International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048
Volume 6, Issue 11, pp 52-58, November-2022
https://doi.org/10.47001/IRJIET/2022.611006

# Prediction of Ignition Delay Behavior of Aviation Jet Fuel Model in a Constant Volume Adiabatic Reactor Relevant to Gas Turbine Conditions

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***Abstract* - Using the Sandia SENKIN code and the CHEMKIN II program, a numerical analysis of the chemical kinetic model of Jet fuel was performed in a constant volume adiabatic reactor at intermediate to high temperatures range of 800 K ≤ TC ≤ 1200 K at lean conditions, equivalence ratios, φ = 0.3 and 0.5 and chamber pressure of 20 and 25 bar. The ignition delay time in this scenario was influenced by pressure, temperature, and the equivalence ratio. The influence of the chamber temperature on the ignition delay time and the trend of negative temperature coefficient behavior was observed at a chamber temperature of between 850 K to 950K. Beyond these set values an Arrhenius behavior was displaced over these ranges of chamber temperatures, as a result, increasing the chamber pressure and equivalence ratio significantly cause a reduction in the ignition delay time for both conditions of pressure and equivalence ratios. It was commonly noted that the model displayed a single-stage ignition delay time and a negative temperature coefficient (NTC) and the ignition delay time is significantly affected by changes in temperature, pressure, and equivalence ratios.**

***Keywords:*** Ignition delay time, Aviation Jet Fuel, Chemical kinetics, Negative temperature coefficient, constant volume, adiabatic reactor.

## I. INTRODUCTION

The gas turbine industry has been introduced to a number of novel combustion technology concepts [1]. These include the lean direct injection (LDI), lean premixed (LPM), or lean premixed prevaporized (LPP) combustion technology, which is now gaining more attention in the gas turbine industry as a potential replacement for the diffusion flame combustor [2, 3]. The dry low emission (DLE) system has also been successful when used with natural gas to meet standard emission requirements. Premixed combustion technology is well-versed in the gas turbine industry. To protect combustor components and reduce pollution emissions, one of the main issues with such technology is avoiding the autoignition phenomenon. The most promising technology for practical applications currently seems to be LLP combustion, which is renowned for its low pollutant emissions when burning liquid fuels like kerosene and fuel oil. [4]. Industries now use the LLP combustor to reduce NOx and boost gas turbine efficiency, and it can be used with both land-based and air-based aero-engines. Premixing the fuel and air upstream of the combustor prevents the formation of the stoichiometric region in LLP combustion, which also eliminates thermal NOx. [5]. One of the problems of LPP combustors is the issue of longer residence times [6, 7]and unsteady flow oscillation known as combustion instability [8]. The LPP combustors operate under fuel-lean conditions, where the rate of combustion is actively driven by the fuel-air ratio. Local extinctions may happen if the fuel-to-air ratio significantly decreases. This instability causes the combustor to become unsteady, which could lead to a spontaneous ignition [9]. These oscillations can reach significant amplitudes and, in extreme cases, cause the combustor catastrophic failure due to excessive structural vibration and heat transfer to the chamber. The expectation of a new aircraft engine is to perform with maximum combustion efficiency as well as provide stability and low emissions. This has increased the need for low NOx turbine engines that apply a lean premixed mode of combustion. Nevertheless, a number of methods have been researched in the literature [10-13] to address the problems with autoignition and flashback in the premixer of LPP combustors. These techniques make an effort to reduce NOx emissions by designing premixers and combustion devices that allowed rapid mixing and combustion before the onset of spontaneous fuel ignition [4]. While other authors [14, 15] work reported in the literature, showed that the fuel is directly sprayed into the premixer so that the liquid fuel droplets vaporize and mix with air at lean conditions.

 

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Volume 6, Issue 11, pp 52-58, November-2022

https://doi.org/10.47001/IRJIET/2022.611006

Consequently, liquid fuels pose a significant challenge in the combustor, particularly in terms of technical requirements such as flash point, freezing point, and autoignition [16, 17]. However, the complexities of fueling system (air and vaporisation premixing) and infrastructure of recent low emission engine has made the burning of liquid fuel a challenge. Because of the refining processes and petroleum feedstocks, conventional jet fuel contains different classes of hydrocarbons and behaves differently [18, 19]. It is primarily derived from crude oil, also known as petroleum jet fuel. It consists primarily of normal alkanes, branched alkanes, cycloalkanes, aromatics, and alkenes, and contains a large number of aliphatic and aromatic hydrocarbon compounds with carbon content C8–C16. Jet fuels consist of alkanes (35 - 45%volume), cycloalkanes (30-35% volume), aromatics (one and two rings, 20-25% volume) and alkenes (less than 5% volume) [19]. Jet fuels are straight-chain such as alkanes with percentage volume of constituent ranging from 35 - 45%, branched-chain such as cycloalkanes with a constituent range of 30-35% by volume, aromatics one and two rings, 20-25% volume and the alkenes which are less than 5% volume [19, 20]. The complexities of jet fuels mean that a direct engine simulation of the chemical kinetic behavior is not feasible [20]. Therefore, commercial fuels are described using a limited number of representative compounds; these are called surrogate mixtures [21]. In this way, it is possible to describe the chemical oxidational process computationally, and well-defined experiments can be performed. The physical and chemical properties of jet fuel should be reproduced by using surrogate fuels. Surrogates are classified into two types; physical surrogates designed to produce the physical properties of fuel and chemical surrogates intended to have a similar chemical composition of the fuel. Comprehensive surrogates are substitutes that mimic the physical and chemical characteristics of fuel. Combustion processes in gas turbine are composed of several stages, including the premixed combustion phase, ignition delay period, and the mixing-controlled combustion or diffusion burn phase[22]. The ignition of the liquid fuel is governed by the physical and chemical process during the ignition delay period, and it is necessary for surrogates models to describe a range of real fuel properties [23, 24]. Both combustion and autoignition are complicated processes that require the interaction of multiple fields of study, such as fluid dynamics, thermodynamics, chemical kinetics, heat and mass transfer, and turbulence. Several facilities, including the flow reactor (FR) [25, 26], static reactor (SR) [27], Jet-stir reactor (JSR) [28, 29], shock tubes (STs) [30, 31], and rapid compression machine (RCM) [19, 32-34], are utilized in literature to obtain ignition delay time (IDT) data. A more detailed analysis is needed to understand the chemical pathway responsible for fuel combustion to increase engine efficiency and minimize greenhouse gas emissions. There is an absolute need to exploit fully the combustion chemistry of jet fuels in a system, which it's run and their behaviors when subjected to a different operating condition of the system. The influence of the fuel on ignition need fully explored with the specific chemistry involved in the autoignition and understood how to predict how long it is safe for fuel and air to mix thoroughly before ignition occurs. The autoignition parameters, which are important for the automotive and gas turbine industries can be better understood using numerical predictions of the ignition delay time and the validation of detailed models. One of the more well-known validation techniques for detailed chemical kinetic mechanisms is to compare the computational predictions of ignition delay times to STs and RCM experiments. Since zero-dimensional computations are free of transport effects, such comparisons can provide a thorough understanding of the underlying chemistry. This present work predicts the autoignition delay time of aviation fuel using the available models from literature at constant volume relevant to practical gas turbine operating conditions

## II. NUMERICAL METHODS

Kinetics modeling of the IDTs is performed using the Sandia SENKIN code [35] in conjunction with CHEMKIN-II software. The conditions behind the reaction chamber were assumed to be zero-dimensional, closed homogeneous adiabatic reactor operating at constant volume. The equations governing reactions in the system are the mass continuity and energy equations. For a closed system, total mass remains constant. Individual species concentrations change but the overall mass remains fixed. Mass, m of the system is therefore given by (1).

$$m = \sum_{k=1}^{K} m_k \qquad (1)$$

$m_k$ is the mass of the k$^{th}$ species and K is the total number of species. The mass fraction for the k$^{th}$ species is:

$$\frac{dY_k}{d_t} = v\dot{\omega}_k W_k \qquad (2)$$

$Y_k$ is the mass fraction, $\dot{\omega}_k$ is the molar production rate, $W_k$ is the molecular weight and $v$ is specific volume. $W_k$ is the net rate of increase of the species k, as a result of competition between reactions which generate and absorb it. Temperature of the mixture is found by considering the 1$^{st}$ law of thermodynamics. For a closed system with no heat transfer, the 1$^{st}$ law reduces to equation 3.

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$$de + pdv = 0 \qquad (3)$$

Internal energy per unit mass is given by:

$$e = \sum_{k=1}^{K} e_k Y \qquad (4)$$

Where $e_k$ is the internal energy of the k$^{th}$ species. Differentiating (4) gives

$$de = \sum_{k=1}^{K} Y_k de_k + \sum_{k=1}^{K} e_k dY_k \qquad (5)$$

For calorically perfect gases, the change in energy per unit mass is $de_k = c_{v,k} dT$ and the specific heat at constant volume of the k$^{th}$ species and T is the mixture temperature. The overall specific heat for the mixture is given by:

$$c_v = \sum_{k=1}^{K} Y_k c_{v,k} \qquad (6)$$

Combining (5) and (6) with the 1$^{st}$ law (3) we get:

$$c_v \frac{dT}{dt} + \sum_{k=1}^{K} e_k \frac{dY_k}{dt} + p\frac{dv}{dt} = 0 \quad (7)$$

Replacing $\frac{dY_k}{dt}$ in the above with equation 2:

$$c_v \frac{dT}{dt} + p\frac{dv}{dt} + v\sum_{k=1}^{K} e_k \dot{\omega}_k W_k = 0 \qquad (8)$$

Equation (2) and (8) can be used to solve problems where the volume is either fixed or is a known function of time. For a mixture at constant pressure, the 1$^{st}$ law reduces to the condition of constant enthalpy (h). The differentiated equation for enthalpy is:

$$dh = de + vdp + pdv \qquad (9)$$

When combined with (3) and removing the $dp$ term

$$dh = 0 \qquad (10)$$

Total enthalpy is then

$$h = \sum_{k=1}^{K} Y_k h_k \qquad (11)$$

The energy equation (8) becomes:

$$c_p \frac{dT}{dt} + v\sum_{k=1}^{K} h_k \dot{\omega}_k W_k = 0 \qquad (12)$$

A rate law specifies the rate of change of concentration of a chemical species in terms of the product of concentration and a rate constant, *k*. The rate constant is independent of concentration but not of temperature and is in the form:

$$k_f = AT^{\beta} exp\left(-\frac{E}{RT}\right) \qquad (13)$$

*E* is the activation energy, $\beta$ is the temperature exponent and *A* the pre-exponential constant.

### 2.1 Chemical Kinetics Models

To be able to accurately predict the reaction progress of a specific fuel under a variety of variables such as pressure, temperature, and equivalency ratio. Comphrensive chemical kinetic mechanisms describing oxidation of the Aachen surrogate [36] is adopted in this simulation for which it has n-decane and 1,2,4-trimethylbenzene component [37]. The surrogate consist of mixture of n-decane 80% and 1, 2, 4-trimethylbenzene 20% by weight, called the Aachen surrogate. This has been chosen for evaluation as a potential substitute for jet fuel. The chemical kinetic mechanism had already been validated from experimental data obtained from shock tube [38], a freely propagating premixed flame [39], and jet stirred reactor [40]. There are 900 elementary reactions and 122 species in the detailed reaction mechanism. Based on formulation data obtained from the GC analysis in published research [32] the equivalence ratios for the jet fuel model were calculated and used in the simulation for all the conditions.

## III. RESULTS AND DISCUSSIONS

### 3.1 Effect of Temperature

Figure 1(a,b,c & d), shows the plot of temperature as a function of time for Jet fuel /air mixture at chamber pressure (PC) of 20 & 25 barat lean condition φ = 0.3 and 0.5, and chamber temperature (TC) in the range of 800 K ≤ TC ≤ 1200 K simulated in a constant volume adiabatic reactor. The effect of temperature is seen on the ignition delay time as a function of time as shown in Figures 1.

In Figure 1(a), within the tested conditions for lean mixtures at chamber pressure of 20 bar and at φ = 0.3. As the chamber temperature was increased from 850 K to 950 K, there was an increase in the ignition delay time as demonstrated in Figure 1(a). This trend illustrates the NTC behavior, which was predicted by the kinetic model at that condition. Beyond the temperature range of 850 K to 950 K,

 

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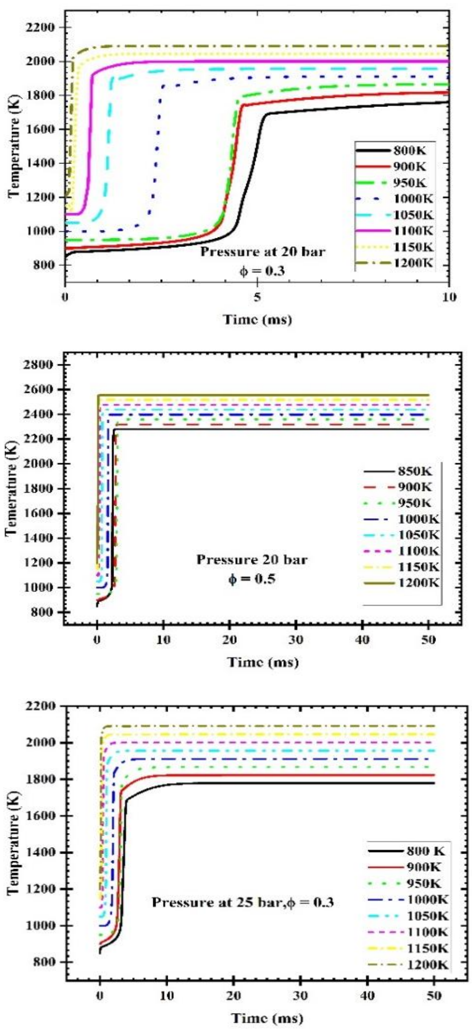
https://doi.org/10.47001/IRJIET/2022.611006

Arrhenius behaviour was observed as the temperature was increased a reduction in the ignition delay time was seen. At this condition studied, a single stage ignition delay time was predicted by the kinetic model in literature [37]. Similar trend was also observed in Figure 1(b,c,&d),where the kinetic model predicted NTC behaviour between the temperature range of 850 K to 950 K and beyond this limit an Arrhenius behaviour was observed. The plot of IDT against the $1/T_C$ as depicts in Figure 3(a & b). The plot shows that at both equivalence ratio of φ = 0.3 and 0.5 and chamber pressure of 20 bar and 25 bar. As the $T_C$increases from 850 K to 950 K, the NTC behavior was seen as the ignition delay time increases within these temperature ranges. Beyond the temperature of 950 K , an Arrhenius behavior was observed as the chamber temperature, Tc, increases leading to a reduction in the IDT as seen in Figure 3(a &b). It has noticeably been revealed that at the NTC region, the reactivity is controlled by the low-temperature chain branching: $R + O_2 \leftrightarrow RO_2 \leftrightarrow QOOH\ (+O_2) \leftrightarrow OOQOOH \rightarrow 2OH$ + product. The reaction pathway is governed by the $R + O_2 \leftrightarrow RO_2$ equilibrium and the rate of isomerization $RO_2 \leftrightarrow QOOH$.

(a)

(b)

(c)




(d)

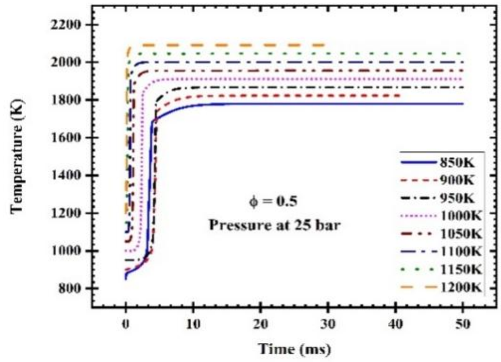



**Figure 1: Shows the effect of temperature on the IDT at (a-b) φ = 0.3, pressure = 20 bar and 25 bar. (c-d) φ = 0.5, pressure = 20 bar and 25 bar**

### 3.2 Effect of Pressure

The effect of pressure on the ignition delay time is shown in Figure 4 (a & b) at equivalence ratio, φ = 0.3 & 0.5. In Figure 2(a) shows the effect of pressure at φ = 0.3, increasing Pc from 20 bar to 25 bar lead to slight reduction in the ignition delay time.

(a)

(b)

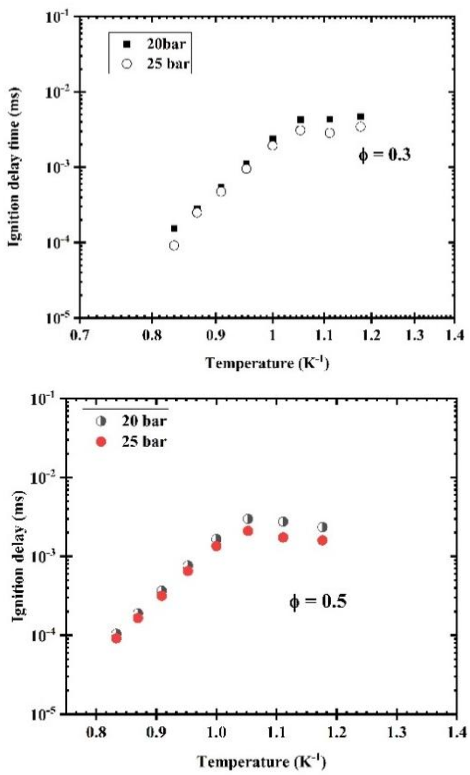



**Figure 2: Shows the effect of pressure on the IDT at (a) φ = 0.3 and (b) φ = 0.5**

At the same time as depicts in Figure 2(b) at higher equivalence ratio, φ = 0.5, increasing pressure, increases reactant concentration thus increases the reaction rate thereby practically reducing ignition delay. Likewise, increasing the pressure in the chamber results in higher temperatures and pressures, which accelerate the speed of molecules and

ISSN (online): 2581-3048
Volume 6, Issue 11, pp 52-58, November-2022
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increase the number density of molecules, resulting in a higher rate of chemical reactions and a reduction in the ignition delay time.

### 3.3 Effect of Equivalence ratio

Figure 3(a & b) also depicts the influence of equivalence ratio on the ignition delay times for Jet fuel model at Pc = 20 bar& 25 bar. However, the effect of changing initial fuel mole fraction on the ignition delay at both conditions of pressure = 20 bar & 25 bar indicate an increase in the initial fuel concentration (that is increasing the equivalence ratio) which leads to a slight decrease in the ignition delay time. The mixture reactivity increases with an increase in equivalence ratio thereby leading a slight reduction in the ignition delay time as demonstrated in Figure 3(a &b). Such behaviour is consistent with other typical hydrocarbon behaviors in literature [32].

(a)

(b)

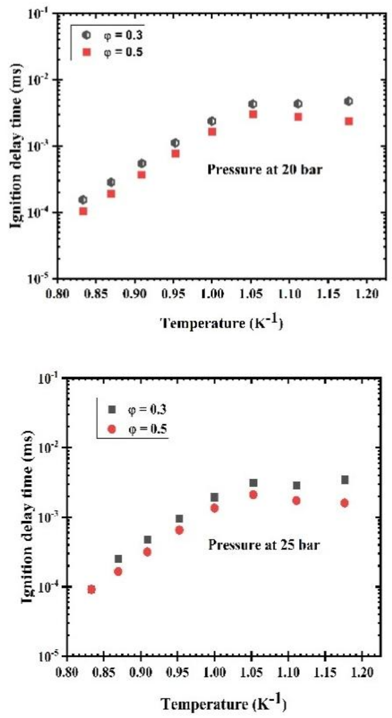


**Figure 3: Shows the effect of equivalence ratio on the IDT at φ = 0.3 and 0.5, pressure = 20 bar and 25 bar**

## IV. CONCLUSION

A reaction kinetics model which comprises 900 elementary reactions and 122 species was used to simulate Jet fuel using a computer-based SENKIN code in conjunction with CHEMKIN II software in a constant volume reactor relevant to gas turbine conditions. It was observed that at $\varphi$ = 0.3 and 0.5, Pc = 20 and 25 bar and Pc at 800 K $\leq$ TC $\leq$ 1200 K. It was observed that the effect of increasing the temperature, pressure, and equivalence ratio has shown to decrease monotonically with of IDTs. Within the conditions studied the chemical kinetic model displays a single-stage ignition delay time and NTC behavior displayed between the temperature range of 850 K and 950 K, further beyond 950 K, an Arrhenius behaviour was seen. Similarly, increasing the equivalence ratio leads to increase in the reactivity, which reduces the ignition delay time? Increasing chamber pressure means higher temperatures and pressures that accelerate the speed of molecules and number density of the molecules thus increasing the frequency of collision resulting in higher rate of chemical reactions that led to a reduction in the ignition delay.

The results presented here would need to be validated against experimental data in order to enhance the development of a chemical kinetic model that would help replicate the combustion of Jet fuel. Future work would consider the reaction pathways and the sensitivity of reaction model.

## ACKNOWLEDGEMENT

We would like to take this opportunity to extend our appreciation to the Federal Government of Nigeria, and more specifically, the office of the Tertiary Educational Trust Fund (TETFUND), for their contribution of funds in the form of an Institutionally Based Research (IBR) grant in order to assist us in carrying out this research. Additionally, we would like to express our gratitude to Mr. Isaac Abuh for diving access to the ICT center, CRUTECH.

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ISSN (online): 2581-3048
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**Citation of this Article:**

Nyong, O. E, Ene, E.B, Igbong, D.I, Ebieto, C.E, Ana, R.R, Igbolo, B, Akpan, U.V, “Prediction of Ignition Delay Behavior of Aviation Jet Fuel Model in a Constant Volume Adiabatic Reactor Relevant to Gas Turbine Conditions” Published in *International Research Journal of Innovations in Engineering and Technology - IRJIET*, Volume 6, Issue 11, pp 52-58, November 2022. Article DOI https://doi.org/10.47001/IRJIET/2022.611006

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