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Study on Ignition Delay and Reaction Mechanism of RP-3/Air Combustion Adding $C_6F_{12}O$

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ABSTRACT: RP-3 jet fuel is the main fuel for aircraft in China, and it is also a source of fire. $C_6F_{12}O$ (Novec 1230) has an outstanding fire extinguishing performance and minimal environmental impacts. In this study, the application of $C_6F_{12}O$ in the inhibition of RP-3 jet fuel fire was considered, and the ignition delay time (IDT) of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$ was measured using a shock tube. In addition, the results showed that the IDT of $C_6F_{12}O$ was 500−900 μs and less sensitive to temperature compared with those of common fuels in the range of 1150−1958 K, and the influence of $C_6F_{12}O$ on the IDT of RP-3 jet fuel was influenced by many factors including temperature, the concentration of $C_6F_{12}O$, and the stoichiometric ratio of RP-3 jet fuel. According to the experimental results, the mechanism of $C_6F_{12}O$ was verified and modified, and then integrated with the mechanisms of RP-3 jet fuel; the integrated mechanism can well predict the IDT of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$. This work provides a good basis for the chemical kinetics analysis of the inhibition of RP-3 jet fuel combustion by $C_6F_{12}O$.
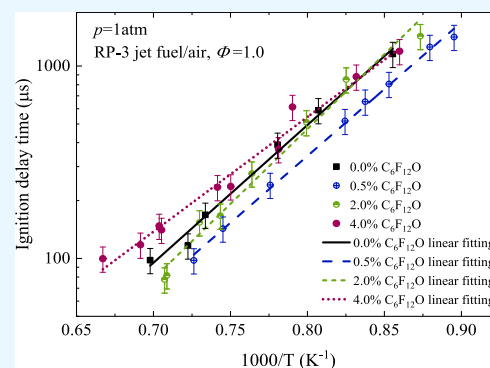
1. INTRODUCTION

Due to its characteristics of high ignition point and high combustion calorific value, RP-3 jet fuel is the main fuel used by civil and military aircraft in China. But at the same time, RP-3 jet fuel is also a major source of danger in fuel leakage fire accidents,[1] resulting in fire and explosion. When aircraft carrying RP-3 jet fuel or the terminals storing RP-3 jet fuel suffer from environmental disasters or wartime attacks, it is easy to catch fire and lead to disastrous consequences, and cause heavy loss of personnel and property. Therefore, it is particularly important to carry out scientific and reasonable research on the combustion inhibition of RP-3 jet fuel and explore the inhibition mechanism of new clean and efficient extinguishants on the combustion of RP-3 jet fuel.

Until now, there have been many achievements in the research of RP-3 jet fuel combustion. IDT measurements have been carried out under different equivalence ratios and pressure conditions.[2−4] In addition, many kinds of proportions of RP-3 jet fuel surrogates ranging from single component to multiple components have been proposed, and the corresponding detailed chemical-kinetic mechanisms have been established.[2,5−10] These studies greatly promoted the development RP-3 jet fuel in combustion control including the promotion in engine and inhibition in fire.

Halon was previously commonly used as an extinguishant for civil and military aircraft but is now being phased out due to environmental concerns. Although many studies have been devoted to finding alternatives to halon over the past 30 years, a perfect solution has not been found that meets all the requirements.[11] $C_6F_{12}O$ (Novec 1230) is expected to be a long-term alternative to halon as a fluorinated extinguishant due to its outstanding fire extinguishment performance[12,13] and minimal environmental impacts.[14]

Several theoretical and experimental studies have been performed on $C_6F_{12}O$.[15] Linteris et al.[16] developed the kinetic mechanism to describe the behavior of $C_6F_{12}O$ in hydrocarbon flames, which has been widely used in its chemical kinetic analysis. The prediction accuracy of the $C_6F_{12}O$ mechanism on laminar flame velocity is verified in several pieces of literature.[17−21] Xing et al.[22] performed a series of reactive force field molecular dynamics (ReaxFF MD) simulations to investigate $C_6F_{12}O$ pyrolysis and calculated its pre-exponential factor and apparent activation energy. The thermodynamic and transport properties of $C_6F_{12}O$ in the range of 300−30,000 K were calculated based on local thermodynamic equilibrium conditions by Li et al.[23] The detailed chemical mechanism and kinetics of $C_6F_{12}O$ reacting with the H radical have been explored by Zhong et al.,[24] providing a detailed theoretical information for uncovering the mechanism of the H radical reacting with other halogen substituted hydrocarbons. Pan's experiment showed that $C_6F_{12}O$ can effectively suppress the ethanol−gasoline vapor explosion (E10).[25] Pagliaro and
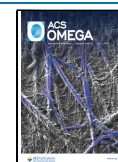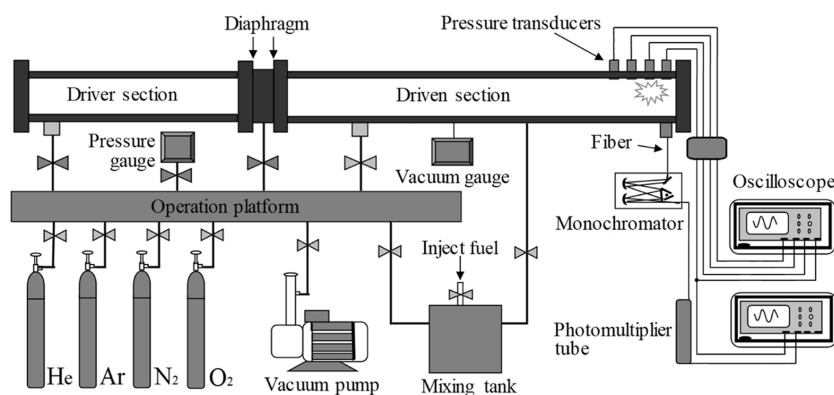
Figure 1. Schematic diagram of the shock tube experimental system.

Linteris studied the effect of the interaction between $C_6F_{12}O$ and the diffusion flame structure of a cup burner on flame extinguishing by numerical simulation and experimental methods.[18] In addition, the inhibition effect between HFC-227ea and $C_6F_{12}O$ on thermal runaway propagation was compared in confined space through experiments, and the results showed that $C_6F_{12}O$ can exert a better cooling effect.[23] However, the experiment of Pagliaro et al.[27] showed that a low concentration of $C_6F_{12}O$ added to lean ($\Phi = 0.6$) methane/air flames can increase the explosion pressure and enhance the reactivity. To thoroughly understand this unexpected behavior, Ren et al.[28] calculated the chemical and physical effects caused by $C_6F_{12}O$. The results show that under thin CH_4/air conditions, $C_6F_{12}O$ helps to increase the equivalence ratio, thereby increasing the flame speed chemically but physically cooling the mixture, and when the actual equivalent ratio of the $C_6F_{12}O/CH_4$/air mixture is greater than 1.20, $C_6F_{12}O$ produces an overly rich fuel mixture, which chemically reduces the flame rate. Additionally, the fire extinguishing device[29] and fire extinguishing integrated system[30] of $C_6F_{12}O$ were developed, and the application of $C_6F_{12}O$ in suppressing the thermal runaway propagation of lithium-ion batteries[26,31−35] has been studied a lot in recent years.

In general, the current research on $C_6F_{12}O$ has been involved in many aspects, and its enhanced combustion in some cases has caused concern. However, the flammability properties of $C_6F_{12}O$ itself[28] and its pyrolysis products[22] still lack in-depth research, with no experimental studies been carried out on its ignition characteristics and its impact on the ignition characteristics of fuel. Also, the prediction ability of the $C_6F_{12}O$ mechanism on ignition characteristics lacks validation and improvement. Considering the application of $C_6F_{12}O$ in the inhibition of RP-3 jet fuel fire, the ignition delay time (IDT) of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$ was measured in this study using a shock tube. According to the experimental results, the mechanism of $C_6F_{12}O$ was verified and modified and then integrated with the mechanisms of RP-3 jet fuel the integrated mechanism can well predict the IDT of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$.

2. FUNDAMENTALS OF THE METHOD

2.1. Experimental Methods. All IDT experiments were carried out in a shock tube as shown in Figure 1. The stainless-steel shock tube comprised a 2 m diver section, a 0.1 m double-diaphragm, and a 5 m driven section with an inner diameter of 10 cm. In the double-diaphragm bursting mechanism, different thicknesses of polycarbonate diaphragms were used to reach

various pressures of reflected shock waves. The details of the shock tube device have been introduced elsewhere.[2,36]

The mixtures of RP-3 jet fuel/air adding $C_6F_{12}O$ (99.96% purity) were prepared in advance in a 40 L heated stainless-steel tank according to Dalton's law of partial pressure. In this study, air refers to synthetic air with 21% O_2 (99.999% purity) and 79% N_2 (99.999% purity). The initial pressures of gas phase fuel and oxygen were measured by a capacitance manometer. The prepared mixture was required to stand for at least 2 h to ensure sufficient mixing before the first ignition experiment. The detailed compositions of experimental mixtures are summarized in Table 1. The concentration of

Table 1. Detailed Compositions of the Experimental Mixtures

mixture	Φ_{RP-3}	$C_{C_6F_{12}O}$ (%)	RP-3 %	$C_6F_{12}O$ %	N_2 %	O_2 %
1	0.5	0.0	0.5	0	59.70143	15.87
2	0.5	0.5	0.5	0.379756	59.70143	15.87
3	0.5	4.0	0.5	3.14881	59.70143	15.87
4	1.0	0.0	1	0	59.70143	15.87
5	1.0	0.5	1	0.379756	59.70143	15.87
6	1.0	2.0	1	1.54772	59.70143	15.87
7	1.0	4.0	1	3.14881	59.70143	15.87
8	2.0	0.0	2	0	59.70143	15.87
9	2.0	0.5	2	0.379756	59.70143	15.87
10	2.0	4.0	2	3.14881	59.70143	15.87
11	0	2.0	0	1.542274	59.70143	15.87

extinguishant C is the percentage of gaseous volume in air, $C = V_{extinguishant}/(V_{extinguishant} + V_{air}) \times 100\%$. To ensure the fuel in the gas phase, the gas tank was heated and kept at 373 K. The shock tube was kept at room temperature as the partial pressure of RP-3 jet fuel and $C_6F_{12}O$ in the shock tube was much lower than their respective saturated vapor pressures.

Four fast-response piezoelectric pressure transducers (PCB 113B) spaced at approximately 20 cm intervals over the last 1 m of the shock tube were used to obtain three shock wave velocities. The shock velocity at the end wall was derived from the linear extrapolation of these three velocities. The one-dimensional normal shock model of CHEMKIN-Pro 17.0 software[37] was applied to calculate the temperature and pressure behind the reflected shock waves. In addition, a quartz optical fiber was installed on the same section as the last pressure transducer to detect the light emitted during ignition. The signal from the fiber was introduced to a grating monochromator coupled with a photomultiplier tube to detect

the CH* emission signals at 431 nm. Two digital phosphor oscilloscopes were used to record the pressure and emission signals.

The IDT of RP-3 jet fuel, τ_{RP-3}, was defined as the time interval between the pressure jump caused by the reflected shock wave and the rise of CH* emission, as shown in Figure 2. The IDTs of $C_6F_{12}O$ in the air at atmospheric pressure were
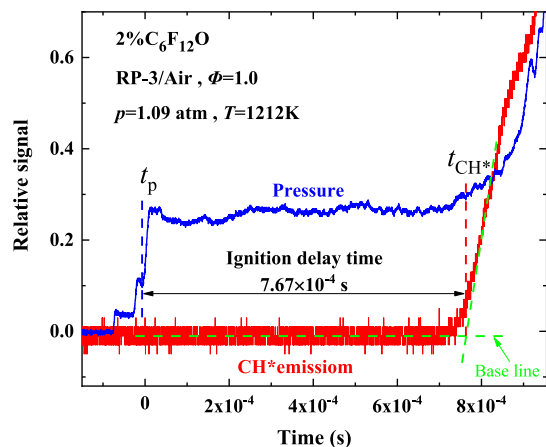

Figure 2. Definition of the IDT of RP-3 jet fuel.

measured. Since the H element is not involved in the whole reaction, it is impossible to judge the ignition time based on the optical signal of OH* or CH*. In addition, it is found through experiments that the total optical signal has a long slow strengthening stage under most working conditions, and the ignition delay measured by the total optical signal under several working conditions is negative, which is totally contrary to the fact. Therefore, it is difficult to measure the ignition time of $C_6F_{12}O$ by a light signal. However, there were obvious signals of a sharp rise of pressure in the experiments, and the experimental results show a certain rule. Based on the above phenomenon, the moment when the pressure starts to rise sharply was chosen as the ignition moment of $C_6F_{12}O$, and its IDT of $C_6F_{12}O$, $\tau_{C_6F_{12}O}$ was defined as shown in Figure 3. To test the IDT uncertainty of this shock tube system, RP-3 jet fuel ignition has been determined previously more than 10 times at a high temperature where the IDT is about 1 ms, and the uncertainty of IDT is within 15%. The IDTs reported in this study are available in the Supporting Information.
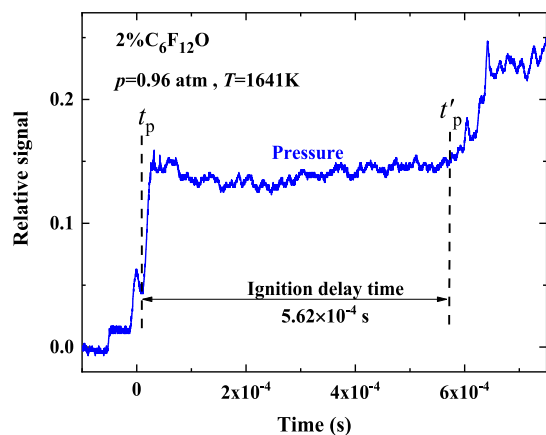

Figure 3. Definition of the IDT of $C_6F_{12}O$.

2.2. Mechanism Construction. To develop the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$, the detailed mechanism of RP-3 developed in our previous work[7] was adopted. That mechanism can predict the IDT of RP-3 jet fuel satisfactorily. To reduce the computation, the mechanism of RP-3 was reduced to 549 species and 3675 reactions. Then, the reaction mechanism of $C_6F_{12}O$, which was developed by Linteris et al.,[16] was added into the RP-3 skeletal mechanism. While integrating the two mechanisms, the reduplicative reactions were eliminated, and it was found that these reactions belong to the C_0-C_4 core mechanism. In the combustion mechanism of RP-3 jet fuel, the core mechanism has been optimized recently and verified more widely than that in the reaction mechanism of $C_6F_{12}O$. Therefore, the thermodynamic parameters and chemical reaction rate coefficients were selected according to the priority of RP-3 jet fuel over $C_6F_{12}O$.

All the simulations in this paper were performed in the perfectly closed homogeneous batch reactor model in the CHEMKIN-Pro 17.0 software.[37] In this study, a typical pressure gradient with the linear relation of $(dP/dt)(1/P) = 2\%$ ms^{-1} was used in ignition simulations. In the mechanism reduction, the IDT of RP-3 jet fuel/air at a stoichiometric ratio adding 2.0 and 4.0% $C_6F_{12}O$ under the pressure of 1 atm and the corresponding concentrations of CF_2, CF_3, and C_3F_7 were chosen as the targets. The absolute error tolerance of IDT was set as 1.0×10^{-6}, the absolute error tolerance of concentration of the three species was set as 1.0×10^{-7}, and the relative error tolerance was set as 20%. After the reductions of DRGEP → DRG → DRGPFA → DRGEP + sensitivity → DRG + sensitivity → DRGPFA + sensitivity → DRGEP + optimization → DRG + optimization → DRGPFA + optimization → FSSA in turn, the reduced combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ was obtained containing 109 species and 517 reactions.

3. RESULTS AND DISCUSSION

3.1. Experimental Results. The ignition delay time under stoichiometric ratios at atmospheric pressure measured in this
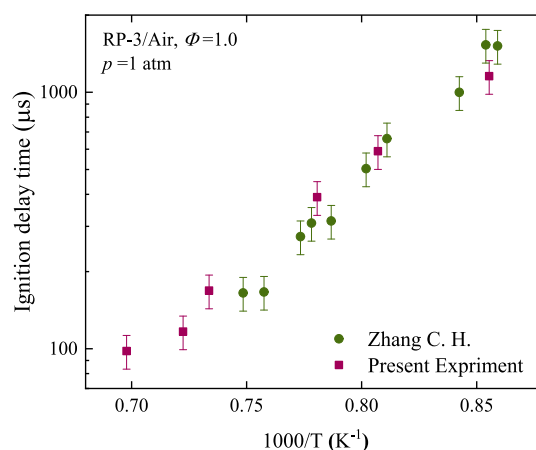

Figure 4. Contrast between the present and previous experimental data under the same conditions.

paper is shown in Figure 4. Compared with the data obtained by Zhang Changhua in 2015 using the same experimental system and the same definition of ignition delay time, it can be seen that the two are close in value size, but have a difference
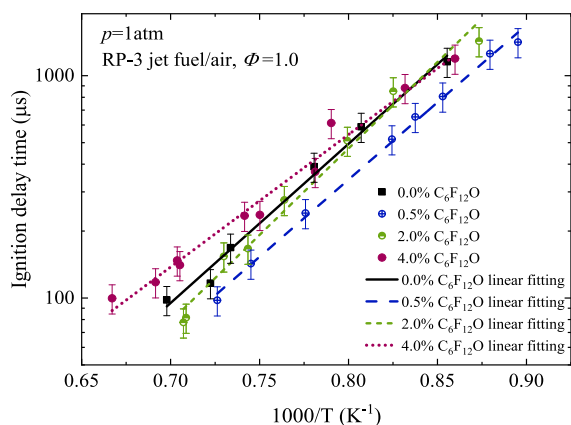
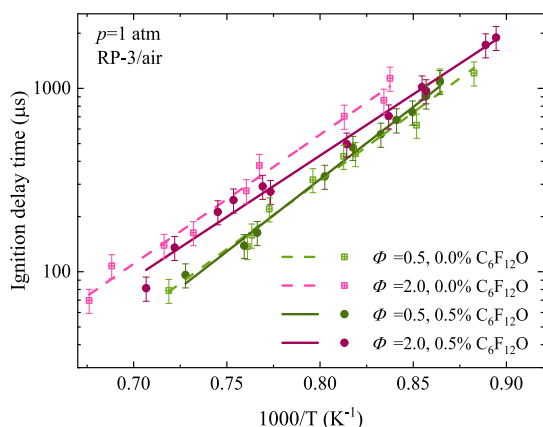**Figure 5.** IDTs of RP-3 jet fuel at different $C_6F_{12}O$ concentrations.

Figure 8. The IDTs of $C_6F_{12}O$, 92# gasoline, and RP-3 jet fuel.

Figure 6. IDT of RP-3 jet fuel adding 0.5% $C_6F_{12}O$.

Figure 9. Contrast between $C_6F_{12}O$ IDTs calculated by the original mechanism, present mechanism, and experimental data.

Table 2. Modification Details of the $C_6F_{12}O$ Mechanism

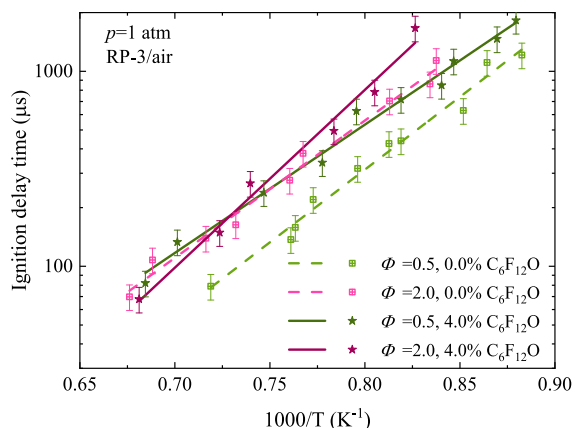| no	reactions $[k = AT^n \exp(-E/RT)]$	original A	optimized A
1	$CO + F + M = CF/O + M$	3.09×10^{19}	1.24×10^{20}
2	$CF_3 + O = CF_2:O + F$	1.54×10^{13}	3.85×10^{12}
3	$CF_4 + M = CF_3 + F + M$	9.00×10^{34}	2.50×10^{33}
4	$CF_3 + O_2 = CF_3O + O$	2.26×10^{9}	8.00×10^{9}
5	$CF_2 + O_2 = CF_2:O + O$	2.00×10^{13}	5.00×10^{11}
6	$CF_2 + O = CF/O + F$	2.45×10^{13}	5.80×10^{13}
7	$CF/O + F = CF_2:O$	1.00×10^{12}	1.40×10^{12}
8	$2CF_3(+M) = CF_3-CF_3(+M)$	9.69×10^{10}	1.40×10^{11}
9	$CF_3(+M) = CF_2 + F(+M)$	1.00×10^{15}	1.00×10^{14}
10	$CF_3-CF_2 + F = 2CF_3$	3.16×10^{13}	7.90×10^{12}
11	$C_2F_5COC_3F_7 => C_3F_7 + C_2F_5CO$	8.50×10^{16}	2.00×10^{16}
12	$CF_3COF + CF_3 = CF_3CO + CF_4$	2.00×10^{12}	2.00×10^{11}
13	$CF_3-CF_3 + CF_3 = CF_4 + CF_3-CF_2$	3.00×10^{12}	1.00×10^{12}
14	$C_3F_7 + O_2 = C_3F_7O + O$	1.03×10^{20}	5.03×10^{19}
15	$C_3F_7 + O = CF_3COF + CF_3$	2.40×10^{13}	3.00×10^{15}
16	$C_2H_4 + F = C_2H_3 + HF$	1.00×10^{14}	5.00×10^{13}
17	$CF_2 + H = CF + HF$	3.98×10^{13}	2.00×10^{13}
18	$CF_3 + H = CF_2 + HF$	5.33×10^{13}	9.00×10^{13}
19	$CF_2 + H = CF + HF$	3.98×10^{13}	2.00×10^{13}
20	$CF + C_2H_4 => C_2H_2 + CH_2F$	1.00×10^{13}	4.00×10^{13}
21	$CH_3 + CF_3 = CH_2:CF_2 + HF$	5.53×10^{19}	1.10×10^{20}
22	$C_2H_4 + F = CH_2:CHF + H$	2.00×10^{13}	8.00×10^{13}
23	$C_2H_4 + F = C_2H_3 + HF$	1.00×10^{14}	5.00×10^{13}
24	$CF_3COF + H = CF_3CO + HF$	2.00×10^{13}	6.00×10^{13}

Figure 7. IDTs of RP-3 jet fuel adding 4.0% $C_6F_{12}O$.

in slope, which may be caused by different sources of RP-3 jet fuel.

The effects of $C_6F_{12}O$ on the IDT of RP-3 jet fuel/air at stoichiometric ratios and high temperatures are depicted in Figure 5. For comparison, the IDTs of RP-3 jet fuel just in pure air were measured as well. It can be seen that after adding $C_6F_{12}O$ in the air, the IDT of RP-3 jet fuel still followed the rule of Arrhenius law in the temperature range of 1100−1500 K, showing a strong linear relationship. However, the effects of different $C_6F_{12}O$ concentrations were different, or even opposite. The IDT of RP-3 jet fuel decreased at low concentrations of $C_6F_{12}O$ (0.5%); however, it was extended
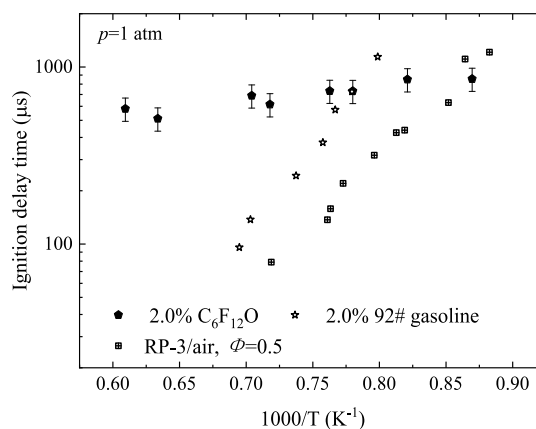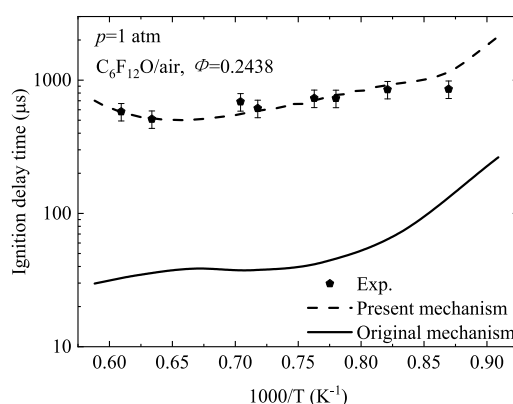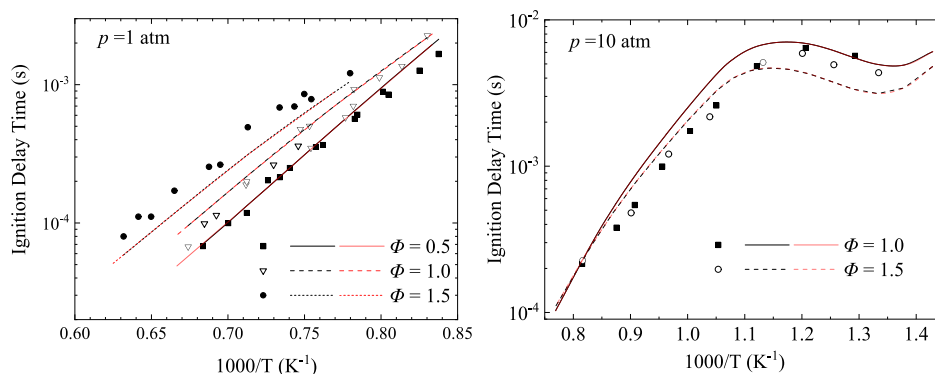
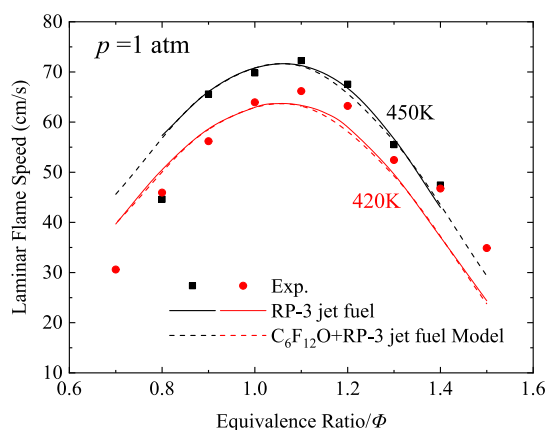**Figure 10.** Contrast of IDTs of RP-3 jet fuel.

Figure 11. Contrast of laminar flame speed of RP-3 jet fuel.

at 4.0% concentration, which was close to the effective extinguishing concentration. Moreover, the effect of $C_6F_{12}O$ was highlighted with the increase of temperature at 4.0% concentration, which means the sensitivity of IDT to temperature was weakened from the perspective of the slope. When the concentration of $C_6F_{12}O$ was in the middle (2.0%), the effect on the IDT of RP-3 jet fuel was not obvious, with just a small reduction.

The variation rule above was obtained under the stoichiometric ratio conditions of RP-3 jet fuel in air. Further experimental studies were conducted to determine whether this rule can be extended to lean and rich combustion. The IDTs of RP-3 jet fuel in the air at stoichiometric ratios of Φ = 0.5 and 2.0, respectively, on adding $C_6F_{12}O$ concentrations of 0.5 and 4.0% are shown in Figures 6 and 7. As shown in Figure 6, when the air contains 0.5% $C_6F_{12}O$, the IDTs of RP-3 jet fuel become shorter under rich combustion conditions, but show little variation under lean combustion conditions. Therefore, it can be inferred that a low concentration of $C_6F_{12}O$ (0.5%) will shorten the IDT of RP-3 jet fuel only when air is relatively scarce. As can be seen from Figure 7, the effects of $C_6F_{12}O$ with higher concentration (4.0%) on the combustion of RP-3 jet fuel are different in the range of 1130−1480 K under different stoichiometric ratios. For lean combustion (Φ = 0.5), the effect of $C_6F_{12}O$ is to extend the IDT, which gets close to that of RP-3 jet fuel combustion in the air with Φ = 2.0. For rich combustion (Φ = 2.0), adding 4.0% extinguishing agent $C_6F_{12}O$ leads to an increase in the slope between IDT and the reciprocal of temperature, that is, IDT is more sensitive to temperature. From the concrete value,

the temperature of about 1380 K is the critical point for the extension and shortening of IDT. If the temperature is higher than this temperature, the IDT will be shortened, and vice versa.

Based on the above analysis, it can be seen that the influence of $C_6F_{12}O$ on the IDT of RP-3 jet fuel is generated by multiple factors including the concentration of $C_6F_{12}O$ in air and the temperature and stoichiometric ratio of RP-3 jet fuel. All of these can affect the direction and amplitude of the change of IDT. Under high temperature conditions, the sensitivity of IDT of RP-3 jet fuel to temperature was weakened to some extent after adding $C_6F_{12}O$ in the air, but it was enhanced when a high concentration (4.0%) was applied to rich combustion (Φ = 2.0). The IDTs of RP-3 jet fuel were shortened by a lower concentration of $C_6F_{12}O$ (0.5%), and the maximum reduction is achieved when Φ = 1.0. A higher concentration (4.0%) of the $C_6F_{12}O$ prolongs the IDTs of RP-3 jet fuel, and the effect was most obvious at Φ = 0.5.

However, the parameters that can be measured through the experiment and the data that can be obtained are limited. Constructing the mechanism of $C_6F_{12}O$ is another method for understanding the influence of $C_6F_{12}O$ on the combustion process and the specific routine of extinguishing the fire from the level of chemical dynamics. As $C_6F_{12}O$ itself is flammable under certain conditions,[16,22] the experiment of IDT was conducted. However, the pressure and light signals were both unobvious at the stoichiometric ratio Φ = 1.0, and it was considered that $C_6F_{12}O$ failed to ignite under that condition. The experimental results that vary regularly with temperature were obtained at the stoichiometric ratio Φ = 1.0 (i. e. C = 2.0%), and the results are shown in Figure 8. In the figure, the IDTs of 92# gasoline[38] under the same condition and those of RP-3 jet fuel at the stoichiometric ratio Φ = 0.5 are added for comparison. As can be seen from the figure, the IDT of $C_6F_{12}O$ was 500−900 μs in the range of 1150−1958 K and decrease just slightly with an increase in temperature. The change rate of the IDT of $C_6F_{12}O$ was much lower compared with those of common fuels, such as 92# gasoline and RP-3 jet fuel, and it can be seen that the IDT of $C_6F_{12}O$ was less sensitive to temperature within that temperature range.

3.2. Modification and Verification of Mechanisms. To verify the predictive ability of the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ on the ignition characteristics, the IDTs of $C_6F_{12}O$ in air at p = 1 atm and Φ = 0.24 were calculated first, and the calculation and experimental results are shown in Figure 9. The mechanism can capture the evolution
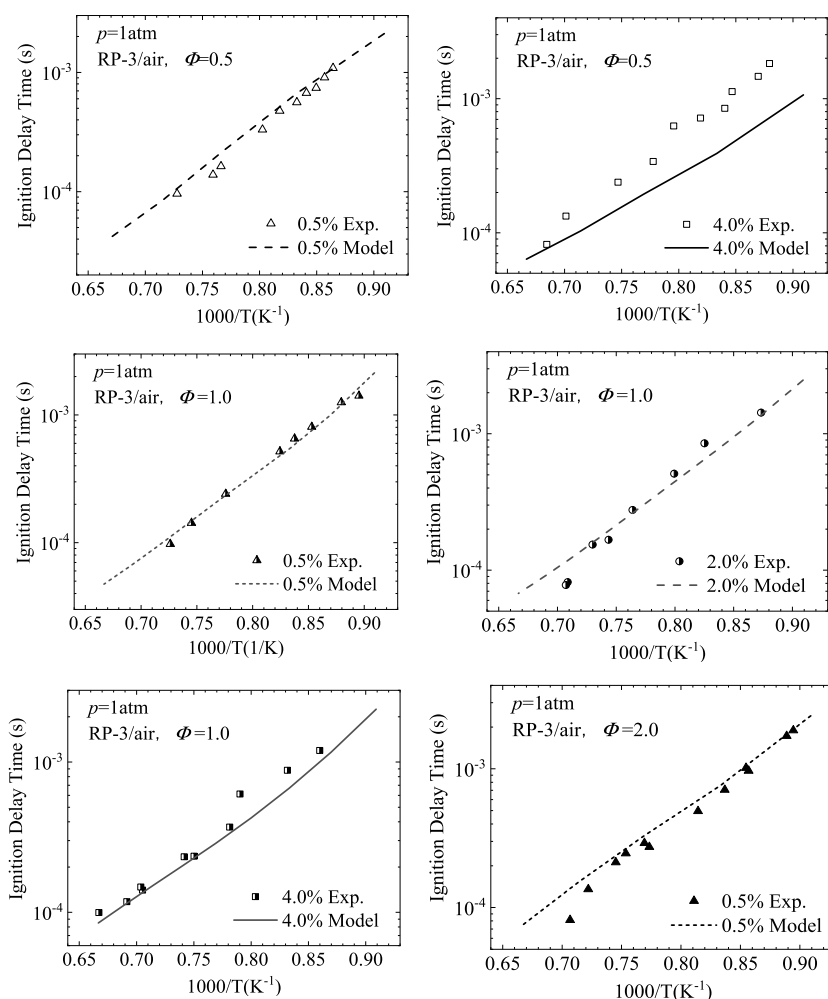
Figure 12. Contrast between calculated data and experimental data of RP-3 jet fuel IDTs in the air adding $C_6F_{12}O$.
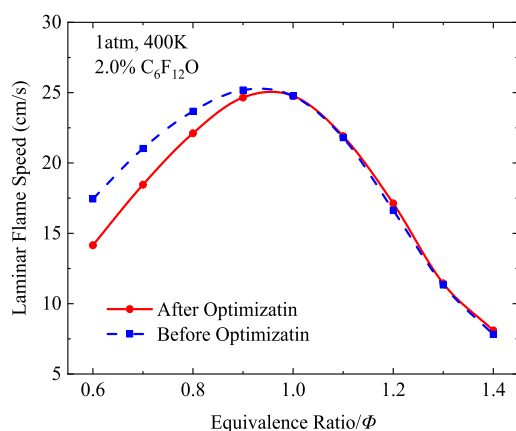

Figure 13. Contrast of RP-3 jet fuel laminar flame speed in air with $C_6F_{12}O$ calculated by the original and optimized mechanism.

trend of IDT on the initial temperature but seriously underestimate IDT at the whole temperature region.

To improve the prediction accuracy, the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ was optimized by adjusting the rate constants of the reactions of $C_6F_{12}O$. Some reactions have been selected to update their rate constants; the optimized reactions and their updated rate constants are shown in Table 2. The performance of the optimized

mechanism is also shown in Figure 9 for comparison; the comparison show that the simulation results on the IDT after optimization are in good agreement with the experimental results , and the optimization greatly improves the ability of the mechanism to predict ignition characteristics.

The IDTs of RP-3 jet fuel in the air were calculated as well to verify the predictive ability of the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ on ignition characteristics. The contrast between the mechanisms of RP-3 jet fuel and RP-3 jet fuel adding $C_6F_{12}O$ is shown in Figure 10; the experimental results of 1 atm in this study and that of 10 atm from Mao's work[39] are added as benchmarks. It can be seen that the results of each condition simulated by the two mechanisms are completely consistent, and the ignition delay time obtained by the experiment can be predicted. It means that the integration did not affect the ability to predict the IDT of RP-3 jet fuel.

To investigate the prediction accuracy of flame propagation characteristics of RP-3 jet fuel by the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$, the contrast between the mechanisms of RP-3 jet fuel and RP-3 jet fuel adding $C_6F_{12}O$ were conducted, and the experimental results were also added as benchmarks. The contrast is shown in Figure 11; it can be seen that the calculation results of the two mechanisms are almost the same, which indicates that integration did not affect the ability to predict the flame propagation characteristics of RP-3 jet fuel.
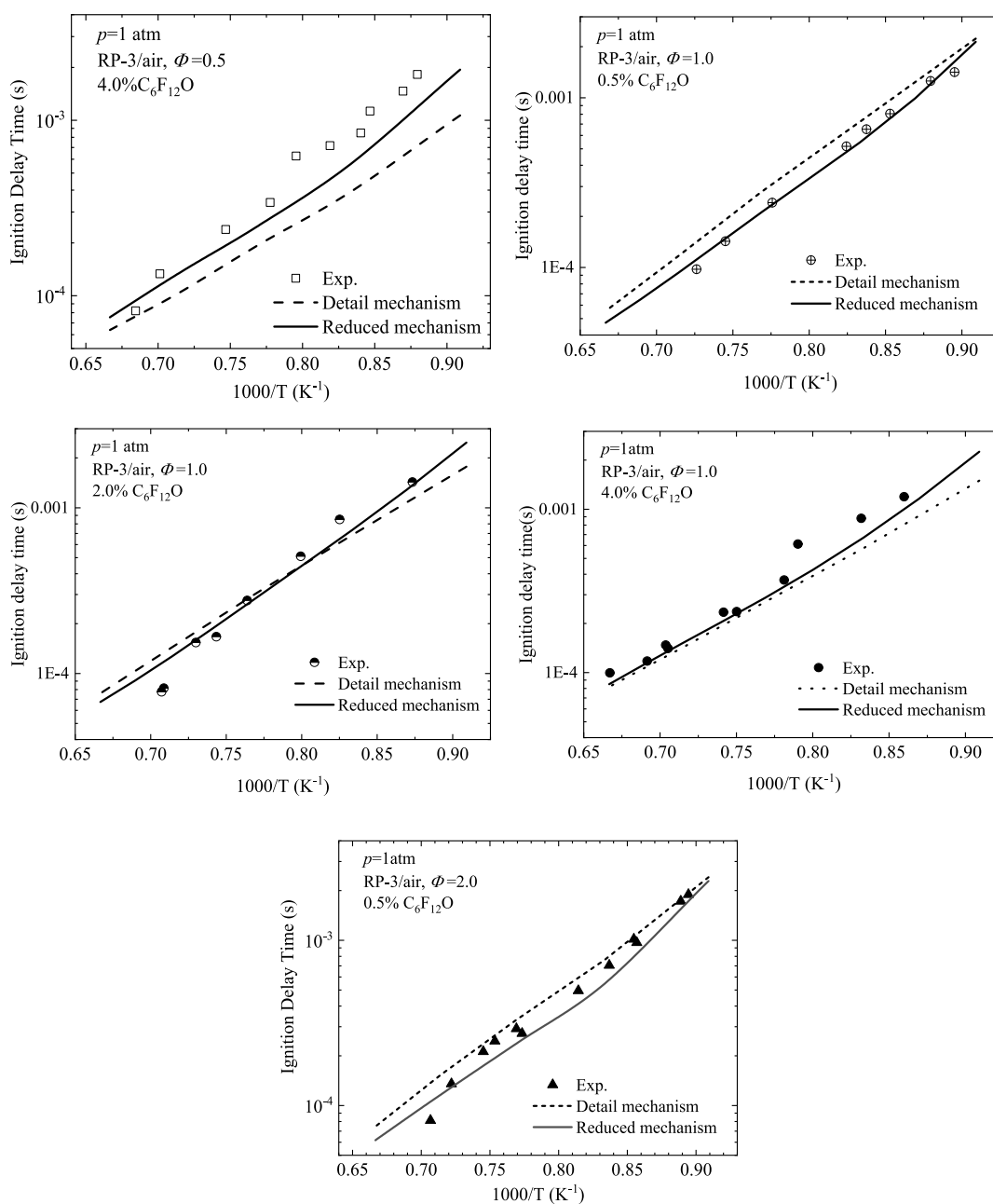
Figure 14. Contrast between the IDTs calculated by the reduced mechanism and detailed mechanism.

Finally, to verify the reliability of the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ in predicting ignition characteristics, the IDTs under experimental conditions in this study were calculated and compared with the experimental value, as shown in Figure 12. It can be seen that the simulation results have little difference with the experimental results in terms of variation trend and numerical value. In general, the combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ in this study can well predict the ignition characteristics of RP-3 jet fuel in the air containing $C_6F_{12}O$.

The reliability of the original mechanism of $C_6F_{12}O$ in predicting flame propagation has been verified by previous studies.[17,19,20] Whether the modified and optimized mechanism can maintain this predictive ability needs to be verified. Therefore, the original mechanism and the optimized mechanism are respectively used to calculate the laminar

flame velocity under the same conditions. Taking 1 atm, 400 K, and 2% $C_6F_{12}O$ concentration as examples, the comparison between them is shown in Figure 13. As can be seen from the figure, in the case of oil-rich combustion ($\Phi = 1.0-1.4$), the result of optimized mechanism is very similar to the original mechanism; while in the case of oxygen-rich combustion, the gap is a little larger, but not more than 18.9%, which is acceptable. In general, the optimized mechanism maintains the reliability of laminar flame speed prediction.

While reducing the mechanism of RP-3 jet fuel adding $C_6F_{12}O$, the IDT experimental result was chosen as the target, and the prediction ability of the reduced mechanism is close to and even better than the detailed mechanism, as shown in Figure 14. It means that in addition to reducing the scale of the mechanism, the reduced mechanism can predict the ignition characteristics more accurately. The reduced mechanism of

RP-3 jet fuel adding $C_6F_{12}O$ developed in this study can be combined with a fluid dynamics model to carry out a fluid numerical simulation based on chemical dynamics, which will provide great help for the design and evaluation of the fire protection system for petroleum.

4. CONCLUSIONS

In this study, the IDT of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$ was measured using a shock tube, and the results showed that the IDT of $C_6F_{12}O$ was 500−900 μs and less sensitive to temperature compared with those of common fuels in the range of 1150−1958 K, and the influence of $C_6F_{12}O$ on the IDT of RP-3 jet fuel was influenced by many factors. The concentration of $C_6F_{12}O$ in air and the temperature and stoichiometric ratio of RP-3 jet fuel can affect the direction and amplitude of the change of IDT. Under high temperature conditions, the sensitivity of IDT of RP-3 jet fuel to temperature was weakened to varying degrees after adding $C_6F_{12}O$ in the air, except that at high $C_6F_{12}O$ concentration (4.0%) applying to oil-rich combustion ($\Phi = 2.0$). The IDT of RP-3 jet fuel was decreased by a low $C_6F_{12}O$ concentration (0.5%), with the greatest decrease observed at $\Phi = 1.0$. Higher concentration (4.0%) of $C_6F_{12}O$ prolonged the IDT of RP-3 jet fuel, with the most obvious increase at $\Phi = 0.5$.

The combustion mechanism of RP-3 jet fuel adding $C_6F_{12}O$ was developed by integrating the mechanisms of RP-3 jet fuel and $C_6F_{12}O$. According to the IDT of $C_6F_{12}O$/air, some reactions from the mechanism of $C_6F_{12}O$ were modified, and the modified mechanism of RP-3 jet fuel adding $C_6F_{12}O$ can well predict the IDT of $C_6F_{12}O$/air and RP-3/air adding $C_6F_{12}O$ without affecting the ability of predicting flame propagation. After a series of reductions, the modified mechanism was reduced to 109 species and 517 reactions, which still performed well.

Through the study on ignition delay and reaction mechanism of RP-3/air combustion adding $C_6F_{12}O$, the IDT of $C_6F_{12}O$ in air and the IDT of RP-3 jet fuel at different concentrations of $C_6F_{12}O$ were obtained through experimental study for the first time, and the study provided a good basis for the chemical kinetics analysis of inhibition of RP-3 jet fuel combustion by $C_6F_{12}O$..

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.3c01888.

Reduced mechanism of RP-3 jet fuel adding C6F12O (.INP format) (PDF)

Thermodynamic datafile (.DAT format) (PDF)

Transport datafile (.DAT format) (PDF)

Experimental results of ignition delay times (PDF)

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Notes

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