

A Comprehensive Combustion Kinetics Modeling Study of Iso-Octane and Air Mixtures

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ABSTRACT

The oxidative behavior of the iso-octane (2,2,4-trimethylpentane) has been studied in a range of experimental facilities in order to investigate the relatively unexplored combustion chemistry of the title species and to provide combustor relevant experimental data. The ignition of iso-octane/air and iso-octane/O₂ mixtures was studied at temperatures of 600–1300 K, pressures of 1–50 atm, and equivalence ratio 0.5 to 2. This study has been conducted analytically using a kinetic scheme with 994 elementary reactions and 201 species. Cantera (an object oriented software for reacting flow) software is used in this study.

Keywords: Iso-octane, shock tube, kinetics modeling, diluent, ignition delay.

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INTRODUCTION

The design and development of new combustion engines are driven by increasingly stringent legislated emissions and fuel economy targets. Now a days this has led to pursuit of alternative approaches to internal combustion engine combustion which can migrate significantly from conventional premixed-charge flame propagation (spark ignition) and diffusion-controlled flame oxidation (compression ignition) [1]. Advanced approaches of engine operation have potential to dramatically enhance engine performance while concurrently reducing engine pollutions. Advanced engine working strategies comprise low temperature and fuel lean conditions which empower higher compression ratios and may reduce the need for exhaust gas after treatment. Homogeneous charge compression ignition is a low temperature combustion method that has been the focus of numerous experimental and computational studies in the past decade. Many articles review

research progress on homogeneous charge compression ignition and other advanced engine strategies including discussions of important limitations of current scientific understanding, demonstration of operating modes, and new approaches in engine technology.

Methods of modern internal combustion engines often encompass mixed modes of combustion, in which flames and auto ignition process are simultaneously contributing to combustion and heat release rates. For example, during spark assisted compression ignition a spark plug is used to initiate a flame into the nominally homogeneous or partially stratified fuel/air charge in an internal combustion engine. Spark assisted compression ignition has been demonstrated to expand high and low load operation beyond homogenous compression charge ignition boundaries. However, methods to optimize spark assisted compression ignition and other mixed modes of combustion are limited by

the lack of fundamental understanding of flame propagation and auto ignition interactions at conditions relevant to advanced engine strategies. Moreover, advanced combustion strategies like HCCI, SACI and GDI often consider highly dilute operation as a means to achieve high efficiency goals and meet emerging and more strict emissions requirements.

These methods typically target either fuel lean or stoichiometric conditions. The combination of high levels of dilution and fuel lean mixtures is particularly challenging, as flame propagation and heat release rates decrease dramatically compared to undiluted stoichiometric conditions.

There is also a significant lack of fundamental combustion data, such as flame speeds and flammability limits at the state and reactant mixture conditions important to advanced combustion in internal combustion engines. This gap complicates optimizing engine operation, especially the development and validation of theory and models which accurately describe mixed modes of combustion [2]. Consequently, the aim of the current study is to characterize flame and auto ignition interactions of iso-octane and air mixtures at premixed, moderate temperature and pressure conditions relevant to advanced engine strategies.

ISO-OCTANE

Iso-octane (2,2,4-trimethylpentane) a primary reference fuel to octane rating in spark ignition engines, has drawn considerable interest as a model compound for branched alkane components found particularly in gasoline [3], but also those found in diesel [4], and jet fuel [5]. Due to its relevance to practical liquid fuels, iso-octane has been the subject of many experimental and kinetic model studies. Experimental investigations of iso-octane oxidation and ignition have been carried out in shock tubes, rapid compression machines,

flames, jet stirred reactors and flow reactors [6]. By this experimental investigations a variety of kinetic measurements have been made including ignition times, radical species concentrations, stable species concentrations, and flame speeds.

SHOCK TUBE

Shock tubes are a common choice for the investigation of ignition phenomena due to the nearly instantaneous heating of the reactant mixture by the shock wave, the near adiabatic constant volume behavior of shock tube reflected shock environment, the ability of shock tubes to access a range of conditions of interest to practical combustion devices, and the ease of applying optical diagnostics to shock tube experiments. When studying the ignition of a fuel compound in a shock tube, the choice of reactant mixture is impotent and there are several options depending on the goal of the choice of diluents gas.

KINETIC MODELING

To build up a chemical kinetic model, a number of assumptions have to be made. The assumptions which are made in the specific way that the conditions simulated correspond to the conditions that are in effect in the experimental side. The complete reaction mechanism (944 reactions and 201 species) which involve in the combustion of iso-octane is proposed and validated with LLNL (Lawrence Livermore National Laboratory) detailed mechanism as shown in Figure 1.

Software: CANTERA object oriented software for reacting flows is used to simulate the results.

CRITERIA FOR FINDING IGNITION DELAY

Ignition delay time (t) is the time which corresponds to the maximum rate of reactions between CO and O atoms. Induction period is the time at which the risen temperature had completed about half, often defined as the time required for a small

(that is 1–5%) temperature or pressure rise. Bowman [7] found that ignition delay time to vary inversely with approximately the first power of the fuel concentration, to be only slightly dependent upon oxygen concentration and to decrease with increasing pressure and temperature. It is the

time to reach the concentration value of OH to 1×10^{-9} moles/cc .It is the time required to start the decomposition of H_2O_2 . Figure 2 shows the criteria applied for finding out the induction or ignition delay period.

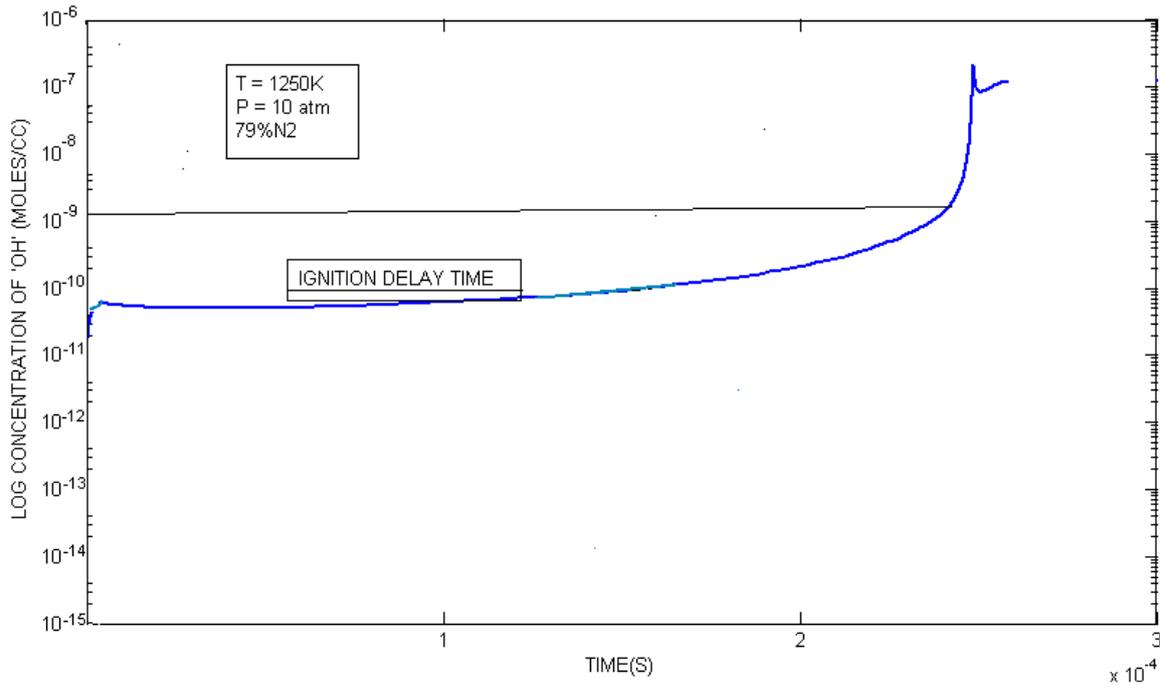


Fig 1. Ignition criteria.

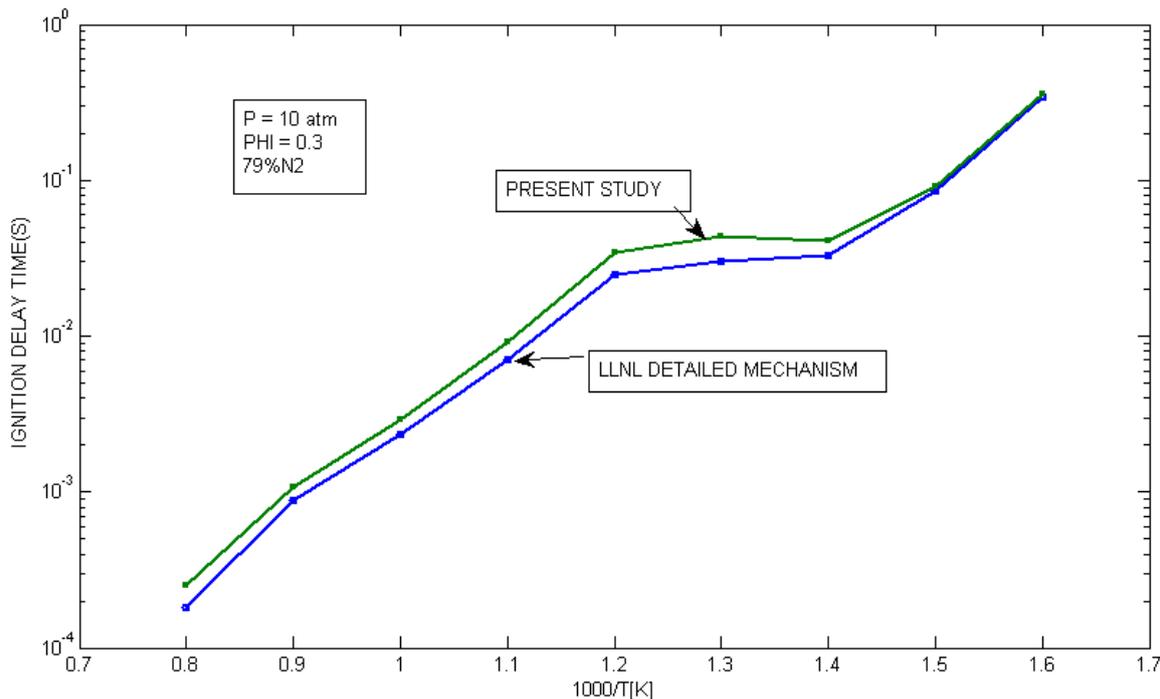


Fig. 2. Validation of the reaction mechanism.

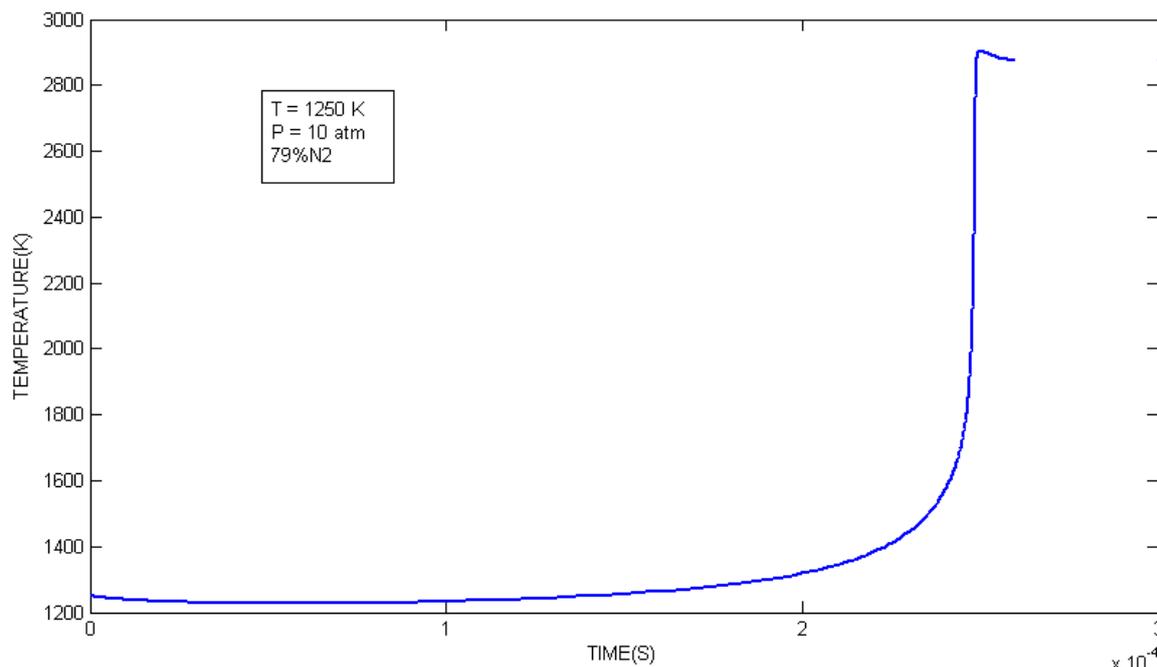


Fig. 3. Temperature profile.

TEMPERATURE PROFILE

The temperature profile is shown in Figure 3. To plot this variation is initial temperature 1250K, initial pressure 10 atm and initial $\phi=0.3$. From the graph it has been observed that the initial dip of temperature occurs. This is due to initiation reaction which is endo-thermic that initially dips and gradually rises until a region when the curve shoots up. These sets of endothermic reactions require a large amount of energy. The heat that is required for this endothermic reaction is drawn from the surrounding thus causing the temperature to dip. Once the reaction is complete, a fraction of fuel breaks down in to molecular weight hydrocarbons or the radicals, the temperature steadies on. Once the radicals are formed by the pyrolytic the propagation reaction starts. The Endothermic reaction proceeds slowly until the self ignition temperature is achieved. Once the temperature is attained, the ignition occurs. The fuel breaks down completely at this stage and the combustion process speeds up. In the curve, it is the region at which the curve steps down. The time between the initial input time and this corresponding initial

input time gives the induction period, of course the chemical ignition delay. The curve steps up and then maintains a particular value. After a while it can be observed that the temperature goes on decreasing because at this stage there is no fuel to burn to energy. Hence temperature reduces.

The condition to plot this variation is initial temperature 1250K, initial pressure 10 atm and initial $\phi=0.3$. We can see that at the point of ignition delay, there is a steep increase in temperature and pressure. Sufficient oxygen is not available to start spontaneous combustion at high equivalence ratio, which increases the ignition delay time.

VARIATION OF IGNITION DELAY WITH TEMPERATURE

The variation of ignition delay [8, 9] with temperature is plotted on the Figures 4 and 5. The ignition delay drops when temperature rises. As a result pressure, density of fuel, oxygen mixtures increases, increases and hence the probability of fuel particle coming in contact with the reacting radicals also increases. From the

Figure 4, we found that, for higher temperature the ignition delay time is decreased. There is profound influence on ignition delay when the initial temperature is increased by 100K.

SPECIES CONCENTRATION PROFILE

Concentration profiles of major species of C_8H_{18} are show in Figure 6. During the

combustion of iso-octane at the point of ignition, the fuel curve steps down. It shows ignition process occurs very fast.

From the Figure 6, the consumption of O_2 is due the combustion of iso-octane, at the point of ignition. The concentration profile of H_2O_2 steps down because it is also considered as the ignition criteria of iso-octane.

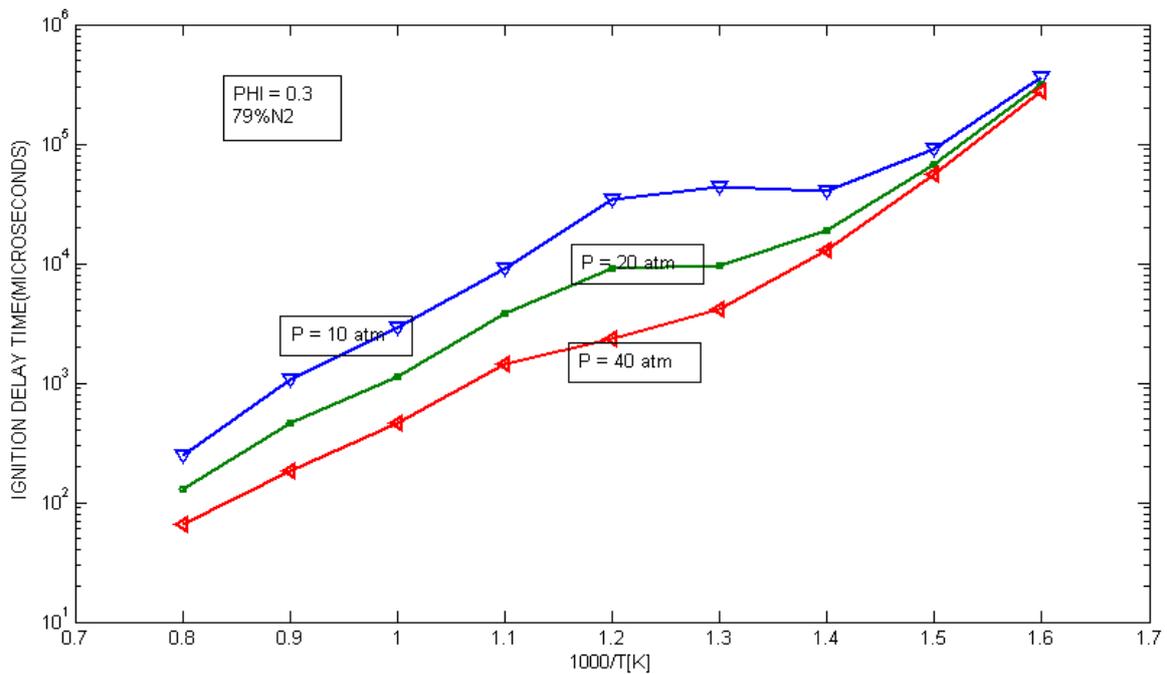


Fig. 4. Variation of ignition delay with temperature.

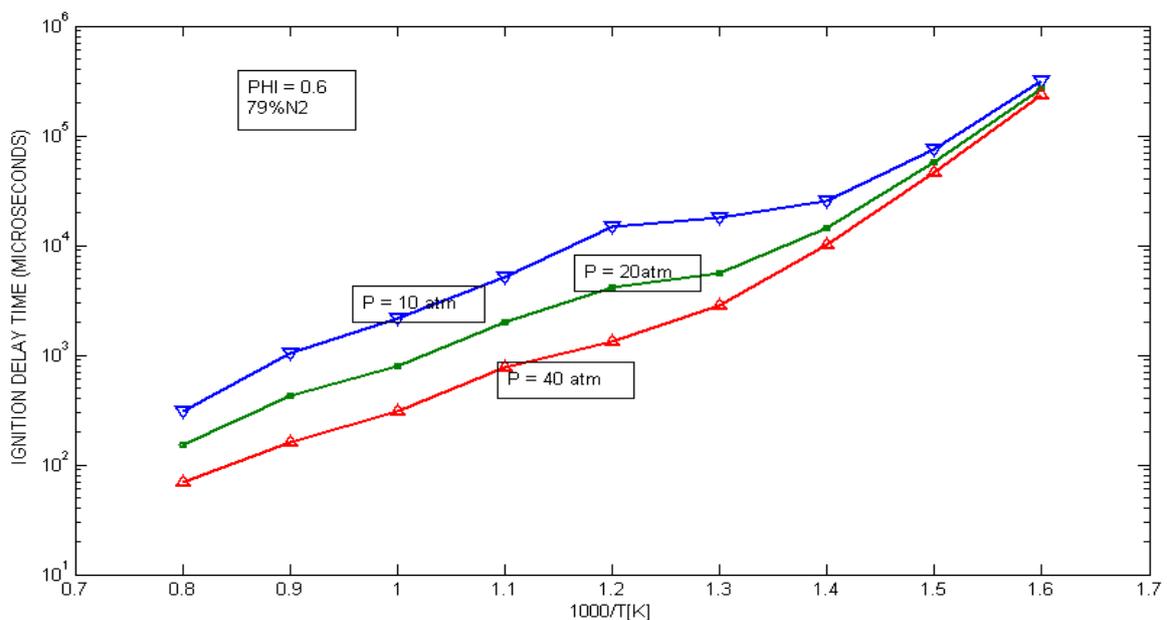


Fig. 5. Variation of ignition delay with temperature.

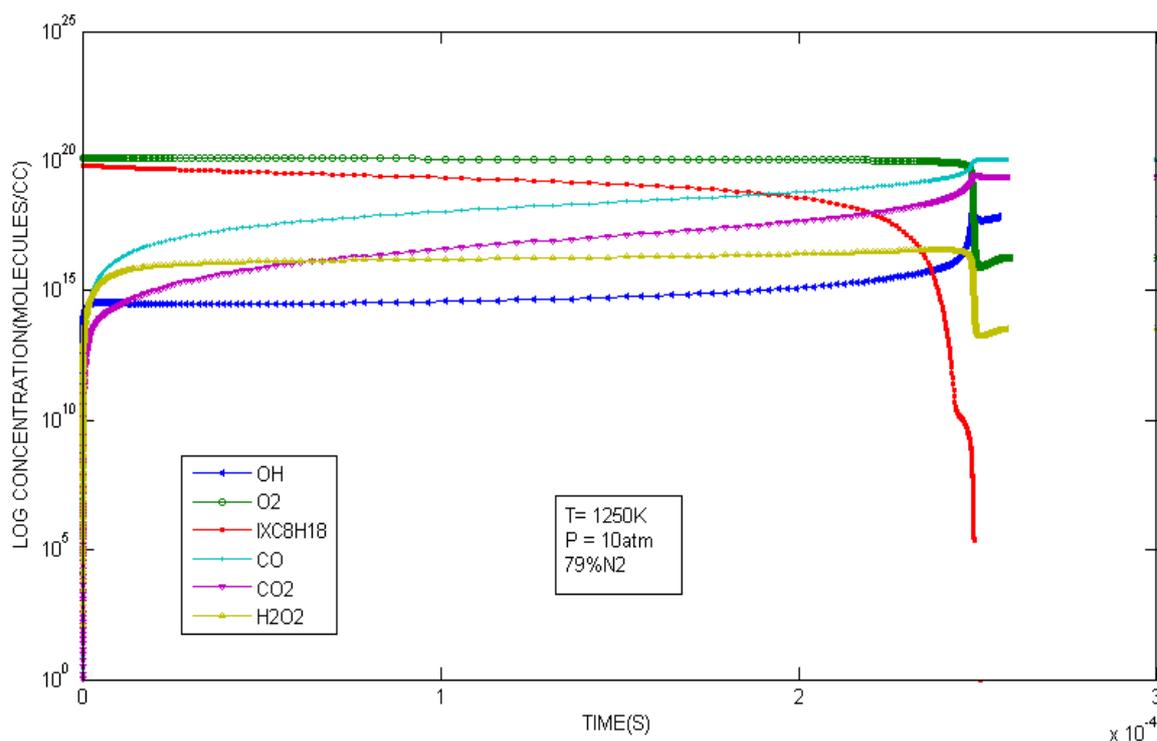


Fig. 6. Species concentration profile.

INFLUENCE OF DILUENTS GASES

Monatomic argon is often used as a diluent gas because its lack of a vibrational mode eliminates consideration of the time scale for vibrational relaxation when calculating the post shock conditions. Additionally, reflected shock pressure profiles for argon mixtures usually display less noise due to the lack of sidewall bifurcation relative to nitrogen relative to nitrogen. Hence, optimized reflected shock conditions are typically obtained using dilute mixtures in argon. However, dilute mixtures in argon are dissimilar in composition to those used in combustion engines, where air is typically the oxidizer and at stoichiometric conditions the fuel concentration is near 1 Mol%. Therefore, experiments performed in air and at elevated pressures are desired for the validation of oxidation mechanisms used at combustion engine conditions [3]. The choice of diluents gas can also influence shock tube ignition measurements through the diluent heat capacity. As heat is released during the radical growth period prior to ignition the temperature rises more quickly for a monatomic diluent than for a diatomic diluent, which accelerates the

ignition process. However, the influence of replacing nitrogen with argon an ignition time measurements is typically considered to be small.

Influence of O₂

From Figures 7–9, it is observed that concentration level of lean mixture of O₂ is maximum as O₂ is consumed more for oxidation of soot. At stoichiometric mixture and fuel rich conditions O₂ has no role for soot oxidation.

Influence of OH

At stoichiometric and fuel rich conditions OH radical are responsible for the oxidation of soot is plotted in Figures 10–12. The concentration levels of OH radical are very high in stoichiometric and fuel rich conditions as compared with lean mixture condition. At lean mixture condition Soot is formed by both OH and O₂.

Theoretically temperature becomes maximum at equivalence ratio of unity but using the proposed mechanism it is found that maximum temperature occurs at equivalence ratio of 1.2 as shown in Figure 13.

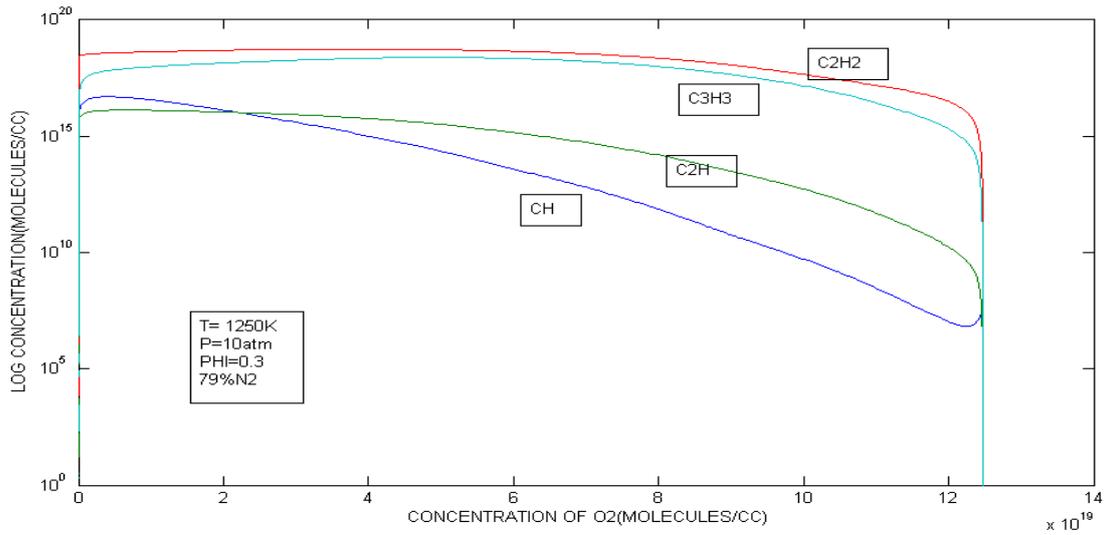


Fig. 7. Variation with O₂ (lean mixture).

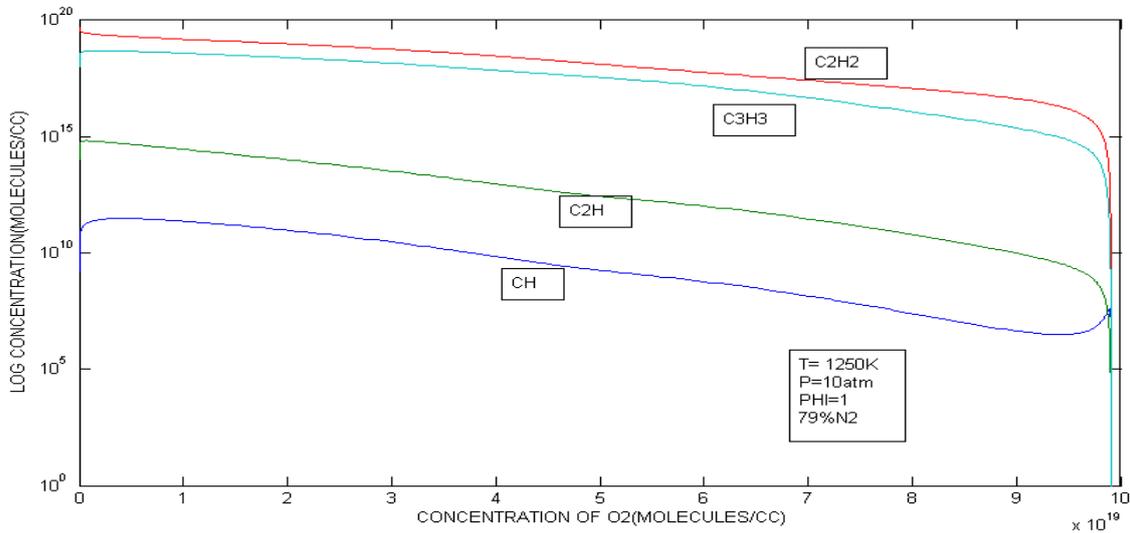


Fig. 8. Variation with O₂ (stoichiometric mixture).

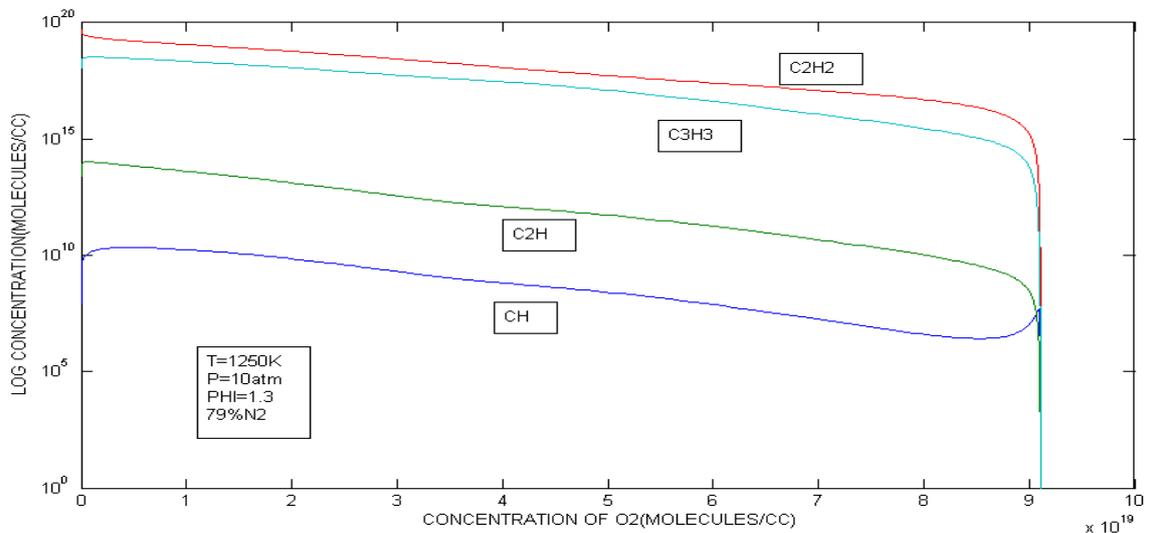


Fig. 9. Variation with O₂ (rich mixture).

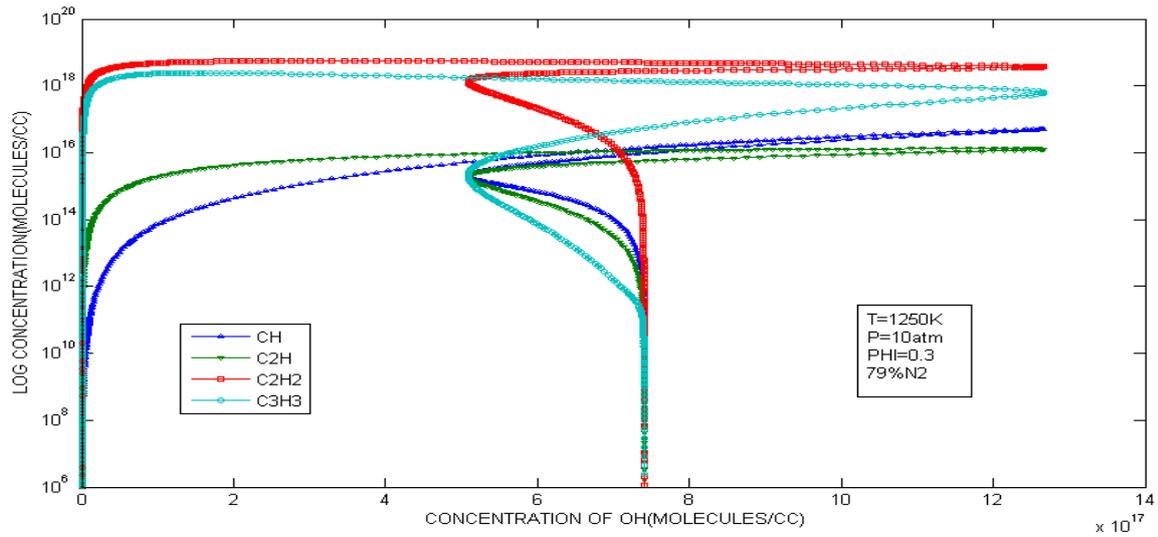


Fig. 10. Variation with OH (lean mixture).

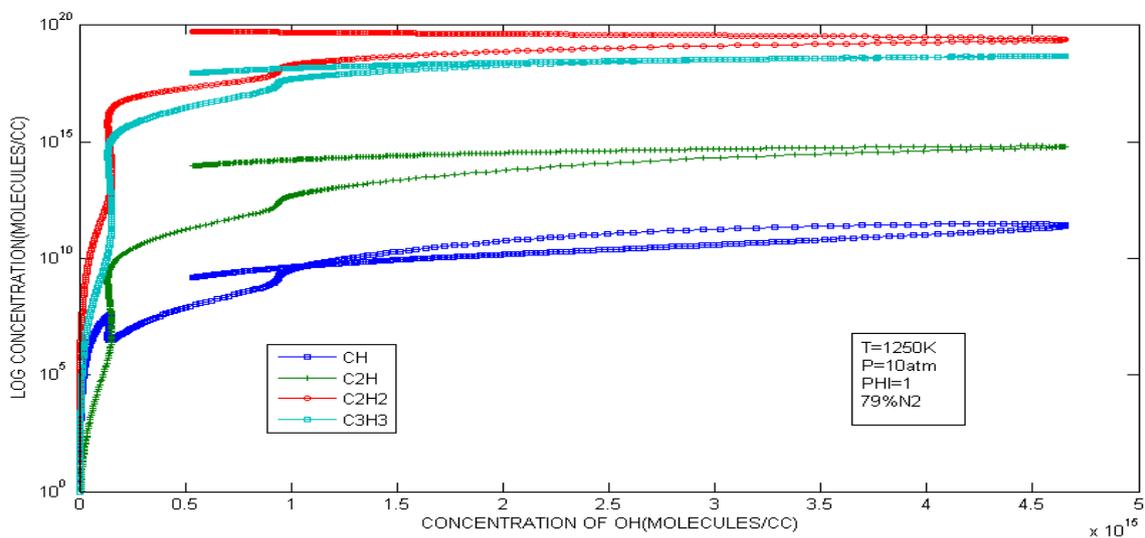


Fig. 11. Variation with OH (Stoichiometric mixture).

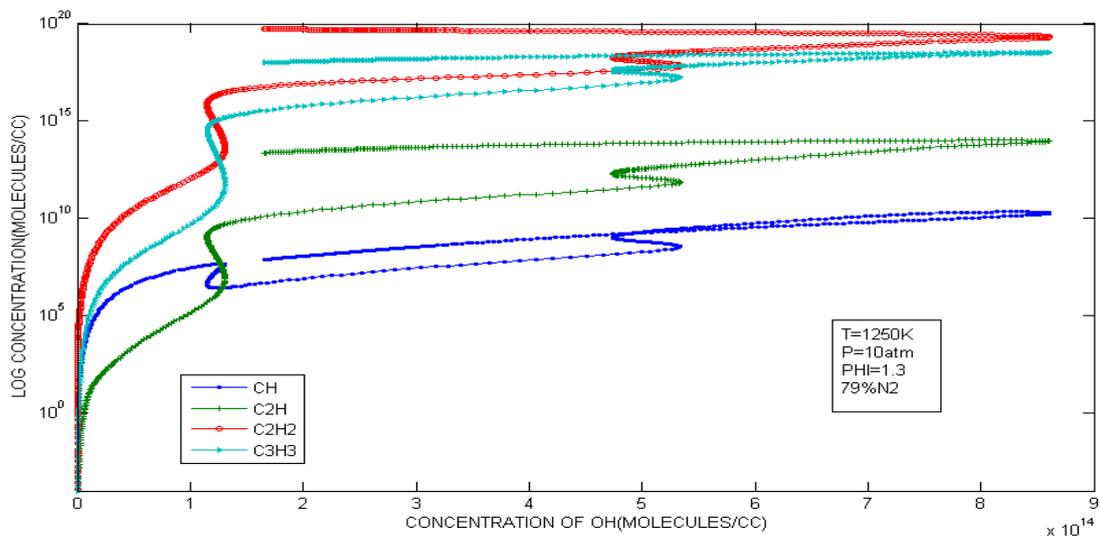


Fig. 12. Variation with OH (rich mixture).

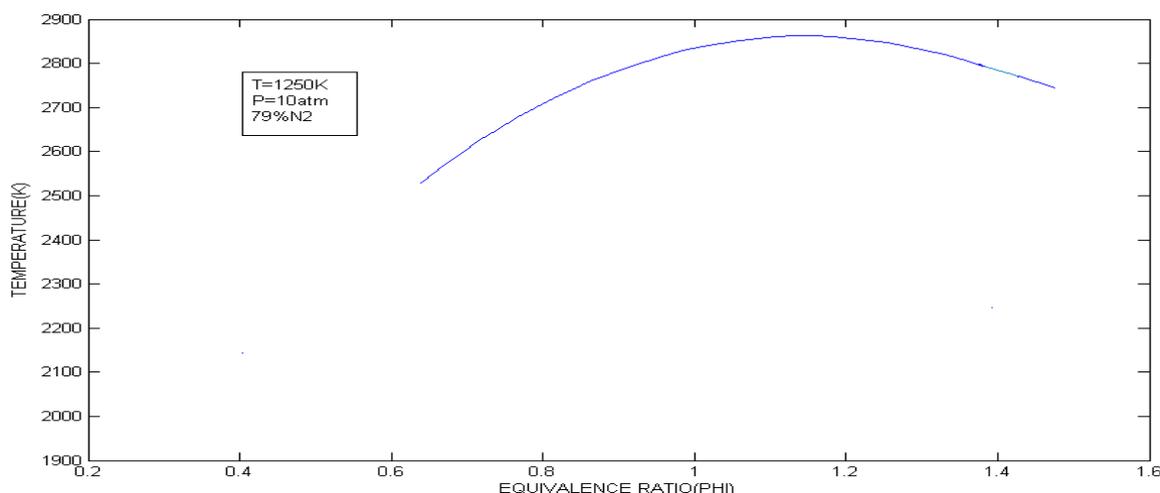


Fig. 13. Variation of temperature with equivalence ratio.

CONCLUSION

The study on the combustion kinetic modeling of iso-octane has been conducted. A reaction mechanism containing 994 reactions among 201 species was proposed and the ignition delay times at various initial conditions of temperatures, pressures and equivalence ratio are determined. The conditions which are used to determine the ignition delay is the time at OH concentration reaches 1×10^{-9} moles/cc. The measured iso-octane/O₂ ignition times agreed well with the previously published results. The difference in measured ignition time for mixtures containing argon and nitrogen as the diluents gas can be attributed to the differing heat capacities of the two diluent species and the level of induction period in which heat releases prior to ignition. At high temperatures, a hydrogen atom transfer reaction was found to be dominant unimolecular decomposition path-way of iso-octane. The reactions of hydrogen atom with the fuel are also found to be important in predicting ignition delay time experiments. The results obtained here are found to be agreeable with previous studies described here.

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