the smaller hydrocarbons, are not strongly affected by the presence or absence of small amounts of heavier ($\sim C_{20}$) fuel components that may be volatilized ($T_1=100$ C and $T_1=150$ C) or may not be totally volatilized ($T_1=80$ C) in the experiments. The possibility of fuel cracking from long mixing times at elevated temperatures is a concern for jet fuels. However in the current experiments, no measurable change in ignition delay time data was observed for fuel/air mixing times between 2.5 to 8 hours.

Ignition delay time measurements were also performed using JP-8 at similar temperatures and pressures. A comparison study of the measured ignition delay times for Jet-A/Air and JP-8/Air mixtures for an equivalence ratio of 1.0, show very good agreement between ignition delay times for both fuels at the high and low temperatures. The low scatter data obtained enables discernment of small differences in ignition delay times in fuel types. However, JP-8 ignition delay times appears to be approximately 10% shorter than Jet-A for temperatures near 1000K.

When experimental conditions vary over a wide range of pressures, assuming a power-law dependence to the pressure scaling leads to a more uniform graphic presentation of the ignition delay time data. The pressure dependence of ignition delay times in Jet-A/air mixtures is shown in Fig. 3. A simple 1/P dependence was found for ignition delay times from 950K to 1250K for the pressure range 20-50 atm based on the scaling of the data points in Fig. 3. As

discussed earlier, this 1/P dependence has been observed in many previous studies with different experimental facilities. A regression analysis of the current data for Jet-A/air and JP-8/air (Φ =1) shows $\tau_{ign} \sim P^{-0.98}$, which is very close to the 1/P behavior. However, in all the results presented in the current work, we have used the simple 1/P dependence to scale ignition delay times.



Figure 1. Example JP-8/air ignition delay time data (Driver gas: He). Initial reflected shock conditions, 1019 K, 22.2 atm, $\Phi = 1$



Figure 2. Ignition delay times including previous data for Jet-A/air (Φ =1.0).



Figure 3. Variation of ignition delay time with pressure (Jet-A/air, Φ =1.0).



Figure 4. Ignition delay times including NTC region data, (Jet-A/air, $\Phi=1$).

The Ranzi et al. [4] mechanism gives the closest agreement with data under current conditions, when compared to other mechanisms. When modeled using the Violi et al. [1] surrogate composition, predictions at 20 atm are slightly higher than the experiment with the Ranzi et al. [4] mechanism at temperatures above 1000K. Below this temperature, the model shows strong NTC (negative temperature coefficient) behavior due to the large presence of n-dodecane in the surrogate fuel. It is to be noted that detailed mechanisms containing a large number of species and reactions cannot easily be applied to the modeling of combustion behavior of jet fuels in practical systems. Also, further experimental

work including key species time-history measurements are needed to provide more comprehensive kinetic targets for refining the mechanisms and improving predictions.

Jet fuel ignition delay time (τ_{ign}) measurements were also performed at low temperatures (700-850 K). Ignition delay time data variation with initial reflected shock temperature, normalized to 20 atm (assuming $\tau_{ign} \sim 1/P$), are presented in Fig. 4. At these low temperatures, ignition delay times are usually long (> 2 ms) and commonly show negative temperature coefficient (NTC) type behavior, in which the ignition delay time becomes longer as the temperature increases. Interestingly, this more or less S-shaped dependence (NTC) is similar to that reported in n-heptane (a diesel surrogate) in air, and mixtures of iso-octane and heptane in air, by Fieweger et al. [7]. The Ranzi et al. [4] mechanism prediction using the Violi et al. [1] surrogate mixture, rolls off much earlier, but later catches up, retaining the primary feature of the data. At very low temperatures (below 700K), ignition delay times increase with decreasing temperature, as seen both in the data and the model.

Comparison between pressure increases in non-reactive (pure N₂) and reactive (Jet-A/air, Φ =1.0) mixtures, shows a higher pressure increase with time in the latter case due to the pre-ignition energy release caused by chemical reactions. In the non-reactive case, for the temperature range from 700-850 K at a pressure close to 20 atm, a simple relation could be established for the reflected shock pressure increase and the incident shock attenuation. At the current side-wall location (10 mm from end-wall), we found a linear relation between change in reflected pressure with time (dP/dt) and the incident shock attenuation rate (%/m). This relation could be used to estimate the total temperature increase due to non-ideal effects from the arrival of reflected shock wave till the onset of ignition, even in the case for reactive mixture cases. In the current experiments for Jet-A/air ignition delay times below about 4 ms, the maximum increase in temperature was estimated to be only 21 K (using an isentropic assumption as recommended by Petersen and Hanson [8]). However, it is to be noted that ignition delay times are relatively insensitive to small variations in the temperature in the NTC region as the ignition delay times in this region are nearly flat (see Fig. 4.)

The present data will be incorporated into the larger Fundamental Shock Tube Kinetics Database currently being developed at Stanford University.

4 Acknowledgements

This work was supported by the Army Research Office under contract No. DAAD19-01-1-0597. The authors would like to thank T. Edwards of the Air Force Research Laboratory, Wright-Patterson and P. Schihl of the Army Research Laboratory for supplying fuel tested in this work.

References

- [1] Violi A et al. (2002). Experimental formulation and kinetic model for JP-8 surrogate mixtures. Combustion Science and Technology, Vol. 174, Nos. 11-12, pp 399-417
- [2] Edwards T, Maurice LQ (2001). Surrogate Mixtures to Represent Complex Aviation and Rocket Fuels. Journal of Propulsion and Power, Vol. 17, No. 2, 461-466
- [3] Dean AJ et al. (2005). Ignition of aviation kerosene at high temperatures. Proceedings of the 20th International Colloquium on the Dynamics of Explosions and Reactive Systems, 31 July- 5 Aug 2005
- [4] Ranzi E et al. (2006). URL: http://www.chem.polimi.it/CRECKModeling/kinetic.html
- [5] Petersen EL (1998). A shock and diagnostics for chemistry measurements at elevated pressures with application to methane ignition. Ph.D. Thesis, Stanford University, Stanford, CA
- [6] Vasu SS et al. (2006). Shock Tube Ignition Delay Times and Modeling of Jet Fuel Mixtures. 42nd AIAA/ ASME/ SAE/ ASEE Joint Prop. Conf. and Exhibit, July 9-12, 2006, Sacramento, USA, AIAA-2006-4402
- [7] Fieweger K et al. (1997). Self-ignition of S.I. engine model fuels: a shock tube investigation at high pressure. Combustion and Flame, Vol. 109, 1997, pp 599-619
- [8] Petersen EL, Hanson RK (2001). Nonideal effects behind reflected shock waves in a high-pressure shock tube. *Shock Waves*, Vol. 10, No. 6, pp 405-420