

Article

Numerical Investigation of the Ignition Delay Time of Kerosene Premixed Combustion in an SI Engine

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Abstract: SI engines are installed widely in small aircrafts as they have good fuel economy. Currently, these SI engines are fueled with gasoline, although their safety can be improved if kerosene is used. However, the combustion performance of kerosene cannot fulfil the requirements due to the differences in physicochemical properties. This study investigates the ignition delay time of kerosene at a pressure range of 15–35 bar and a temperature range of 600–1000 K. A detailed chemical reaction mechanism is employed for the premixed combustion process. Under the initial conditions of 1000 K and 35 bar, with an equivalence ratio of 1, the total ignition delay time of kerosene is 0.401 ms. The NTC range of kerosene is determined as roughly 750–920 K. Subsequently, the chemical reaction paths with an equivalence ratio of 0.8, 1, and 1.2 and an initial pressure of 15, 20, and 25 bar were analyzed. The rate-determined elementary reactions were obtained based on a sensitivity analysis. The difference between kerosene and gasoline are also compared, and the rate-determining reactions that affect the ignition of kerosene and gasoline are discussed. The results of this study can provide a reference for the combustion performance improvement and knock suppression of SI engines fueled with kerosene.

Keywords: kerosene; ignition delay time; SI engine; premixed combustion; chemical reaction path



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1. Introduction

Spark-ignition (SI) engines are the power sources of small aircrafts such as helicopters and unmanned aviation vehicles (UAVs). Premixed combustion is applied for SI engines using gasoline as the fuel. However, gasoline has a high volatility and low flash point, making it unsafe for aviation applications [1]. Compared with gasoline, kerosene has good low-temperature fluidity, stability, lubricity, and does not easily generate static electricity. To improve the safety of aviation SI engines, it is necessary to investigate the feasibility of using kerosene instead of gasoline.

The combustion characteristics of fuel-air mixtures can be measured under working conditions with a specified temperature, pressure, and equivalence ratio inside a constant volume bomb [2]. Recently, the combustion performances of kerosene mixed with other fuels were studied. Shi et al. supplied kerosene together with diesel fuel in a diesel engine to reduce the ignition delay time and alleviate the cold-starting problem [3]. Hydrogen can be added to the combustion process of kerosene to improve the laminar flame speed [4]. Kindracki et al. [5] controlled the combustion process via regulating the hydrogen blending ratio. In addition, hydrogen is also helpful for the evaporation of kerosene and the following heat-release process [6]. Some investigations analyzed the combustion performance based on engine experiments. Gad et al. [7] mixed biodiesel with kerosene to supply a diesel engine. The results indicated that the emissions were decreased. Ghose et al. [8] blended kerosene with ethanol in a gas turbine, showing that the exhaust temperature dropped, and the CO emission was reduced.

Although the heat value of kerosene is close to that of gasoline, the flame speed of kerosene is evidently lower than that of gasoline. Therefore, a serious knock phenomenon

occurs in SI engines fueled with kerosene [9]. A large ignition delay time of the fuel yields a slow flame propagation and is more vulnerable for knock appearance. The ignition delay time is influenced by the combustion temperature, pressure, and equivalence ratio and can be determined via experiments [10]. Marek et al. [11] measured the ignition delay time of kerosene Jet-A inside a premixed-pre-evaporation tube under the pressure of 0.54–2.5 MPa and temperature of 550–700 K. The results indicated that the ignition delay time was inversely proportional to the pressure. Spadaccini et al. [12] studied the ignition delay times of five liquid fuels using test equipment with a continuous mass flow rate. Liang et al. [13] built a high-pressure shock tube and measured the ignition delay time of kerosene JP-3. The temperature ranged from 820–1500 K and the pressure was 5.5–22 bar. An investigation showed that a serious adsorption of gaseous kerosene in the shock tube occurred [14] and the effects on the measurement of the ignition delay time should be considered. The ignition delay time has a direct connection with the pyrolysis of the fuel. Song et al. [15] studied the thermal cracking process of RP-3 and found that the equivalence ratio had a great influence on the products.

The combustion characteristics of kerosene can be investigated theoretically by the employment of a detailed chemical reaction mechanism. Wang et al. [16] designed a reduced mechanism containing 106 species and 382 elementary reactions. The kerosene was represented by the mixture of n-decane, n-propyl cyclohexane, and n-propyl benzene. The results indicated that the mechanism had a high precision on the prediction of the ignition delay time, species concentrations, and flame speed during the high-temperature combustion process. Honnet et al. [17] used a surrogate fuel for kerosene and developed a chemical reaction mechanism. The feasibility was validated by the experiments of a shock tube and a rapid compression machine. Xiao et al. [18] designed a detailed reaction mechanism for RP-3 containing 109 species and 946 elementary reaction steps. Ma et al. [19] conducted a shock tube experiment to validate the chemical reaction kinetics model for RP-3. The results indicated that the ignition delay time was reduced with an increase in the temperature, pressure, and mole fraction of kerosene, as well as with a decrease in the equivalence ratio. Sun et al. [20] analyzed the combustion characteristics of small alkenes based on a sensitivity method and compared with the measured data of the ignition delay time. The established chemical reaction mechanism can be integrated with the fluid flow and heat transfer simulation in CFD software. Thus, the entire combustion process can be evaluated [21]. Additionally, to accelerate the numerical computation, an artificial neural network method could be induced [22].

Recently, Tay investigated the reaction mechanism of kerosene for a compression ignition engine [23–25]. A chemical reaction mechanism composed of 123 species and 586 elementary reactions was proposed in [23], which was used to simulate the combustion of the mixture of diesel and kerosene. The results from the shock tube tests validated the reliability of the mechanism and a high precision of the heat release rate was predicted. Subsequently, a reduced mechanism with 48 species and 152 reactions was developed in [25]. The experimental results of a constant volume bomb and an optical engine verified the accuracy of the mechanism. Later, Tay et al. [26] investigated the soot production based on the developed mechanism. Series experiments were conducted to validate the mechanisms. In [27], the combustion characteristics of the diesel-kerosene mixture were measured on a direct-injection diesel engine. In [28], the results of the heat release rate and the flame propagation were measured on a shock tube and an optical engine and compared with the simulated data.

Table 1 lists the initial conditions of some investigations about the ignition delay time of kerosene. The initial pressures were mostly concentrated in the medium- and low-pressure ranges, up to 25 bar. With regard to the SI engines, although the temperature range is roughly the same across the literature, the in-cylinder pressure at the top dead center will be more than 30 bar, and sometimes even reach 60 bar. Therefore, it is necessary to investigate the combustion characteristics of kerosene under such a high-pressure condition.

The initial pressure range studied in this paper is set to 15–35 bar, which is much higher compared with that of Table 1.

Table 1. Comparison of the ranges for the initial pressure and temperature of kerosene in the literature.

Temperature (K)	Pressure (Bar)	Reference
550–900	3	[29]
298	0.2–1	[30]
700–1200	20	[31]
673–973	1–25	[32]
1000–1700	1–3	[33]

Most of the developed chemical reaction mechanisms for kerosene were based on the working conditions of a gas turbine engine or a diesel engine. The premixed combustion process of the kerosene-air mixture inside an SI engine is quite different from these engines. Therefore, when kerosene is used as a substitute fuel for gasoline, it is useful to obtain the combustion characteristics of kerosene, such as the ignition delay time in the proper pressure range. This is critical for the suppression of the knocking phenomenon of SI engines fueled with kerosene. Therefore, the reaction mechanism of kerosene premixed combustion based on the working conditions of an SI engine needs to be explored. The rate-determined steps should be identified, and the effects of the working parameters need to be estimated. In this study, a chemical reaction mechanism is used to simulate the combustion characteristics of kerosene inside the SI engine and the ignition delay time is employed to evaluate the combustion performance. The influences of the initial temperature, pressure, and the equivalence ratio of the mixture are discussed. Then, a sensitivity analysis approach is used to analyze the reaction path and the rate-determined steps are obtained. The results are also compared with that of the gasoline fuel and the differences are discussed. The outcomes of this study provide a reference for the combustion performance improvement of an SI engine fueled with kerosene.

2. Methodology

Table 2 lists the main physicochemical properties of kerosene and gasoline. Significant differences exist between these two fuels, especially for the flash point, kinematic viscosity, and autoignition temperature. The low flash point of gasoline can also be seen, making it difficult in aviation applications that have a rigid requirement on security.

Table 2. Comparison of the properties of kerosene and gasoline.

Physicochemical Property	Kerosene	Gasoline
Fuel composition (C/H)	C7~C16	C5~C11
Density (kg/L)	0.80~0.84	0.70~0.75
Flash point (°C)	45~51	−45~−25
Theoretical air-fuel ratio	14.7	14.8
Kinematic viscosity (mm ² /s)	1.841	0.8
Boiling point (°C)	185	30~220
Spontaneous ignition point (°C)	380~425	510~530

An adiabatic constant-volume premixed combustion is assumed for the combustion of kerosene in the SI engine. Based on the zero-dimension reaction model in the chemkin software, the reduced chemical reaction mechanism of Tay [28] is employed. There are 48 species and 152 elementary reactions. The zero-dimensional homogeneous model in chemkin is adopted. It is assumed that the fuel and air are uniformly mixed in the combustion chamber. Thus, the combustion reactions are constant volume adiabatic reactions. The initial operation parameters, such as the temperature and pressure, are specified according to the practical measured data from an engine test [9]. Unlike gas turbines, SI engines

cover a wider pressure range. The pressure range was set to 15–35 bar. The corresponding temperature was set from 600 to 1000 K. There are several definitions for the ignition delay time during the autoignition process of kerosene. The first ignition delay time is defined as the time from the beginning of the reaction to the first peak of the pressure change rate. The second ignition delay time is the time from the first peak to the second peak of the pressure change rate. In this study, the overall ignition delay time is the sum of the first and second ones.

The ignition delay times of Jet-A and JP-8 were determined using the chemical reaction mechanism and compared with the results of the literature [34,35]. The kerosene-air mixture was stoichiometric, and the pressure was 20 bar. Figure 1 shows the results, in which the tendencies are similar and the negative temperature curve (NTC) is manifested obviously as the temperature increases. Although the deviations under the low temperature are slightly higher, the maximum error is less than 0.3 ms. Hence, the mechanism can be used for the following premixed combustion simulation. In this study, a numerical simulation method is used. The advantage is that a qualitative estimation of the ignition delay time can be obtained with a low cost. In addition, the detailed chemical reaction paths can be analyzed using sensitivity analysis to obtain the rate-determining reactions. However, this method needs to be combined together with the experimental study to give a more accurate estimation.

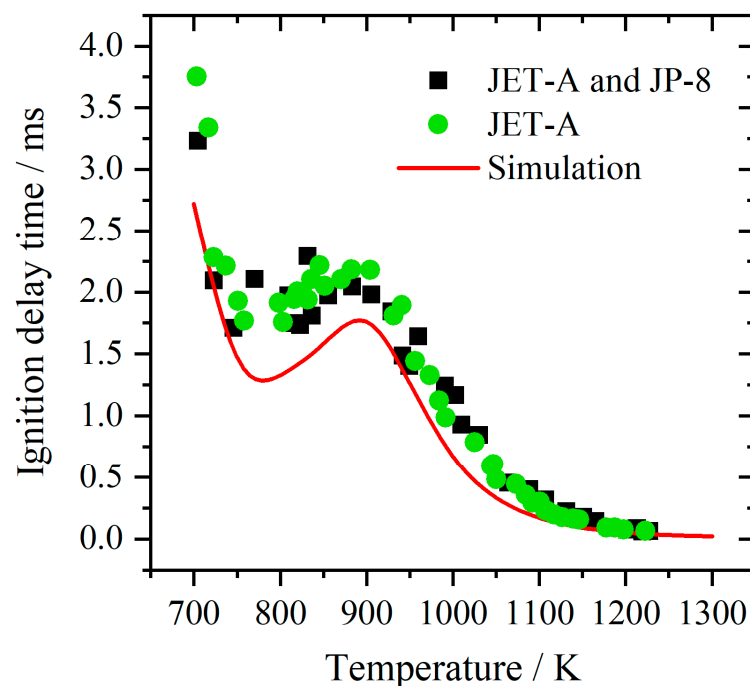


Figure 1. Validation of the chemical reaction mechanism of kerosene.

3. Results of Ignition Delay Time

3.1. Ignition Delay Time of Kerosene

The results of the first ignition delay time as a function of the temperature are shown in Figure 2a, with an initial pressure of 15–35 bar. As the temperature increases, the first ignition delay time decreases primarily. When the initial temperature is less than 800 K, the first ignition delay time decreases monotonously as the initial temperature rises. When the initial temperature is in the range of 800–900 K, the first ignition delay time shows an NTC phenomenon although the magnitude is not significant. The first ignition delay time decreases as the initial temperature rises in the range of 800–910 K, but the decreasing magnitude was reduced. When the initial temperature is greater than 900 K, the first ignition delay time reduces as the temperature increases. On the other hand, as the initial

pressure increases from 15 bar to 35 bar, the first ignition delay time drops monotonously. The reduction is more evident when the initial temperature is getting higher.

The overall ignition delay times of kerosene are compared in Figure 2b under different initial pressures. The overall ignition delay time first decreases and then increases as the initial temperature rises for a fixed initial pressure. When the initial temperature is less than 750 K, the overall ignition delay time drops as the temperature increases. When the temperature is greater than 750 K, an inverse tendency is displayed because it is in the NTC region. The temperature range of the NTC region is 750–920 K for kerosene. As the initial pressure increases, the overall ignition delay time also decreases slightly, and large variations occur in the high-temperature region.

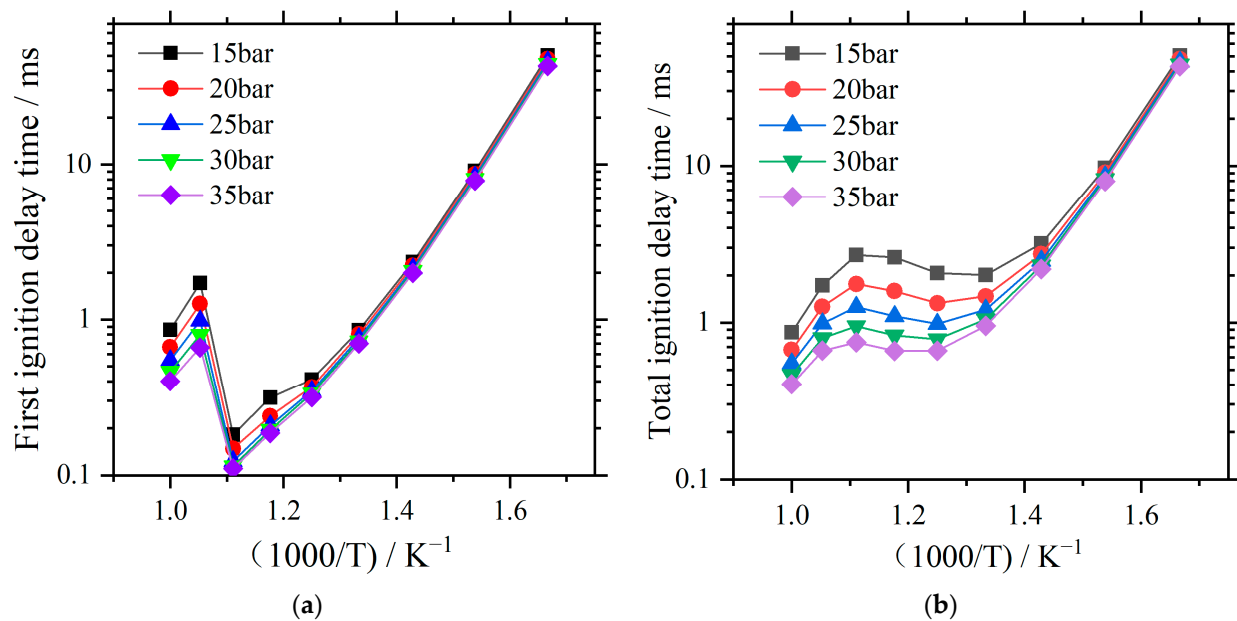


Figure 2. Results of the ignition delay time of kerosene under different pressures: (a) first ignition delay time; (b) overall ignition delay time.

3.2. Comparison with Gasoline

Gasoline is the conventional fuel of an SI engine. In this study, the combustion performance of gasoline is also determined and compared with the results of kerosene. The shell-D mechanism [31] was used. The ignition delay times for the gasoline-air premixed combustion were calculated under the same temperatures and pressures as kerosene. Figure 3 shows the simulation results and the comparison with the experimental data from [36]. The simulated ignition delay time has a high consistency with the experimental data and the NTC region can be observed. When the initial temperature is low, the deviation is relatively high. However, a small deviation is shown under the high-temperature region. The average deviation is about 0.16 ms. Therefore, this mechanism can be used for the following simulation of the gasoline-air premixed combustion.

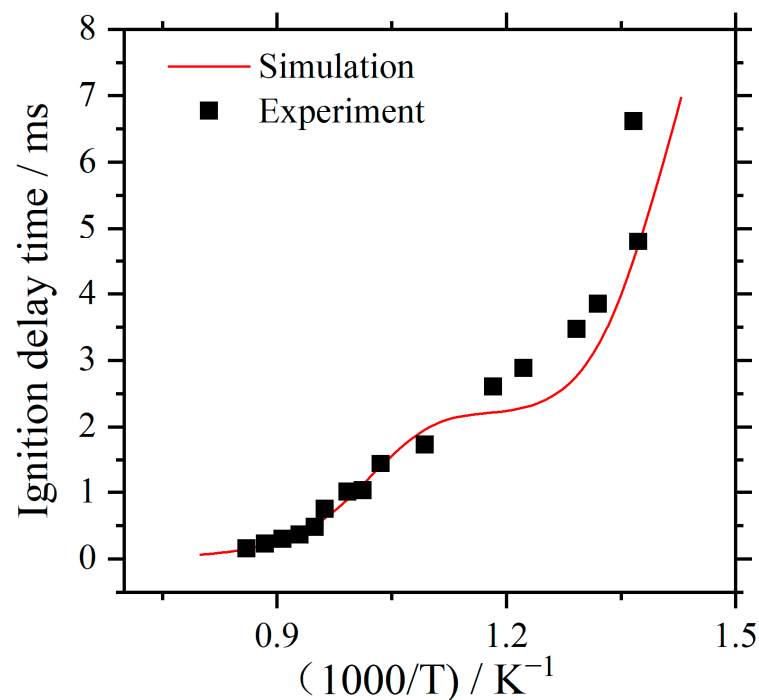


Figure 3. Validation of the chemical reaction mechanism of gasoline.

Figure 4 shows a comparison of the ignition delay time of kerosene with gasoline under the initial pressure of 15, 35, and 60 bar, respectively. When the initial pressure is low, the ignition delay time of kerosene is smaller than that of the gasoline under the same temperature. This deviation decreases as the temperature increases. When the initial temperature is greater than 1000 K, the ignition delay time of kerosene is almost the same with that of the gasoline. On the other hand, as the initial pressure increases, the discrepancy of the ignition delay time between these two fuels reduces. When the initial pressure is 60 bar, the ignition delay times are very close for the two fuels. A small ignition delay time may not be beneficial for the knock control. It is shown that the ignition delay time of kerosene can be increased under the high-pressure conditions. If the in-cylinder pressure could be controlled to avoid the region where the ignition delay time of kerosene is too small, the severe knock of kerosene premixed combustion might be alleviated.

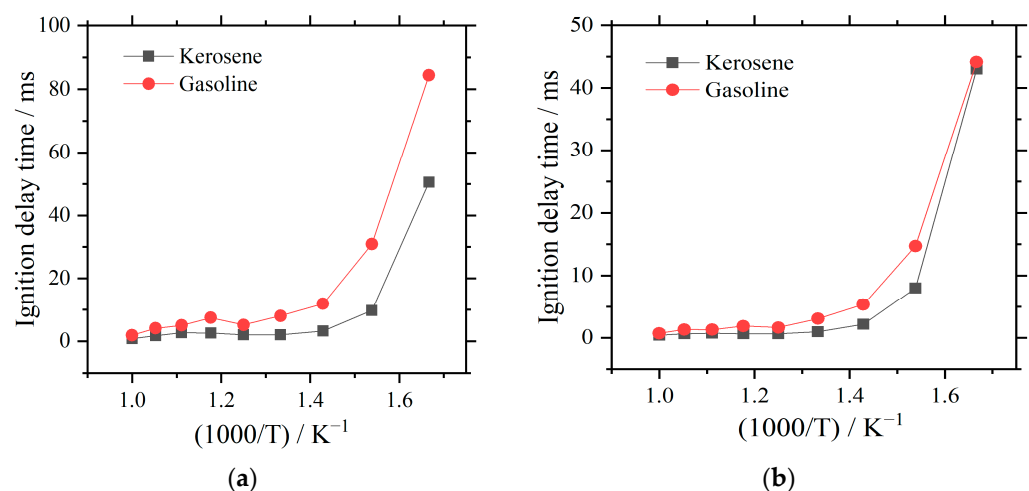


Figure 4. Cont.

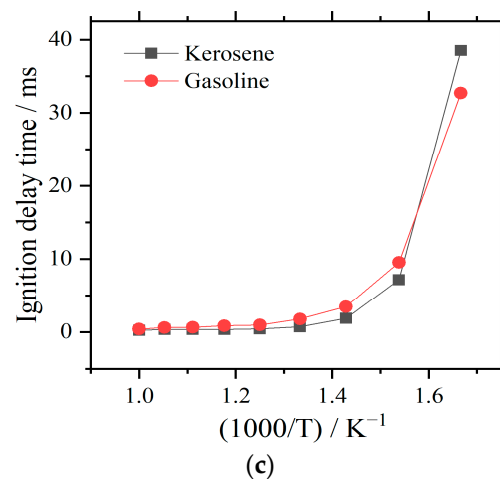


Figure 4. Comparison of the ignition delay time between kerosene and gasoline: (a) initial pressure of 15 bar; (b) initial pressure of 35 bar; (c) initial pressure of 60 bar.

4. Chemical Reaction Path Analysis

4.1. Effect of Equivalence Ratio

The most important reactions could be found based on the sensitivity analysis method. The time-dependent chemical kinetics behavior of the homogeneous kerosene-air mixture was simulated first. Then, the first-order sensitivity coefficients were determined with respect to the rate parameters of the elementary reactions. In such a way, how important certain reaction pathways are can be obtained. Figure 5 shows the results when the initial pressure is 20 bar and the initial temperature is 800 K. The equivalence ratios are set to 0.8, 1, and 1.2. In this figure, the sensitivity coefficients were normalized. A positive sensitivity coefficient means a longer ignition delay time and the autoignition of kerosene is suppressed and vice versa. Table 3 lists the corresponding detailed elementary reactions. In Table 3, the reactions R9, R91, and R121 have an evident suppression effect on the chemical kinetics. It can be seen that the most important reactions that suppress the autoignition are the pyrolysis of kerosene and oxidation. The relatively stable species CH_2O and HO_2 are generated via these reactions and the overall reaction rate slows down. On the other hand, the elementary reactions that accelerate the autoignition are the generation of OH and other active species. For the kerosene premixed combustion, reactions R7, R5, and R9 are the most important rate-determining reactions. As the equivalence ratio decreases, the sensitivity coefficient of each reaction increases slightly. However, the orders of these elementary reactions are the same.

Table 3. Lists of the important reactions of kerosene.

Reaction Number	Reaction Equation
Rxn#7	$\text{OOKERO}\#\text{OOH} = \text{KERO}\#\text{KET} + \text{OH}$
Rxn#5	$\text{KERO}\text{-OO} = \text{KERO}\#\text{OOH}$
Rxn#6	$\text{KERO}\#\text{OOH} + \text{O}_2 = \text{OOKERO}\#\text{OOH}$
Rxn#4	$\text{KERO}\text{-} + \text{O}_2 = \text{KERO}\text{-OO}$
Rxn#2	$\text{KERO} + \text{OH} = \text{KERO}\text{-} + \text{H}_2\text{O}$
Rxn#98	$\text{CH}_3 + \text{HO}_2 = \text{CH}_3\text{O} + \text{OH}$
Rxn#117	$\text{CH}_3\text{O} + \text{M} = \text{CH}_2\text{O} + \text{H} + \text{M}$
Rxn#72	$\text{H}_2\text{O}_2 + \text{OH} = \text{HO}_2 + \text{H}_2\text{O}$
Rxn#64	$\text{HO}_2 + \text{OH} = \text{H}_2\text{O} + \text{O}_2$
Rxn#103	$\text{CH}_3 + \text{HO}_2 = \text{CH}_4 + \text{O}_2$
Rxn#121	$\text{CH}_3\text{O} + \text{O}_2 = \text{CH}_2\text{O} + \text{HO}_2$
Rxn#91	$\text{CH}_2\text{O} + \text{OH} = \text{HCO} + \text{H}_2\text{O}$
Rxn#9	$\text{KERO}\text{-} + \text{O}_2 = \text{KERO}\# + \text{HO}_2$

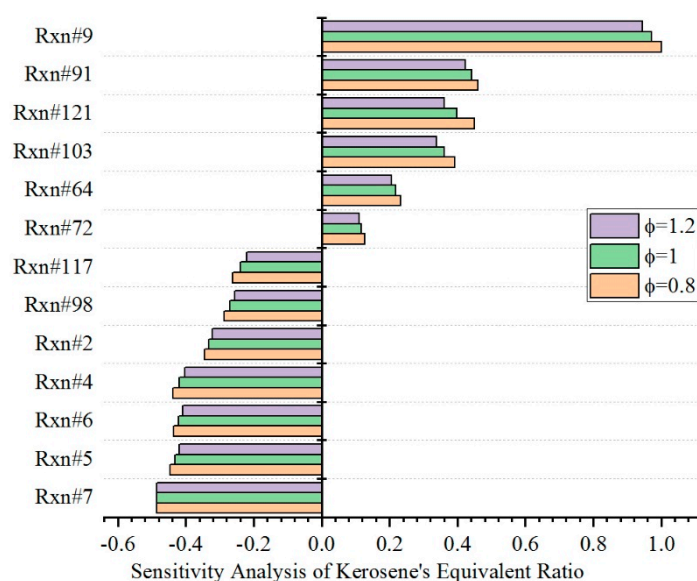


Figure 5. Sensitivity analysis of kerosene under different equivalence ratios.

The main reaction paths of kerosene are depicted in Figure 6, with an initial pressure of 20 bar and an initial temperature of 800 K. The equivalence ratios of 0.8, 1, and 1.2 are represented by the black, red, and blue colors, respectively. The reaction paths for the different equivalence ratios are consistent. Only the proportions of the branched chain reactions and the amounts of reactants and products are changed. The kerosene molecule mainly reacts with the radicals OH and H. The groups C_3H_6 and C_2H_5 are produced via two steps of thermal cracking. Afterwards, the species CH_2O and H_2O are generated after the elementary oxidation reactions. Meanwhile, the intermediate species C_2H_4 and C_2H_3 can also react with radicals such as OH, and CH_2O is produced. Finally, CH_2O will react with OH further and CO_2 and H_2O are obtained.

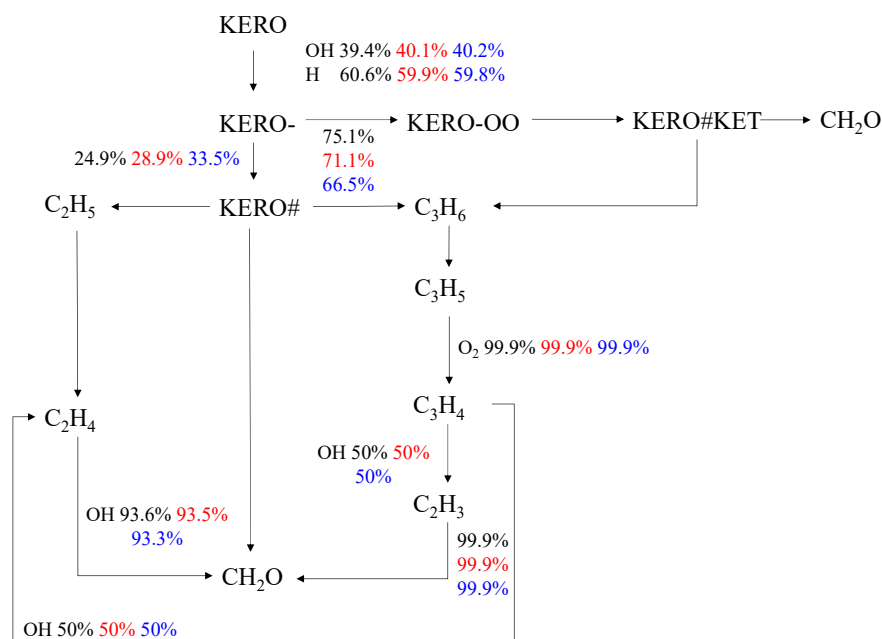


Figure 6. Effects of equivalence ratio on the chemical reaction path of kerosene (T = 800 K; P = 20 bar; black: $\Phi = 0.8$; red: $\Phi = 1$; blue: $\Phi = 1.2$).

The homogeneous premixed combustion of gasoline is compared with the kerosene under the same operation conditions. Table 4 lists the 10 main important reactions of gasoline based on the sensitivity analysis. Figure 7 shows the detailed results of the sensitivity analysis. The initial pressure is 20 bar and the initial temperature is 800 K. The sensitivity coefficients of the reactions vary slightly under different equivalence ratios and no regular pattern appears. The reactions R9, R2, R6, and R16 are the main reactions accelerating the combustion process while the reactions R4 and R28 are the most important reactions that suppress the ignition process. Reaction R4 can be seen as the rate-determining step.

Table 4. Lists of the important reactions of gasoline.

Reaction Number	Reaction Equation
Rxn#2	$\text{SDC}_8\text{H}_{14} + \text{H} = \text{H}_2 + \text{SDC}_8\text{H}_{13}$
Rxn#4	$\text{SDC}_8\text{H}_{14} + \text{OH} = \text{H}_2\text{O} + \text{SDC}_8\text{H}_{13}$
Rxn#6	$\text{SDC}_8\text{H}_{14} + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{SDC}_8\text{H}_{13}$
Rxn#8	$\text{SDC}_8\text{H}_{12} = 0.1333333\text{C}_2\text{H}_4 + 0.1466667\text{C}_3\text{H}_6 + 0.0733333\text{iC}_4\text{H}_8 + 0.5\text{C}_6\text{H}_6 + 0.5\text{C}_6\text{H}_5\text{CH}_3 + 1.5\text{H} + 0.5\text{CH}_3$
Rxn#9	$\text{SDC}_8\text{H}_{13} + \text{O}_2 = \text{SDC}_8\text{H}_{13}\text{O}_2$
Rxn#16	$\text{SDC}_8\text{H}_{12}\text{O}_3 = \text{CH}_2\text{O} + \text{OH} + \text{CO} + 0.0111111\text{C}_2\text{H}_4 + 0.0122222\text{C}_3\text{H}_6 + 0.0061111\text{iC}_4\text{H}_8 + 0.4166667\text{C}_6\text{H}_6 + 0.4166667\text{C}_6\text{H}_5\text{CH}_3 + 1.5\text{H} + 0.5\text{CH}_3$
Rxn#28	$\text{H} + \text{O}_2(+\text{M}) = \text{HO}_2(+\text{M})$
Rxn#30	$\text{OH} + \text{OH}(+\text{M}) = \text{H}_2\text{O}_2(+\text{M})$
Rxn#83	$\text{CH}_2\text{O} + \text{OH} = \text{HCO} + \text{H}_2\text{O}$
Rxn#93	$\text{CH}_3 + \text{HO}_2 = \text{CH}_3\text{O} + \text{OH}$

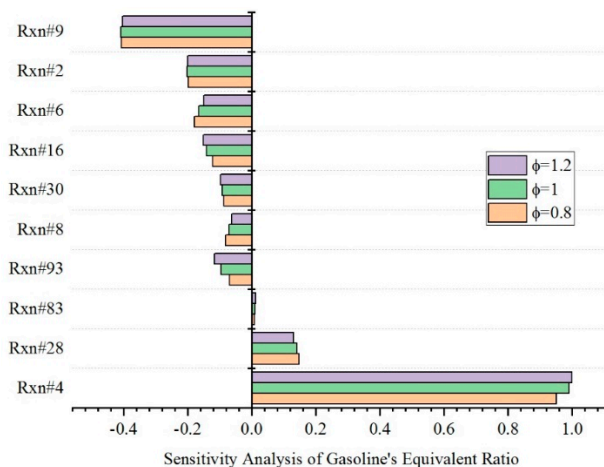


Figure 7. Sensitivity analysis of gasoline under different equivalence ratios.

Figure 8 shows the main reaction paths of gasoline at an initial pressure of 20 bar and an initial temperature of 800 K. The reaction chains of gasoline are apparently less than that of kerosene. The main reactions are the oxygen addition reactions and the cracking of the carbon chains. The equivalence ratio will influence the proportions of the thermal cracking reactions. As the equivalence ratio increases from 0.8 to 1.2, these proportions are increased gradually. More groups of C_3H_6 and C_2H_4 are generated. As a result, the decomposition rate of C_8H_{13} is almost doubled.

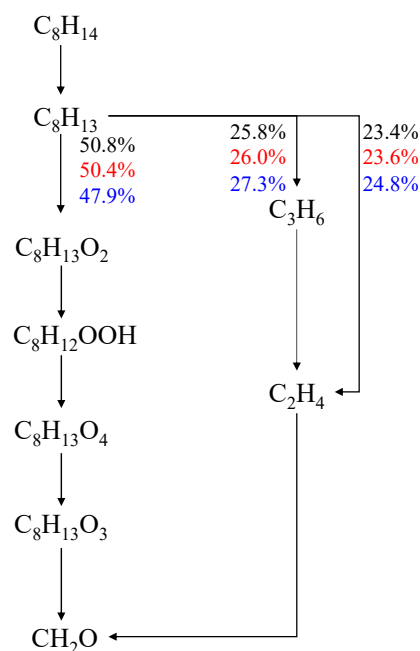


Figure 8. Effects of equivalence ratio on the chemical reaction path of gasoline. ($T = 800$ K; $P = 20$ bar; black: $\Phi = 0.8$; red: $\Phi = 1$; blue: $\Phi = 1.2$).

4.2. Effects of Initial Pressure

The initial pressure of the homogeneous kerosene-air mixture has a great effect on the ignition delay time as the above Section 3 describes. Herein, the effects of the initial pressure on the chemical reaction paths are analyzed further and the rate-determined reactions are estimated. Figure 9 shows the results of the sensitivity analysis for kerosene under different initial pressures. As the pressure increases, the sensitivity coefficients of the reactions decline. An increment in the initial pressure is helpful for the acceleration of the chemical reaction rates. Therefore, the sensitivity coefficients decrease. The main reactions that will shorten the ignition delay time are R7, R5, R6, and R4. The reactions R9, R91, R121, and R103 will extend the ignition delay time and is useful for the suppression of knock phenomenon of kerosene.

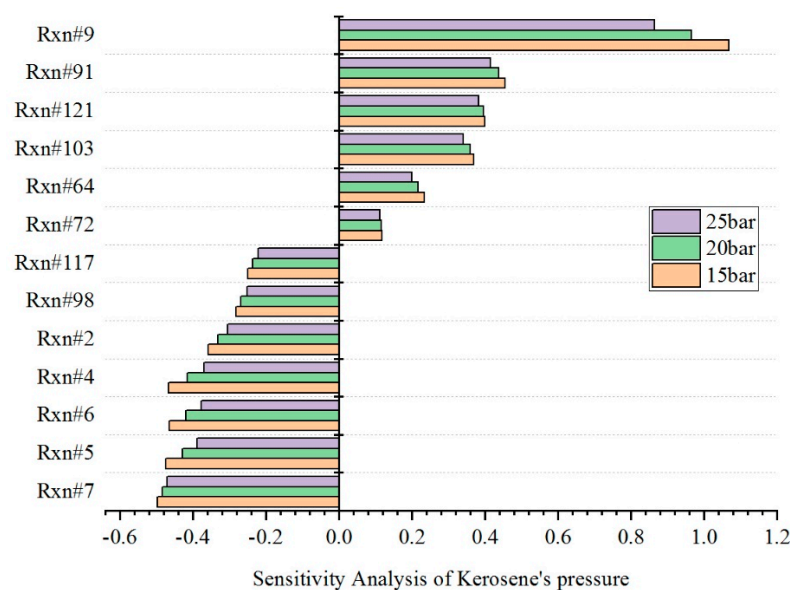


Figure 9. Sensitivity analysis of kerosene under different initial pressures.

The effects of the initial pressure on the chemical reaction paths of kerosene are displayed in Figure 10. The corresponding temperature is set at 800 K and the stoichiometric mixture is used. As the initial pressure increases, the main reaction paths changes. The proportion of the reaction between the KERO group and OH rises. Accordingly, the oxygen addition reaction on the KERO group also increases and the amount of KERO-OO enlarges. The results indicate that the initial pressure has a great effect on the first several steps of the kerosene decomposition.

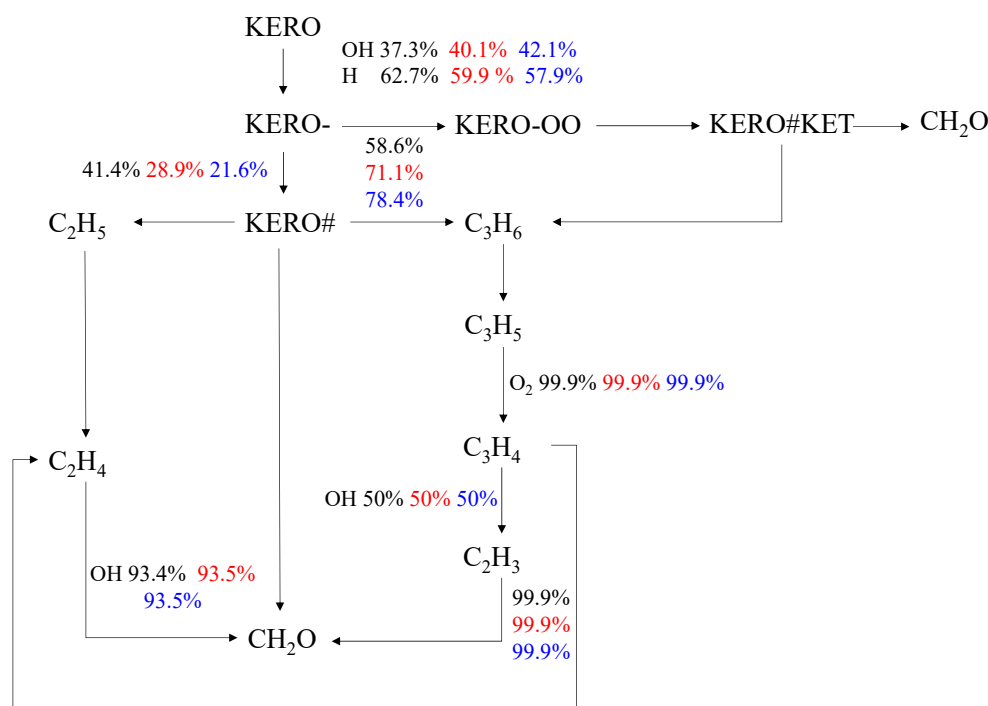


Figure 10. Effects of initial pressure on the chemical reaction path of kerosene ($T = 800$ K; $\Phi = 1$; black: $P = 15$ bar; red: $P = 20$ bar; blue: $P = 25$ bar).

As a comparison, the effect of the initial pressure on the gasoline premixed combustion is shown in Figures 11 and 12. First, the results of the sensitivity analysis are displayed in Figure 11. Similar with the case of kerosene, the overall chemical reaction rates increase and the sensitivity coefficients decline as the initial pressure rises. Therefore, the difference in the ignition delay time between kerosene and gasoline is alleviated. The reactions R8 and R83 are the two main reactions that will extend the ignition delay time while the reactions R9, R6, R4, and R2 will lead to a small ignition delay time.

The main chemical reaction paths are depicted for gasoline under different initial pressures. As the initial pressure increases from 15 bar to 25 bar, the chemical reaction rate ascends and the decomposition rate of C_8H_{13} is increased three times. The oxygen addition reaction of C_8H_{13} enlarges while the proportions of the decomposition reactions of C_3H_6 and C_2H_4 decrease.

The kerosene fuel is a complicated mixture of many components. A surrogate fuel with similar physical and chemical properties is often used to represent kerosene in many investigations [17,37,38]. Recently, Wu et al. [39] developed a surrogate with 7 species that is composed of aromatics, 2-ring cycloalkanes, 1-ring cycloalkanes, iso-alkanes, and n-alkanes, exhibiting a good match on the physical-chemical properties and ignition characteristics. Won et al. [40] tried a quantitative structure-property relation approach to design a surrogate with a similar combustion property. However, the kerosene fuel is represented by $C_{10}H_{22}$ in this study and the chemical reaction mechanism developed by Tay et al. was employed. This mechanism was validated under the working conditions of a diesel engine and shows

a high fidelity in the pressure range of this study. The investigation on the effects of the components of the surrogate for kerosene is beyond the scope of this study.

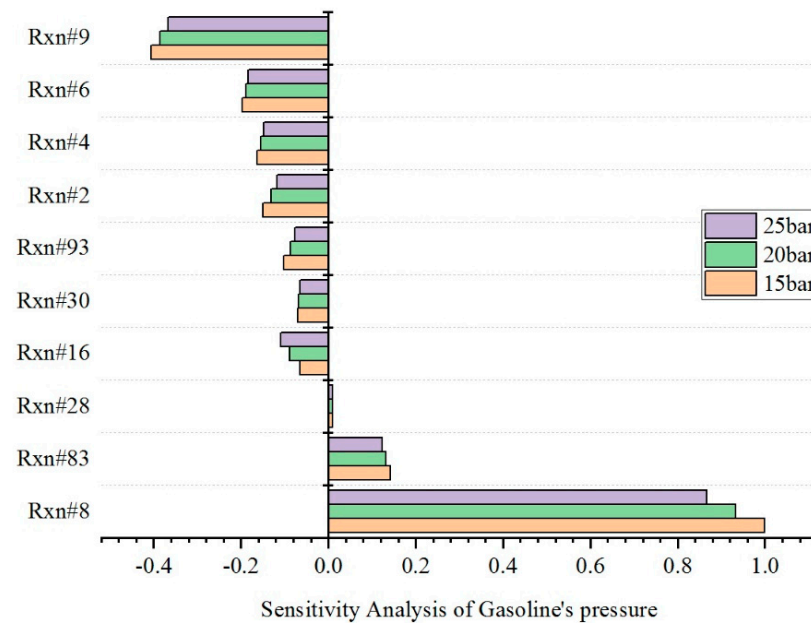


Figure 11. Sensitivity analysis of gasoline under different initial pressures.

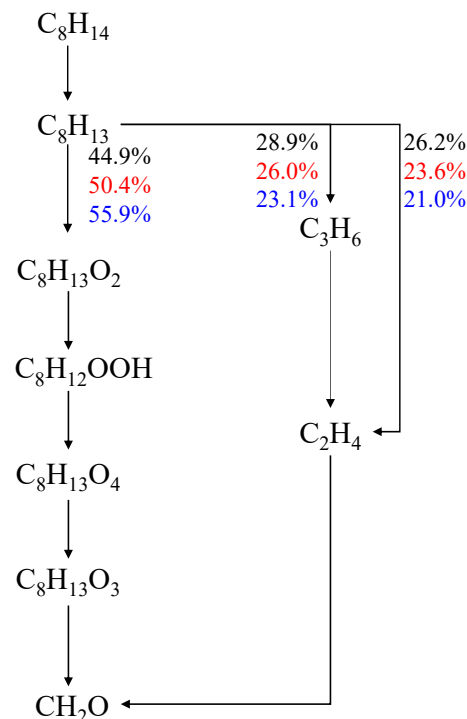


Figure 12. Effects of initial pressure on the chemical reaction path of gasoline ($T = 800$ K; $\Phi = 1$; black: $P = 15$ bar; red: $P = 20$ bar; blue: $P = 25$ bar).

5. Conclusions

In this study, the chemical reaction mechanism of a homogeneous kerosene-air mixture was investigated for an SI engine application. The detailed reaction mechanism was setup and the effects of the initial temperature and pressure were analyzed. The most important reactions were determined based on a sensitivity analysis. Additionally, the results from

kerosene were compared with those of gasoline and the differences were analyzed under the same conditions.

The initial pressure has a great effect on the ignition delay time of kerosene. When the initial pressure is less than 35 bar, an obvious NTC region occurs in the temperature range of 750–920 K. Under the initial condition of 1000 K and 35 bar, the total ignition delay time of kerosene is 0.401 ms for the stoichiometric mixture. As the initial pressure increases, the chemical reaction rates increase and the ignition delay time declines. The discrepancy in the ignition delay time between kerosene and gasoline also decreases. The results of the sensitivity analysis indicate that the sensitivity coefficients basically reduce as the initial pressure increases. The equivalence ratio and the initial pressure will influence the proportions of the main branched chain reactions while the main reaction paths are almost consistent. With regard to the ignition delay time of kerosene, the most important reactions that will shorten the ignition delay time are R7, R5, R6, and R4. The main reactions that will increase the ignition delay time are R9, R91, R121, and R103. To suppress the severe knock of the kerosene in an SI engine, methods need to be explored that could reduce the effects of the reactions R7, R5, R6, and R4 or strengthen the reactions R9, R91, R121, and R103.

SI engines fueled with kerosene have good application prospects in the fields of small UAVs, high-altitude UAVs, and small ships. However, the knock issue must be solved at first. Therefore, further studies are required in the future. The abovementioned key reactions need to be tested to reduce the knocking phenomenon. Meanwhile, with regard to the numerical simulation, a constant volume adiabatic reaction was employed in this study. For SI engines, the combustion process can be considered as a constant volume combustion basically due to the rapid propagation of the flame front. To achieve a more accurate estimation of the ignition delay time, the engine module in chemkin can be used to simulate the conditions approximating the practical operating conditions of an engine. Alternatively, the detailed mechanism can be integrated with 3D simulations as well. In such a way, the real combustion process can be estimated more accurately, and a better understanding of the combustion mechanism can be achieved.

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