

Auto-ignition of Diesel Fuel at High Temperatures and Pressures

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1 Introduction

Most aviation fuels are mixtures of a large number of hydrocarbons and the chemical kinetic processes occurring in combustion of such fuels at high temperatures have not been sufficiently validated. There is scarcity of data on auto-ignition of heavy fuels at high temperatures and pressure. Only limited data have been reported for ignition of Diesel fuels in jet-stirred reactors [1] and in shock tubes [2]. Thus, there is an obvious lack of experimental data for high-temperature combustion and auto-ignition of Diesel fuel and its surrogates in air. The objectives of this study are as follows:

- to investigate systematically combustion and ignition properties of Diesel No.2 at 4.7 – 10.4 atm, temperatures 1065 - 1838 K, and stoichiometries $\phi = 0.5 - 2$;
- to compare auto-ignition of premixed Diesel fuel/Air mixtures with a Jet-A/air mixture at equivalent post-shock conditions,
- to obtain reference data on ignition of Diesel fuel/Air mixtures at high temperatures itself.

2 Experimental setup

Stainless steel heated shock tube of 76 mm in diameter was used in the experiments. The wall thickness was 9 mm. The length of the tube was 6.0 m. The tube channel was calibrated with accuracy of 0.005 mm. Four independent current circuits provided an independent heating of the four shock tube sections to ensure the uniform temperature distributions along the tube length with accuracy $\pm 5^{\circ}$ C. For shock tube tests presented in this report the initial temperature of the tube was kept between 100 - 110^o C.

The commercial No. 2 Diesel fuel was used for these studies. The density of used Diesel sample was (0.8237 \pm 0.01) g/ml at 26^o C. The runs were performed in stoichiometric $\phi = 1$, lean $\phi = 0.5$, and rich $\phi = 2$ Diesel fuel /Air mixtures within the range of post-shock pressures of 4.7 – 10.4 atm and temperatures of 1065 – 1838 K (Table 1).

Figure 1 presents the drawing of the test section for studies in Diesel fuel/Air mixtures. Pressure variations at different cross-sections of the tube were measured by three high-frequency PCB

pressure sensors Model 113A24 with a rise time less than $1.5 \mu\text{s}$ and with a 1.5-mm spatial resolution. The end wall PCB pressure transducer measured the reflection time and pressure history behind reflected shock waves in the vicinity of the reflecting surface. For controlling ignition and reaction times the additional ion current sensor was mounted into reflecting surface of the shock tube. To detect arrival times of reaction front two additional ion current sensors were installed along the shock tube channel at different distances from the reflecting wall. This setup ensured obtaining information on propagations of shock and reaction fronts over the length of 340 mm upstream the end wall. Pressure and ion current signals were recorded and processed by an automatic 10-bit data acquisition system connected with a central computer.

Table 1. The experimental conditions for No. 2 Diesel fuel /Air mixtures

Diesel - Air	Equivalence ratio, ϕ	Post-shock Pressure [atm]	Post-shock Temperature [K]	Post-shock Density [kg/m^3]
Mixture 1	1	4.68 – 10.4	1078 -1665	1.49 –2.71
Mixture 2	0.5	5.6 – 9.8	1117 – 1903	1.3 – 2.47
Mixture 3	2.0	5.7 – 10.0	916 – 1838	1.4 – 3.17

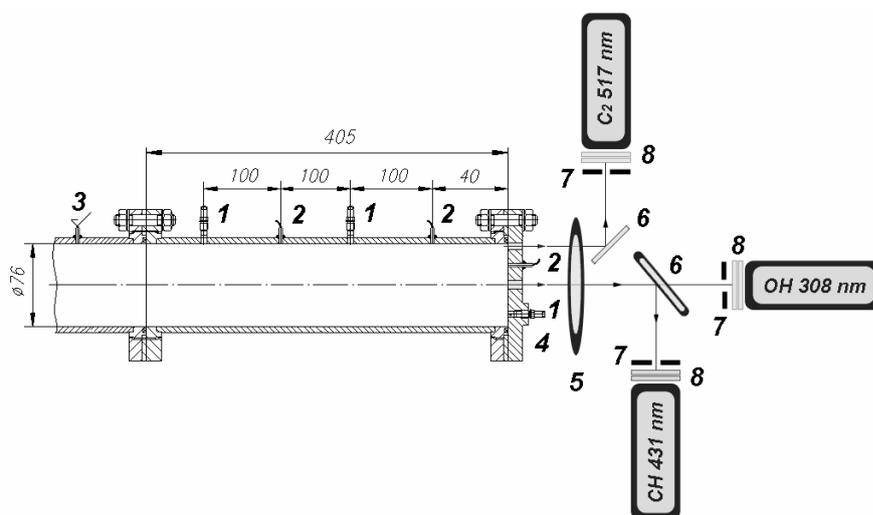


Figure 1. Schematic of the test section for auto-ignition studies in Diesel fuel/Air mixtures in a 76-mm shock tube: 1 – high-frequency PCB pressure transducers; 2 – ion current sensors; 3 – thermocouple; 4 – reflecting wall with inserted quartz rods; 5 – lens $f = 40 \text{ cm}$; 6 – beam splitter; 7 – aperture diaphragms; 8 – doubled monochromatic filters; 9- photomultipliers.

To provide spectroscopic observations two quartz rods of 8 mm in diameter has been mounted into the plane end wall. The first rod ensured emission observations from the gas column of 5 mm in diameter along the centerline of the tube, the second – from the similar gas column along the tube wall in the boundary layer. To fix the instant at which the luminosity commences, both gas volumes ($\varnothing 5 \text{ mm}$) has been imaged onto a photomultiplier detectors installed in a focus of the collecting quartz lens $f = 400 \text{ mm}$. The 1-mm apertures mounted in front of the photomultipliers ensured the angle selection of transmitted radiation and passed only light beams propagating along the shock tube axis. The beam-splitters divided output spectrum into three optical paths to provide the simultaneous co-axial emission observations at several spectral bands. The luminosities of OH radicals (transitions $A^2\Sigma - X^2\Pi$) at wavelength of 308.9 nm and CH radicals (transitions $^2\Delta - ^2\Pi$) at wavelength of 431.5 nm were implemented to measure auto-ignition of the mixture along the centerline of the shock tube. The

luminosity of C_2 radicals (transitions ${}^2\Pi - {}^2\Pi$) at wavelength of 516.5 nm were detected to identify the auto-ignition in the boundary layer. Ignition times were controlled also by pressure and ion current measurements at the reflecting wall.

The ignition or induction time of the mixture was defined as the time difference between shock arrival at the end wall and the onset of emission within measuring gas columns. The applied optical setup was sensitive to the onset of auto-ignition at selected gas volumes and generated induction times of studied mixtures from the beginning of normal reflection of the incident shock wave. To obtain a correct temperature dependence of ignition time on activation energy of the mixture and fuel/oxygen concentrations all comparative shock-tube series were performed at approximately constant post-shock density. It means that fuel, oxygen, and nitrogen concentrations were kept nearly constant within a studied temperature range behind reflected shock waves.

3 Results

It was shown that for studied range of post-shock conditions the reaction rate of Diesel fuel oxidation exhibit a nonlinear Arrhenius dependence with global activation energies ranged from 32.6 kcal/mole at high temperatures (> 1200 K) to 20.4 kcal/mole at low temperatures (1200 K $<$).

For stoichiometries $\phi = 0.5 - 1$, the overall empirical approximation for ignition delays have been derived from the experimental data:

$$\tau(\mu s) = 8.0663 \times 10^{-6} \times \exp\left(\frac{15473}{T}\right) \times [O_2]^{0.28653} \times [Diesel]^{-0.54218} \quad (1)$$

where, τ is the ignition time in (μ sec), T is the post-shock temperature in (K), $[Diesel]$ is the Diesel fuel concentration in (mole/cm^3), and $[O_2]$ is the Oxygen concentration in (mole/cm^3). The global activation energy of Diesel fuel obtained from regression analysis is 30.7 ± 0.26 kcal/mole. Equation (1) gives the excellent agreement with experimental data points for stoichiometries $\phi = 0.5 - 1$. This correlation results in 13 % standard deviation from the fitted induction times.

For a wider stoichiometry range of $\phi = 0.5 - 2$, overall empirical approximation for ignition delays is:

$$\tau(\mu s) = 1.5563 \times 10^{-5} \times \exp\left(\frac{13789}{T}\right) \times [O_2]^{-0.43055} \times [Diesel]^{-0.0404} \quad (2)$$

with the global activation energy of Diesel fuel obtained from regression analysis is 27.3 ± 0.42 kcal/mole. Approximation (2) results in the satisfactory coincidence with experimental observations for $\phi = 2$. This correlation results in 27 % standard deviation from the fitted induction times.

At equivalent post-shock conditions in comparison with Jet-A/Air mixtures, Diesel fuel demonstrates $\approx 3 - 6.4$ times longer induction periods for $\phi = 2$ (Fig.2); $\approx 2.5 - 2.6$ times longer induction periods for $\phi = 0.5$; and ≈ 1.5 times longer induction periods for $\phi = 1.0$ (Fig.3).

Critical post-shock temperatures $T = 1251$ K ($\phi = 1$), $T = 1294$ K ($\phi = 0.5$), and $T = 1260$ K ($\phi = 2.0$) required for strong auto-ignitions of Diesel fuel/Air mixtures were established from experimental measurements. CJ detonation velocities in Diesel fuel / Air mixtures are $V_{CJ} = 1735 \pm 20$ m/s (for $\phi = 2$); 1580 ± 15 m/s (for $\phi = 1$); and 1450 ± 20 m/s (for $\phi = 0.5$).

The obtained data can be used directly for propulsion applications, validations of reaction mechanisms, and for analysis of detonability limits and explosion hazard of Diesel fuel/Air mixtures.

Acknowledgements

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References

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- [2] Haylett DR, Lappas PP, Davidson DF, Hanson RK (2009) Application of an aerosol shock tube to the measurement of diesel ignition delay times. Proc. of the Comb. Inst. 32 (1): 477.

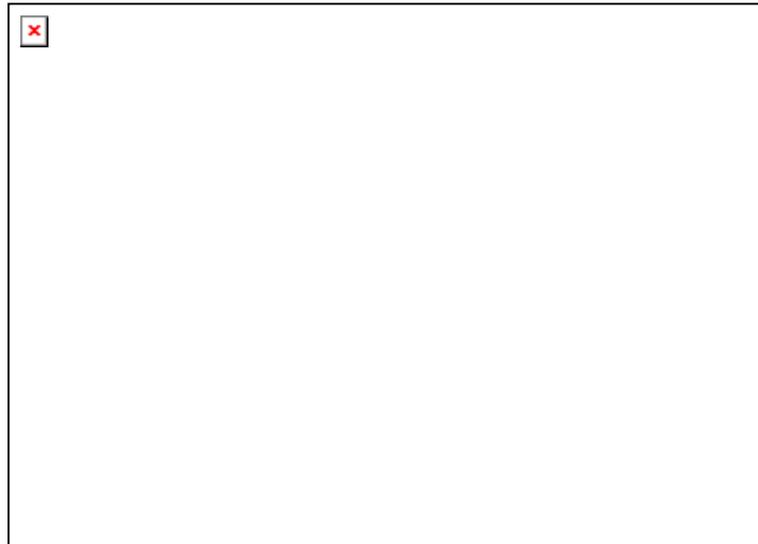


Figure 2. Ignition delay time vs. reciprocal temperature for rich Diesel fuel/ and Jet-A/Air mixtures ($\phi = 2.0$) at equivalent post-shock conditions

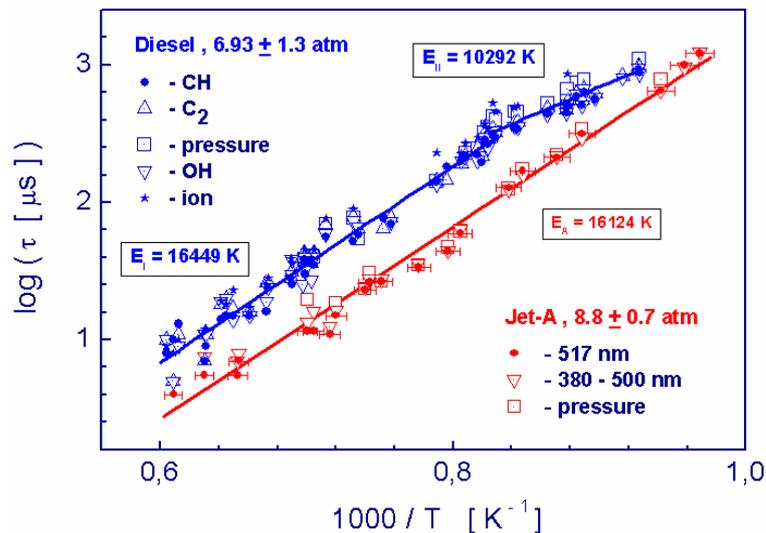


Figure 3. Mean activation energies for stoichiometric Diesel fuel/ and Jet-A/Air ($\phi = 1.0$) mixtures at equivalent post-shock conditions