

Measurement of the Autoignition Delay Time of Multi-Surrogate Paraffinic Fuel at Low-to-Intermediate Temperature Regime

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Abstract - A multi-surrogate fuel known as Bannersol consisting of C_{10} to C_{14} constituents which are representative classes of hydrocarbon found in Jet fuel is investigated in a newly designed pneumatically release rapid compression machine refer as SHEF-PRRCM. The study was carried out at lean and stoichiometric conditions within the compressed temperature range, T_c of 723 K–847 K. The influence of pressure, temperature and equivalence ratio was seen on the oxidation of Bannersol. The results showed that at the conditions studied no evidence of the onset of the negative temperature coefficient (NTC) and two-stage ignition behaviour was observed. A comparison of Bannersol with Jet A-1 showed that Banner has higher reactivity than Jet A-1 mainly attributed to the paraffinic content of Bannersol.

Keywords: SHEF-PRRCM, Bannersol, Ignition delay time, Jet A-1.

1. Introduction

The united nation predicted world population forecast is to grow from 6.5 billion to around 9 billion, and is expected to exceed 11 billion by 2050 [1]. The risk of natural resource depletion [1] and the detrimental effects of pollution on human health and the environment are troubling. Currently, land and air transport are the leading sector with substantial growth in demand for oil, this demand is in response to atmospheric pollution, which is affecting public health due to the dangerous rise in land and air emissions. The same emissions are created by land and air transport; including carbon monoxide sulfur oxides, nitrogen oxides, carbon dioxide, unburned hydrocarbons, and particulate matter. These emissions are known as greenhouse gas (GHG) which causes global climate change. The need to diversify from this fuel-producing GHG into a more friendly fuel with little or no harmful substance is relevant to the world's overall well-being. For proper transit from the conventional fuel to a biomass-based alternative fuel derived from hydro processed fat and oil or coal and natural gas that is processed through Fischer Tropsch technology that is traditionally GHG-free. They are

the most important sustainable fuel, look promising, and are useful for limiting greenhouse gas emissions [2]. To understand the reaction pathway that helps to minimize GHG and improve the efficiency of the system, a comprehensive study of the chemical properties of new novel fuels with respect to combustion (ignition) are compulsorily important to minimize or control hazardous emission from the engine.

Surrogate hydrocarbons are essentially simpler mixtures of hydrocarbons that mimic the physical and chemical properties of complex fuels. They are extensively used in combustion research. Real-world fuels like gasoline, diesel, or jet fuel consist of hundreds or even thousands of different hydrocarbons[3], making their behaviour extremely complex to understand and predict. Surrogate fuels, with a limited number of components, simplify this complexity and allow researchers to study combustion processes more easily and develop more efficient and cleaner engines. The combustion properties of surrogate fuels, such as ignition delay, flame speed, and heat of combustion, are used to calibrate and optimize engine performance. By adjusting the ratio of different components in the surrogate fuel, engineers can tune the combustion process to achieve desired performance characteristics.

Paraffinic fuels, due to their structure, have been studied extensively in literature for their autoignition characteristics. In a study by Pfahl, et al.[4], they investigated n-heptane (a representative paraffin) and found that its autoignition behavior is heavily influenced by temperature, pressure, and air/fuel ratio. The study revealed that at high pressures, the autoignition delay decreased significantly. A comprehensive study by Pitz, et al. [5] developed a detailed chemical kinetic model for n-heptane, which is often used as a surrogate for paraffin fuels. Their model accurately predicted the ignition delay times for a range of pressures and temperatures. Later research by Curran, et al. [5] extended this work by developing a kinetic model for n-decane, another crucial paraffin. They found that n-decane has a longer ignition delay time than n-heptane, which makes it more suitable as aviation fuel. More recently, Dagaut, et al.[6] conducted experiments on a range

of paraffins and developed kinetic models for each. They found that increasing the chain length of the paraffin increased the autoignition delay time. The principal objective of this study is to examine the autoignition characteristics of surrogate fuel, Bannersol at stoichiometric and lean conditions under low to intermediate-temperature ($< 847\text{K}$) conditions in a rapid compression machine (RCM) outside the limits of NTC region. There are still sparse data on low to intermediate temperature combustion of multicomponent fuel from RCM facilitates which has necessitated further tests to build an archive of data to deepen our understanding of the oxidation kinetics of fuel free from aromatics. The autoignition properties of unique solvents is examined to characterize the impact of chemical structure on ignition delays that enhance the understanding of structure reactivity relationships and contribute to the successful integration of next-generation non-petroleum derived fuels into existing aviation systems.

2. Experimental Setup

Manuscript concerning the detailed description and characterisation of SHEF-PRRCM has been described in the previous work [7, 8] but the description of facility would be briefly given to aid the understanding of the reader. The recently developed SHEF-PRRCM [8, 9] is a device used to simulate the compression stroke of a single engine cycle to study the autoignition process in a controllable environment. The fuels mixtures is compressed in a short time scale from initial conditions of initial pressure (P_0), and initial temperature (T_0) to the end of compression, characterised by compressed pressure (P_c) and compressed temperature (T_c). The SHEF-PRRCM is pneumatically operated, triggered by the solenoid valve to activate the pneumatic piston release mechanism (PRM) system and stopped hydraulically. The compression time ranges from 23 to 52 ms, while the majority greater than 60% of pressure/temperature rise occurs in the last 4 ms of compression. The facility is known for a shorter compression time, which decreases the heat transfer during compression stroke that results to a slightly higher compressed gas temperature. It has a compression ratio of up to 20 and the stroke of the machine can vary from 120 to 152 mm, where the clearance is also adjustable. The creviced piston is designed to minimize flow vortex during compression [8, 10, 11]. The desired compressed conditions can be reached by changing initial pressure, initial temperature, and the compression ratio of the facility. The facility has a 420 W power output of FGH052-080L hightemperature fibreglass tape that was rap around the reaction chamber to increase the temperature of the walls and test mixture to desired temperature. The PID controller has a dual-port, which accommodate the heating tape and the K-type thermocouple subsequently used for heating and taking temperatures of the reaction chamber wall. The signal from a piezo pressure

transducer (Kistler 6009) combined with a charge amplifier (Kistler 5007) during each running of experiments recorded by a National Instrument (NI) cDAQ 9223 data collecting card running at a frequency of 100K Hz. As the heat loss during the fast compression process is negligible, the compressed gas temperature at the end of compression T_c is estimated using the adiabatic relation:

$$\ln\left(\frac{P_c}{P_0}\right) = \int_{T_0}^{T_c} \frac{\gamma}{\gamma-1} \frac{dT}{T}$$

Where P_0 is the initial pressure, P_c is the compressed pressure, T_0 is the initial temperature, γ is the specific ratio. The temperature T_c cannot be calculated directly because the specific heat ratio used in the above equation is unknown a function of temperature and mixture composition. The theory assumes that no mixing occurs between the hot core region and the cold boundary layer. The only way heat loss influences the core region is by the expansion of the core region caused by the cooling of the boundary layer as the piston compresses to a constant volume at the end of the stroke.

Specifically, a non-reactive experiment is conducted under similar conditions as that of the reactive experiment by replacing O_2 with N_2 , and the corresponding heat loss parameters are derived for the compression and post-compression duration from the experimental pressure trace. The compressed gas temperature, T_c is numerically estimated by varying the compression ratio to match the experimental pressure trace during the compression and post compression stages. Figure 1.0 shows the sectional view of the current SHEF-PRRCM.

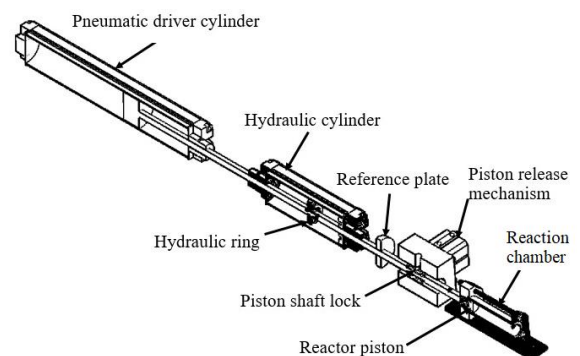


Figure 1: The sectional view of the current SHEF-PRRCM [7]

The gases used are of purity: O_2 : 99.993%, N_2 : 99.999%, Ar: 99.995 %. For the entire experiment, a dry air mixture consisting of 21% O_2 , 79% N_2 was used with diluted argon gas to alter the EOC at TDC. Before the experiment, liquid fuel was transported from the fuel bank to sample glass bottles properly labelled to prevent cross-contamination. The gases are transported from the cylinder to the Teflon gas bags

properly labelled and the leftovers are discarded after each experiment to prevent the possible diffusion of the gas. The fuel and air mixture is volumetrically measured and injected into the heated reaction chamber using syringe and left to homogenise for 1.5 hours. The expected result from an RCM test is the ignition delay, which has to be properly defined for it to be clearly understood. The ignition delay time, defined as the time from the end of compression to the first peak of pressure rise respect to time.

The ignition behaviours are shown in the reactive experimental result illustrated in Fig 2; Atypical pressure history, $P(t)$, measured from the SHEF-PRRCM for Bannersol/air mixtures at stoichiometric and $P'(t)$ is the time derivative of the measured pressure as a function of time. The ignition delay definition appears to have one peak pressure rise signifying a single-stage ignition delay of Bannersol oxidation. The time zero corresponds to the end of compression and the first-stage ignition delay, τ is the time from the end of compression to the maximum rise in pressure, $P'(t)$.

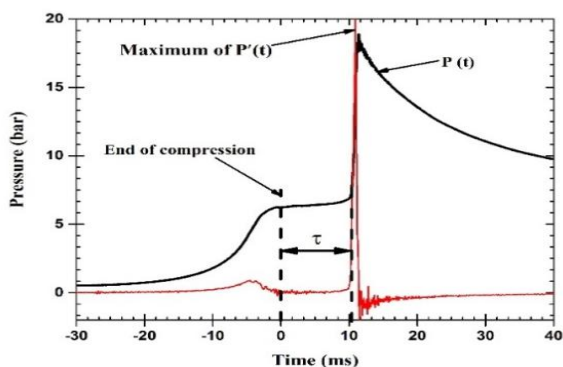


Figure 2: Illustrate ignition delay definition used in this study. $P(t)$ is the pressure as a function of time, and $P'(t)$ is the time derivative of the pressure as a function of time

2.1 Tested fuels and conditions

Figure 3 shows the molecular composition of two test fuels, Aviation Jet A-1 labelled (FST-265638) and a multi component surrogate fuel referred to as Bannersol (Banner NP1014) using the two-dimensional gas chromatographic separation ($GC \times GC$) analysis. The hydrocarbon classification technique used by Stiebich et al. [12]reported that this hydrocarbon group classification technique was useful to analyze each large part of fuel component, and these distributions are close to those reported in other works for analysis of conventional and non-conventional compositions of fuels[13].Fig. 3(a) shows the molecular class of Jet A-1. The main components of Jet A-1, which are based on Stiebich et al.[12] technique are Cyclo-paraffin 37.65 percent, n-paraffin 19.35 percent, iso-paraffin 20.57 percent, Naphthenes 2.85 percent, Alkyl benzenes 15.55 percent, and Indanes and

Tetralin 3.81 percent by weight. Fig 3(b) depicts molecular composition for a multi component solvent which contain no amount of sulphur and aromatics compared to Jet A-1. The fuel is purely paraffinic and has carbon atom ranging from C_{10} to C_{14} . The constituents are 21.18 % decane, 31.31% undecane, 0.2% Tridecane, 37.3 % Tetradecane and about 2.02 % greater than Tetradecane by weight as shown in Figure 3b.

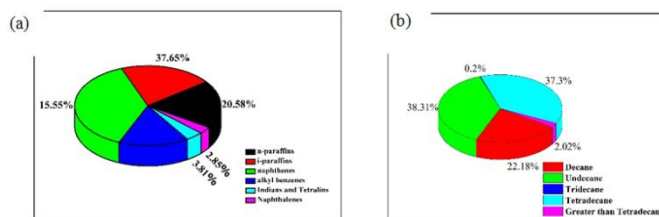


Figure 3: The molecular class composition as identified by ($GC \times GC$) relative signal area percentage analysis (a) Jet A-1 (FST-265638) (b) Bannersol (Banner NP 1014)

Table 1 shows the mixture composition for the test conditions studied. The conditions for the current RCM experiments are selected in order to study Bannersol characteristics under low to intermediate temperature at compressed pressure, $P_c = 6$ and 10 bar at lean and stoichiometric conditions, $\phi = 0.75$ and 1.0. The fuel was supplied by the low carbon combustion centre (LCCC) of the University of Sheffield at purity of greater 99.0% by volume. The air mixtures used was supplied by BOC, UK and the purity of oxygen, nitrogen and argon were greater than 99.993%. Prior to any experiment, the gas mixtures were transported from the cylinder to the Teflon gas bags of 500ml capacity each properly labelled. In addition, the initial temperatures of the chamber wall for all experiment was in the range of 110°C to 140 °C similar to Casey[14] report.

Table 1

Banner NP 1014	Molar Composition (%)			Equivalence Ratio	EOC Pressure (bar)
	O_2	N_2	Ar	ϕ	P_c
0.86	20.82	78.32		0.75	6.10
1.14	20.76	78.10		1.0	6.10
0.86	20.82	58.74	19.58	0.75	6.10
1.14	20.76	58.58	19.53	1.0	6.10

Some selected physical and chemical properties for test fuels are shown in Table 2. For the Jet A-1, and Bannersol, the derived empirical formulas are $C_{11.84}H_{22.72}$ and $C_{11.75}H_{25.49}$. The equivalence ratio of both fuel, however, is calculated based on the derived empirical formula as obtained from the 2D ($GC \times GC$) analysis.

Table 2: Selected Fuel properties

Property	Jet A-1 (FST- 265638)	Banner 1014	NP
Density at 15 °C (kg/m ³)	805.3	755	
Distillation Temp (°C)			
Initial Boiling point	163.8	183	
Final Boiling point	259.1	250	
Kinematic viscosity at 20 °C (mm ² /s)	3.521	1.88	
Molecular formula	C _{11.84} H _{22.72}	C _{11.75} H _{25.49}	
MW(g/mol)	165	167	
Total C(g)	142.3	141.1	
Total H(g)	22.9	25.7	
C _x (mol)	11.84	11.75	
H _y (mol)	22.72	25.49	
%C	86.1	84.5	
%H	13.9	18.2	
HC ratio	1.92	2.17	
DCN	43.74	75	

3. Experimental Results

Ignition delays of Bannersol/air mixtures was studied in a heated RCM at compressed temperature of 723 K ≤ T_c ≤ 847

K, compressed gas pressure, P_C = 6 and 10 bar, and φ = 0.75 and 1.0.

3.1 Combustion of Bannersol/air mixture

3.1.1 Low to Intermediate temperature ignition delay time measurement of Bannersol

Figure 4(a & b) illustrate the Arrhenius plot for Bannersol/air mixture at P_C = 6 & 10 bar, φ = 0.75 and 1.0 and compressed temperature, T_C = 723 K to 847 K. The effect of compressed temperature is seen on the ignition delay time as shown in Figure 3. Within the tested condition for lean and stoichiometric mixture. I observed that the ignition delay time decreases monotonically with temperature increase, traditional low temperature behaviour including an NTC region showing negative slope on an Arrhenius plot was not observed. The monotonic decrease of ignition delay with compressed temperature indicates that there is no NTC region of the ignition delays in the present experiments at both conditions. Figure 3(a & b) also depicts the influence of equivalence ratio on the ignition delay times of Bannersol/air mixture at P_C = 6 & 10 bar. It can be seen that ignition delay time decreases with the increasing the equivalence ratio. However, the effect of changing initial fuel mole fraction on the ignition delay and in both conditions of P_C = 6 & 10 bar, increases the initial fuel concentration (that is increasing the equivalence ratio) decreases the ignition delay. The ignition delay time shows no clear NTC behaviour, and the mixture reactivity increases with increase in equivalence ratio which is consistent with other typical hydrocarbon behaviours [15, 16].

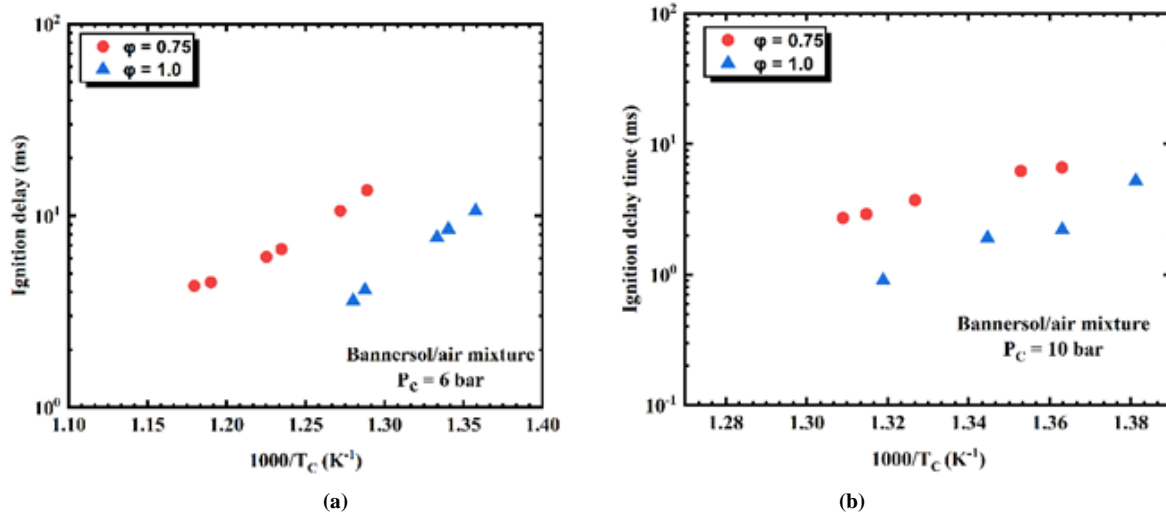


Figure 4: Ignition delay of Bannersol/air mixtures as a function of inverse temperature for varying equivalence ratio. Conditions: φ = 0.75 and 1.0 (a) 6 bar and (b) 10 bar

The influence of pressure on the Bannersol ignition delay time is shown in Figure 5(a & b) at φ = 0.75 & 1.0. In Figure 5(a) at φ = 0.75. Increasing pressure leads to about two fold reduction in the ignition delay compared to figure 4(b) at higher equivalence ratio. Thus at both conditions studied increasing pressure, increases reactant concentration thus increases the reaction rate thereby practically reducing ignition delay.

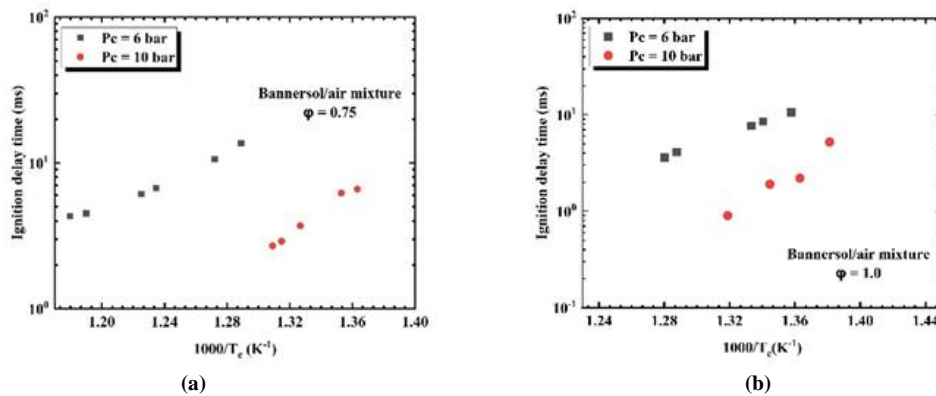


Figure 5: The influence of pressure on ignition delay of Bannersol/air mixture at (a) $\phi = 0.75$ and (b) $\phi = 1.0$

3.2 Comparison of Bannersol and Jet A-1

Figure 6 & 7 shows the Arrhenius plot comparing Bannersol and Jet A-1 at lean and stoichiometric condition, $\phi = 0.75, 1.0$ and $P_c = 6, 10$ bar. In figure 5 (a & b) the ignition delay plot against $1000/T_c$, at $P_c = 6$ bar and $\phi = 0.75, 1.0$. Both Bannersol fuel is seen a slightly lower ignition delay compared to Jet A-1. Bannersol showed to be fairly reactive than the Jet A-1. However, higher pressure as shown in Figure 6 (a & b), Bannersol became more reactive than Jet A-1. The perceived differences in reactivity for both fuels are attributed to their classification groups (n-paraffins, iso-paraffins, and cyclo-paraffins), hydrogen-to-carbon ratio and the chemical structure of hydrocarbon [17, 18]. And these differences in reactivity can be explained by the relative significance of low temperature chain branching reactions over chain-propagating or chain-terminating reactions. Nevertheless, the proportion of concentration the classification group determines the global rate of low temperature chain branching over the influence of different paraffinic bonding environments on the steadiness of RO_2 and the rate of H-atom transfers in the $RO_2 \leftrightarrow QOOH$ isomerisation.

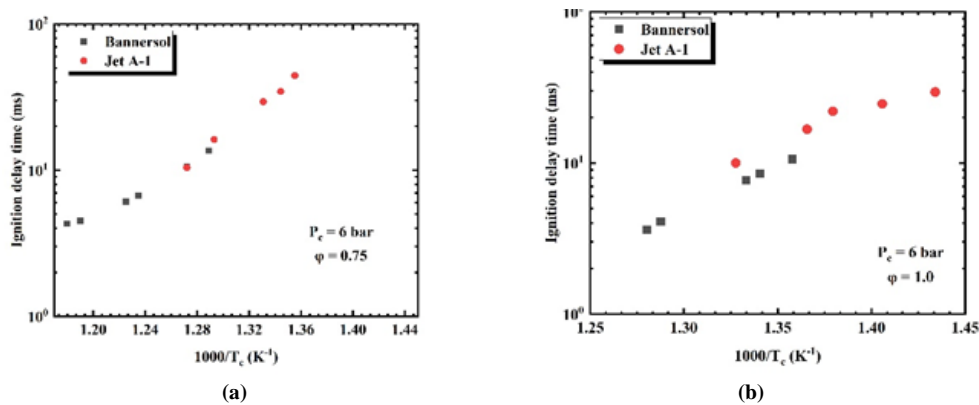


Figure 6: Comparison of ignition delay time of Jet A-1 with Bannersol. Conditions: (a) $\phi = 0.75, P_c = 6$ bar (b) $\phi = 1.0, P_c = 6$ bar

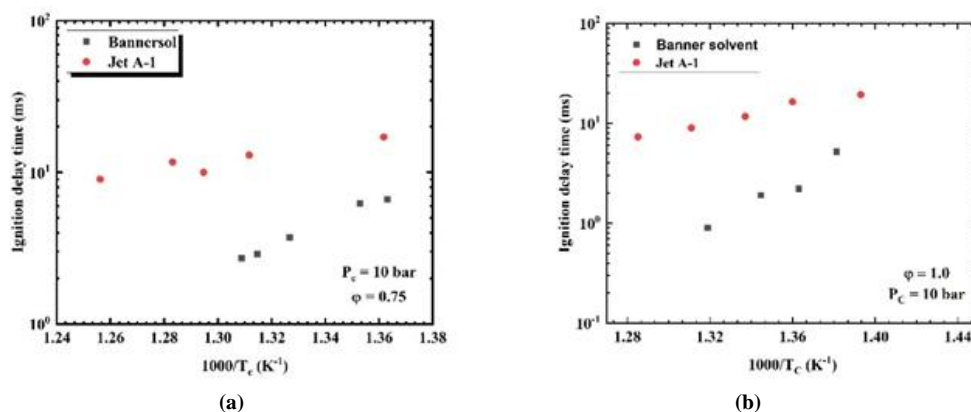


Figure 7: Comparison of ignition delay time of Jet A-1 with Bannersol. Conditions: (a) $\phi = 0.75, P_c = 10$ bar. (b) $\phi = 1.0, P_c = 10$ bar

4. Conclusions

An experimental investigation of Bannersol/air mixture in a heated RCM was conducted at low to intermediate temperatures regime ($723\text{ K} \leq T_c \leq 847\text{ K}$), compressed pressure, $P_c = 6$ and 10 bar and equivalent ratio ratios, $\phi = 0.75$ and 1.0. Within the conditions studied Bannersol displayed a single stage ignition without any trend of NTC behaviour. Paraffinic fuels are a type of hydrocarbon fuel characterized by straight or branched chain molecules. Common examples include n-heptane, n-octane, and n-decane, which are often used as surrogates for real fuels in combustion studies. As the temperature increases, the autoignition delay decreases. This is because higher temperatures accelerate the chemical reactions that lead to ignition. The effect of pressure is more complex. At low to moderate pressures, an increase in pressure tends to decrease the autoignition delay. However, at very high pressures, the autoignition delay may increase due to so-called "negative temperature coefficient" behaviour, but this was not the case at the condition studied. Comparison of Bannersol with Jet A-1 showed that Banner has higher reactivity than Jet A-1 mainly attributed to the paraffinic content of Bannersol. The autoignition delay of paraffinic fuels is a complex parameter that depends on the temperature, pressure, fuel-air ratio, and fuel composition. Understanding this behavior is crucial for the design and operation of internal combustion engines and other combustion devices.

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