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Effects of Ethanol and Methanol on the Combustion Characteristics of Gasoline with the Revised Variation Disturbance Method

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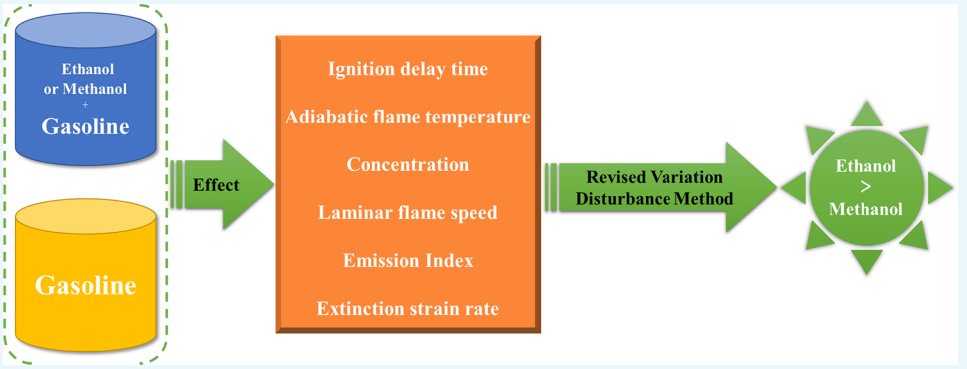

ABSTRACT: This paper proposes a revised variation disturbance method to provide valuable information and reference for fuel design or optimization of internal combustion engines to realize the comprehensive and quantitative evaluation of the effects of blending agents on the combustion performance of primary fuels. In this method, methanol and ethanol are blended into gasoline to form six kinds of alcohol−gasoline (E10, E20, E30, M10, M20, and M30). Then, the ignition delay, adiabatic flame temperature, component concentration, fuel-burning rate, extinction strain rate, and CO emission of gasoline and alcohol−gasoline are studied by system simulation in a wide range of operating conditions. Based on the new variation disturbance method, the effects of methanol and ethanol on the combustion performance of gasoline are next analyzed globally and characterized quantitatively. The comprehensive results of ethanol and methanol on the gasoline's combustion are visually presented. The method proposed in this paper is preliminarily validated based on the analysis of the microscopic mechanism of combustion. The results show that the blending of ethanol and methanol has positive effects on gasoline combustion, and ethanol can rapidly ignite the gasoline in a wide range of operating conditions and is superior to methanol in terms of fuel combustion, stability, and pollutant discharge. Based on the treatment of simulated values of six combustion characteristics selected in this paper and the calculations of the variation disturbance method, the total disturbance values of ethanol and methanol to gasoline combustion are obtained as 0.8493 and 0.2605, respectively. That is, ethanol has a more significant effect on improving the combustion performance of gasoline than methanol. In addition, based on the analysis results of the combustion, it is found that the blending of ethanol enlarges the reaction of notable components in gasoline. This finding also proves the effectiveness and validity of the scientific method utilized in this paper.

1. INTRODUCTION

Presently, fossil fuels are still the primary energy in human society. But with the increase in global energy consumption, energy crisis and environmental pollution have become two urgent problems that have prompted people to look for suitable green renewable energy sources and have spurred research on biofuels such as alcohols and esters around the world. Alcohol fuels such as methanol and ethanol have been successfully used in any conventional, gasoline-powered vehicle such as gasoline engines by blending or pure combustion, and especially, alcohol−gasoline has been well used. For example, utilizing ethanol can improve the thermal efficiency of spark ignition engines and reduce exhaust emissions. When an alcohol fuel is blended into gasoline, the oxygen content of the fuel will increase and is more conducive to combustion. This leads to the contents of aromatic hydrocarbons, sulfur, lead, and other components in the alcohol-containing fuel being much lower than those in gasoline, so it is possible to effectively reduce greenhouse gas emissions and reduce air

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pollution. In addition, adding methanol or ethanol to gasoline will also increase the octane number of fuels so that the engine can work at a higher compression ratio. Therefore, among various biofuels, alcohol fuels have great potential in improving engine performance and reducing pollutant emissions. In addition, the raw materials for preparing alcohol fuels are readily accessible and cheap, and the technology is relatively mature. Therefore, alcohol fuels are regarded as an excellent alternative for fossil fuels.[1−3]

A series of experimental studies and numerical analyses have been carried out on the combustion of alcohol fuels and gasoline in gasoline engines, in addition to many kinetic studies. For example, the pure combustion and blending of alcohol fuels are studied by experimental means and combustion simulation. As a renewable alternative to fossil fuels and the current demand for internal combustion engines, the research on blending alcohol-based fuels is more valuable.[3−7] Therefore, relevant experimental studies on alcohol blending in gasoline have been widely carried out.

Abu-Zaid et al. studied the effect of methanol blending on the gasoline performance in engines. It was thus found that, within the scope of their study, a mixture of 15% methanol and 85% gasoline (by volume) can achieve optimal engine performance with maximum power output and minimum brake-specific fuel consumption.[8] Liao et al. carried out an experimental study on the combustion characteristics of methanol−gasoline at low temperature based on a constant volume combustion bomb. This study proved that a moderate addition of methanol could slightly improve the combustion performance at low temperatures and significantly reduce the emission of HC and CO.[9] Furthermore, Zhang et al. studied the test engine load performance, engine output emission, air−fuel ratio change, and combustion characteristics of methanol−gasoline with different blending ratios in engines. These results showed that methanol−gasoline with a low mixing ratio could better adapt to current engines and vehicles. Their THC, CO emissions, and fuel consumption were lower than those of pure gasoline.[10] Bilgin and Sezer studied the effects of methanol on the performance and fuel cost of gasoline in gasoline engines and also found that methanol blending brought the best performance for engines in terms of effective braking pressure and brake thermal efficiency (bte).[11]

Yao et al. studied the effect of ethanol on the intermediate components and products of gasoline combustion in a low-pressure premixed planar flame by using synchrotron radiation combined with flying molecular beam mass spectrometry. Furthermore, they compared the distribution of typical intermediate components and products, the differences in components, and the changes in temperature between gasoline and ethanol−gasoline in flame and analyzed the effect of ethanol on the anti-explosion performance and emission characteristics of gasoline.[12] Qian et al. studied the combustion of alternative fuels of ethanol and gasoline in dual-fuel spark-ignition engines. It was found that, with the increase in proportion of ethanol in the fuel, the flame duration and rapid combustion duration were prolonged. At the same time, the total amount of nitrogen oxide emission and hydrocarbon emission gradually decreased.[13] Al-Hasan studied the characteristics of ethanol−gasoline mixtures in terms of engine performance and emission. The results showed that blending ethanol with gasoline could improve the braking power, torque, volumetric efficiency, brake thermal efficiency, and fuel consumption while reducing the brake-specific fuel consumption and equivalent air−fuel ratio. In addition, the concentration of CO and HC in the engine exhaust gas decreased, while the concentration of CO_2 increased. It was also found that a fuel blended with 20% ethanol (by volume) achieved the best engine performance at all engine speeds.[14] Qi and Lee studied the combustion and emission of ethanol−gasoline in gasoline engines. The results showed that gasoline had a faster combustion rate and a higher peak heat release rate (HRR) under low engine loads. Comparatively, ethanol−gasoline had a faster combustion rate and a higher HRR under high engine loads. The brake thermal efficiency of ethanol−gasoline was not much different from that of gasoline, but the brake-specific fuel consumption was slightly higher; with the increase in ethanol content in ethanol−gasoline, the CO emission decreased, and the HC emission increased slightly under high engine load, while the NO_x emission depended on engine operating conditions and ethanol content.[15] Liu et al. studied the effects of the chemical kinetic behavior and adiabatic flame temperature of E30 ethanol−gasoline (containing 30% ethanol) on the laminar flame speed at different initial temperatures and analyzed the relative importance of thermal and chemical effects of ethanol at different initial temperatures. It was found that the chemical effect of ethanol was much more apparent than its thermal effect characterized by adiabatic flame temperature.[16] Yang et al. analyzed the laminar flame speed and flame stability of E30 ethanol−gasoline using the high-speed schlieren method and a constant volume burner. The results showed that the laminar combustion rate of E30 was positively correlated with the initial temperature and negatively associated with the initial pressure and dilution ratio. By adding ethanol with a higher volume fraction, the laminar combustion rate increased significantly relative to gasoline and E10, highlighting one of the benefits of ethanol as a blending component of gasoline fuels.[17] Fan et al. studied the combustion performance of three alternative gasoline fuels, including EPRF, ETPRF, and TPRF (made from a mixture of ethanol, toluene, and PRF reference fuel), in a rapid compression machine (RCM). The results showed that the synergetic effect of ethanol during spontaneous combustion and the dependence of flame speed on pressure were better than those of toluene at different mixing ratios of ethanol.[18] Xu et al. studied the effects of methanol and ethanol on the laminar premixed flame of *n*-heptane/toluene mixture as a gasoline alternative fuel by using synchrotron photoionization and molecular-beam mass spectrometry techniques combined with numerical simulation. The results showed that the addition of alcohol had a weak chemical effect on the decomposition of hydrocarbon fuels. It could significantly promote the formation of HO_2 and OH free radicals and inhibit the formation of aromatic hydrocarbons during gasoline combustion.[19] Parag and Raghavan also carried out experimental studies on the effect of ethanol on the combustion rate of fossil fuels.[20]

The effects of alcohol fuels on the combustion performance of gasoline in engines have also been studied. Wei et al. studied the combustion performance of methanol, ethanol, and gasoline in gasoline engines. The results showed that more alcohol fuel participated in the low-temperature reaction than gasoline in HCCI combustion mode. Therefore, it was conducive to the kinetic chemical reaction and shortening of the ignition time and combustion duration. It was also found that alcohol fuels were conducive to reduction of the combustion temperature and NO_x emission of engines.[21] Li

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et al. studied the combustion and emission characteristics of gasoline, respectively blended with methanol, ethanol, *n*-butanol, and isopropanol/*n*-butanol/ethanol (IBE) in an injection-type spark-ignition engine. Comparative experimental studies on different alcohol and alcohol-containing gasoline types with different volume fractions under different operating conditions were carried out.[22] He et al. studied the combustion characteristics of ethanol, *n*-butanol, and their mixture with gasoline in gasoline engines. The results showed that, when the mixture had the same oxygen mass content, *n*-butanol had a better effect on improving the ignition performance of gasoline than ethanol.[23] Iliev studied the performance of methanol and ethanol in engines after blending with gasoline. The results showed that alcohol−gasoline had lower braking power and higher brake-specific fuel consumption than gasoline fuels. The concentration of CO and HC decreased with the increase in mixture percentage of alcohols, but the NO_x emission increased significantly as the mixture percentage of alcohols increased to 30%.[24] Ihracska et al. studied the flame propagation characteristics of premixed fuel−air such as gasoline, iso-octane, E85, and M85 and their differences in engines.[25] Masum et al. studied the possibility of using alcohols with higher carbon numbers such as propanol, butanol, amyl alcohol, and hexyl alcohol as gasoline alternative fuels and compared the performance of gasoline and ethanol−gasoline in engines. It was found that the optimized polyol−gasoline mixture exhibited good performance in terms of fuel characteristics, engine performance, combustion, and emission.[26]

With the development of computers, accurate prediction of the combustion and emission performance of fuels in engines can also be achieved based on efficient numerical simulation. More importantly, the knowledge and understanding of combustion micromechanism can be realized based on combustion simulation results and kinetic analysis. For example, Kalvakala et al. studied the relationship between the tendency of soot and fuel composition and chemical properties during gasoline combustion based on simulation technology.[27] Accurate combustion simulation is based on high-precision alcohol or gasoline combustion models. Therefore, the combustion models of alcohols and alcohol−gasoline have developed rapidly, and the corresponding combustion kinetic models of gasoline and alcohol fuels have also seen rapid development.[28−35]

To summarize, the experimental monitoring and research on the combustion characteristic of gasoline blended with methanol, ethanol, and other small molecular alcohol fuels or additives are relatively mature and extensive. They involve the effects of small-molecule alcohol fuels on gasoline's combustion and emission performance in engines. Most of the above research results are based on engine tests and measurements. It is found that the blending of alcohol fuels can improve the combustion and emission performance of gasoline. However, relevant studies on the degree and trend of the effects of alcohol blending are largely qualitative analyses. In addition, because of the different combustion performance of fuels, most of the above studies focus on a specific combustion characteristic of fuel under certain operating conditions. The effects of blending agents (additives or blending fuel) on the combustion performance of primary fuels are relatively simple. Therefore, the effects of alcohol fuels on gasoline combustion performance need to be quantitatively characterized based on multiple operating conditions and multiple combustion characteristics. Then, a comprehensive evaluation of blending components is critical and has an important guiding significance.

In this paper, a study on the combustion performance of gasoline and small-molecule alcohol fuels such as methanol and ethanol is carried out in the range of engine combustion conditions. A new variation disturbance method is proposed to analyze and quantify the extent of the effects of methanol and ethanol on the combustion performance of gasoline. This provides an intuitive and comprehensive understanding of the effects of fuel blends. Furthermore, based on the combustion path analysis, the method is verified by the combustion micromechanism. This provides a scientific analysis method for evaluating the performance of blending agents and a significant application value for fuel design or optimization of internal combustion engines.

2. METHODOLOGY

2.1. Selection and Verification of the Combustion Model. In this paper, gasoline and two kinds of alcohol−gasoline formed by blending methanol and ethanol into gasoline were studied. For the convenience of numerical simulation and systematical analysis, a three-component gasoline alternative fuel with mole fractions of 69.13% toluene, 18.67% *n*-heptane, and 12.20% iso-octane (the volume fractions are 60.66, 22.65, and 16.69%, respectively), which was proposed by Xu et al. for Chinese No. 92 gasoline, was used.[36] The combustion model used in this paper is a four-component gasoline alternative model (toluene/*n*-heptane/iso-octane/ethanol) developed by Li et al. of KAUST Clean Combustion Research Center in 2019. The model (KAUST-59s mechanism) contains 59 components and 270 reactions and can predict the combustion performance of the four single-component fuels above and the combustion test results of blending fuels such as gasoline.[37] The laminar flame speed of gasoline alternative fuels is simulated, and the simulation results coincide well with the experimental results, as shown in Figure 1, to verify the feasibility of using the KAUST mechanism to predict the combustion characteristics of domestic gasoline. Therefore, through this paper, it is understood that this model is quite suitable for the combustion simulation of ethanol, gasoline, and their mixtures.

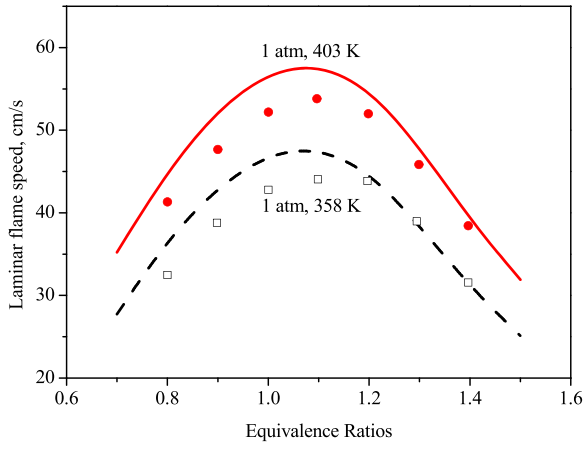

Figure 1. Laminar flame speed of gasoline. Lines represent this work, and the symbols represent the work of Xu et al.[36]

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Since the combustion performance of methanol also needs to be accurately predicted in this paper, it is also necessary to verify the accuracy of the KAUST-59s mechanism in the simulation of methanol combustion; therefore, the ignition delay and laminar flame speed of methanol are simulated in a wide range of operating conditions in this paper based on the mechanism of the 59 components, as shown in Figures 2 and 3.

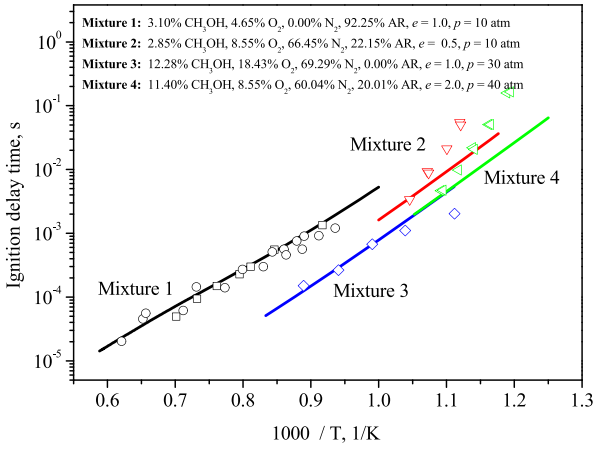

Figure 2. Ignition delay time of methanol. Lines represent this work, and symbols represent the work of Burke et al.[38]

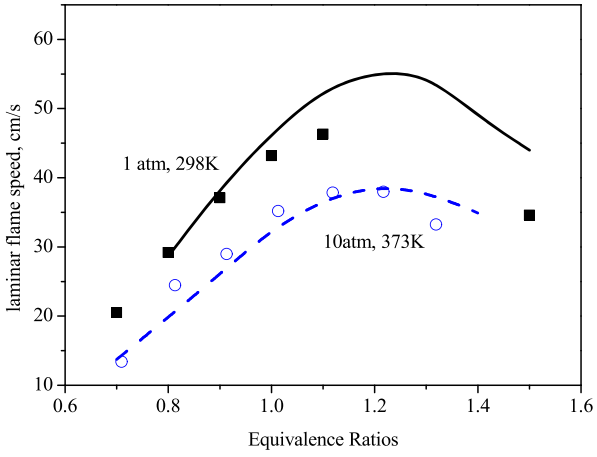

Figure 3. Verification of laminar flame speed of methanol. Lines represent this work, the solid squares represent the work of Sileghem et al.,[39] and the open circles represent the work of Beeckmann et al.[40]

It can be seen from the two figures that the numerical simulation of combustion can well reproduce the combustion results such as ignition and flame characteristics of methanol and accurately present the trend and law of the combustion performance changing with the operating conditions. Therefore, relevant studies on methanol and its effects on gasoline combustion performance can be reasonably carried out based on this mechanism.

2.2. New Variation Disturbance Method. The combustion process of blend fuels (blending agent/primary fuel) can be affected by many factors in addition to the impact of combustion environment factors such as pressure, temperature, equivalence ratio, etc. In addition, the addition of blending agents affects the combustion process and combustion performance of primary fuels. Since a fuel has a wide variety of combustion characteristics, such as self-ignition time, flame temperature, component concentration, component yield, heat release rate, and combustion completeness, and the values and dimensions of each combustion characteristic are quite different, it is obviously disadvantageous to a comprehensive evaluation of the combustion.

The authors first proposed the variation disturbance method in 2019 based on the concept of coefficient of variation. This method eliminates the effects of the numerical scales and dimensions of combustion characteristics and quantifies the effects of blending components by the coefficient of variation.[41] To better describe the extent of effects of blending agents on the overall combustion performance of primary fuels, this paper proposes a new disturbance based on the concept of coefficient of variation and the experience of research on combustion dynamics. This quantity can be used to quantitatively characterize the extent of effects of blending fuels on the combustion performance of primary fuels and comprehensively analyze the disturbance to each combustion characteristic. Finally, the disturbance to each combustion characteristic is summed to obtain the total disturbance (D). The calculation process is shown in eqs 1 − 6. The comprehensive disturbance degree of the effects of fuel blends on the combustion performance of primary fuels can be visually and numerically presented by the value of the disturbance.

$$D = \sum D_i = = \sum \delta_i \omega_i d_i \tag{1}$$

$$\delta_i = \text{return}\ (S_i)\ (\delta_i = 0, \text{if}\ S_i = 0; \text{otherwise}, +1 \text{or} -1) \tag{2}$$

$$\omega_i = \frac{\text{abs}(S_i)}{\sum_{n=1}^{n} \text{abs}(S_i)} \tag{3}$$

$$d_i = \frac{\text{stdev}(|c_{i1}|: |c_{ij}|)}{\text{avg}(|c_{i1}|: |c_{ij}|)} \tag{4}$$

$$S_i = \sum_{j=1}^{j} c_{ij} \tag{5}$$

$$c_{ij} = \frac{V_{ij}^{b} - V_{ij}^{o}}{V_{ij}^{o}} \tag{6}$$

In the above equations, V_{ij} is the magnitude (experimental value or simulated value) of the i-th combustion characteristic of the fuel under the j-th operating condition over a wide range of parameters, where V_{ij}^{b} is the magnitude of disturbance to the combustion of the fuel blends after the addition of blending agents (additives or other alternative fuels), and V_{ij}^{o} is the magnitude of the combustion performance of the original fuel without blending agents; c is the relative variation in the combustion characteristics of blend fuel and initial fuel under all operating conditions; S_i is the cumulative value of c under the operating conditions used and can be used to preliminarily predict the overall effect of the blending of blending agents on the main fuel under various operating conditions; and d_i is the disturbance of the i-th combustion characteristic, where stdev is the standard deviation of the sample, and avg is the standard arithmetic mean of the sample. The disturbance quantity can be used to quantitatively analyze the extent of effects of blending fuel on primary fuels, directly analyze the disturbance to each combustion characteristic, and eliminate the differ-

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Table 1. Proportion of Various Fuels (Molar Ratio)

	fuel						
	gasoline	E10	E20	E30	M10	M20	M30
composition	gasoline	ethanol:gasoline (1:9)	ethanol:gasoline (1:4)	ethanol:gasoline (1:2.33)	methanol:gasoline (1:9)	methanol:gasoline (1:4)	methanol:gasoline (1:2.33)
proportion (alcohol)	0%	10%	20%	30%	10%	20%	30%

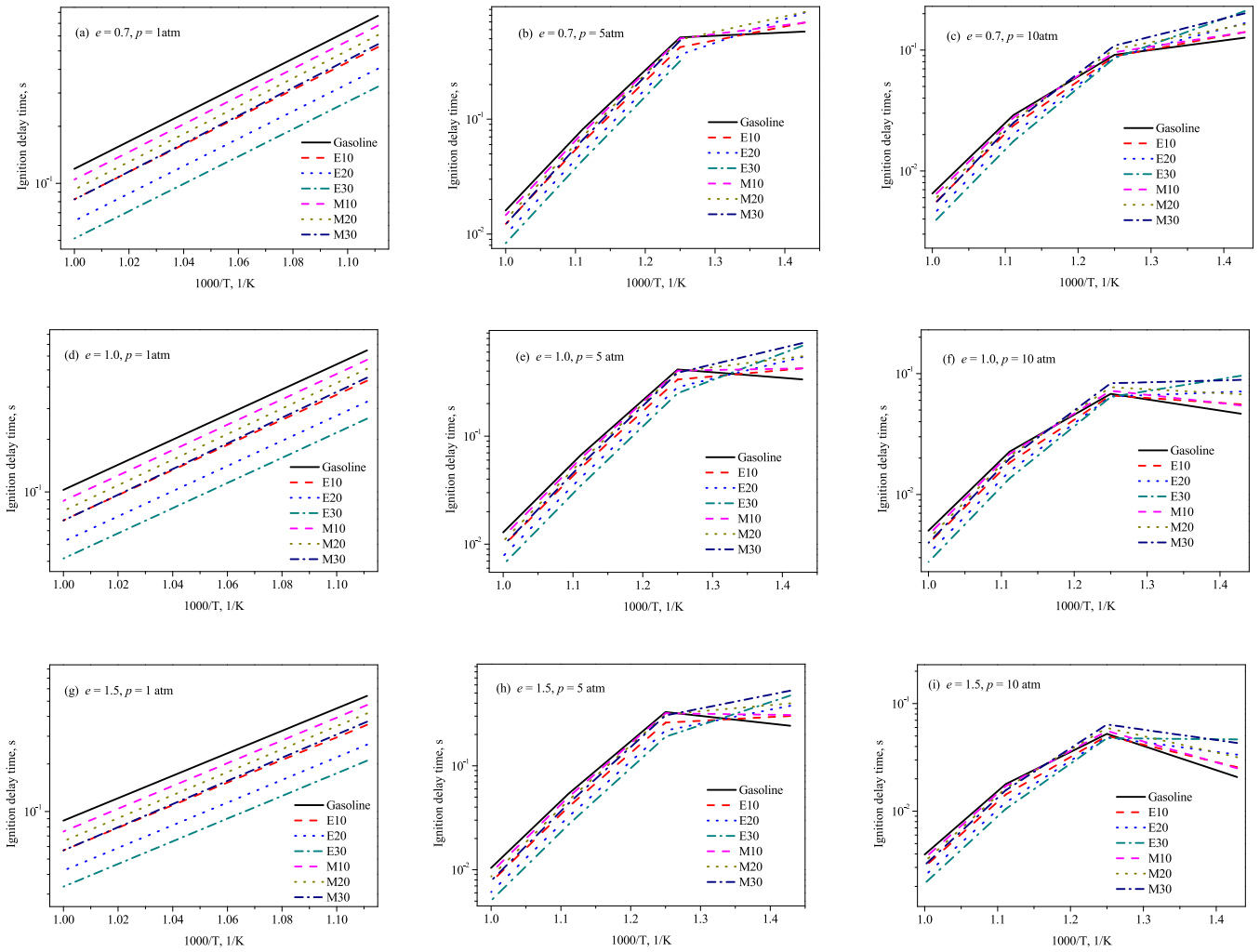

Figure 4. Comparison of ignition delay time of different fuels at (a) $e = 0.7$ and $p = 1$ atm, (b) $e = 0.7$ and $p = 5$ atm, (c) $e = 0.7$ and $p = 10$ atm, (d) $e = 1.0$ and $p = 1$ atm, (e) $e = 1.0$ and $p = 5$ atm, (f) $e = 1.0$ and $p = 10$ atm, (g) $e = 1.5$ and $p = 1$ atm, (h) $e = 1.5$ and $p = 5$ atm, and (i) $e = 1.5$ and $p = 10$ atm.

ences in dimensions and magnitudes of combustion characteristics. Then, the dimensionless total disturbance is obtained by summing the disturbance to each combustion performance. ω_i is the weight of a blending agent in the combustion characteristic. It is used to compare the effects of various additives or blending fuels on the combustion performance of the primary fuel. If n kinds of blending agents are studied, the S_i corresponding to each blending agent needs to be summed to obtain $\sum S_i$, and then the weight ω_i of the blending agent is calculated based on the ratio of S_i and $\sum S_i$; if the effect of only one blending fuel is considered, the weight value is 1. At the same time, the δ function is introduced to characterize the positivity of disturbance. S_i and the value (+1, −1, 0) from the return function are used to preliminarily judge the disturbance effect on the primary fuel, that is, to characterize whether the effect of a blending agent or fuel blend on the combustion performance of the primary fuel is promotive or inhibitive under all operating conditions. When the δ function is +1, it indicates that the blending component has a positive effect on the combustion characteristics of the primary fuel. When the δ function is −1, it shows an inhibitive effect. When the δ function is 0, it indicates no effect. It should be emphasized that the rule of the return value of the δ function should be given based on the knowledge of combustion theory and engineering requirements. For specific applications, refer to the following chapters.

2.3. Fuel Composition. To systematically study the effects of ethanol (C_2H_5OH) and methanol (CH_3OH) on the combustion performance of gasoline, two kinds of molecular alcohols were respectively blended with gasoline at ratios of

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1:9 (molar ratio, 10%), 1:4 (20%), and 1:2.33 (30%) to form six kinds of alcohol−gasoline, which are recorded as E10, E20, E30, M10, M20, and M30 in order, as shown in Table 1. Through systematic comparison and analysis of the combustion simulation results of gasoline and the six kinds of alcohol−gasoline above, it is possible to gain an intuitive understanding of the effects of alcohol blending on the combustion performance of gasoline.

3. RESULTS AND DISCUSSION

3.1. Basic Combustion Characteristics. A numerical study has been performed using Chemkin software.[42] The simulation results are set out as follows: ignition delay time, adiabatic flame temperature, and OH mole fraction, which were conducted in a closed homogeneous batch reactor. The laminar flame speed and EICO were calculated by Premixed Laminar Flame Speed Calculation code. The extinction strain rate was simulated using the Diffusion Opposed-flow Flame code, and the strain rate is defined on the oxidizer side as the gradient of the velocity profile.[43] As one of the critical characteristics of fuels, ignition delay time can directly reflect the burning speed and is also one of the important parameters to judge whether fuels can burn quickly. In this paper, the characteristics of gasoline, methanol−gasoline, and ethanol−gasoline, including ignition temperature, combustion temperature, and OH concentration, are systematically studied based on a zero-dimensional homogeneous reactor at pressures (p) of 1 and 10 atm, equivalence ratios (e) of 0.7, 1.0, and 1.5, and an initial temperature (T) of 700−1000 K. The zero-dimensional constant volume reactor is selected in numerical simulation, and the combustion reaction time is set to 1 s. If the fuel does not burn successfully within 1 s, the numerical simulation under such conditions is considered invalid and is not presented in this paper. Detailed simulation results are provided in Tables S1−S3 of the Supporting Information.

A simulation of the combustion of seven fuels, including gasoline, is shown in Figure 4. The results show that, when the initial pressure is 1 atm, and the temperature is 700−800 K, the fuel cannot ignite in 1 s. As shown in Figure 4a,d,g, at the initial temperatures of 900 and 1000 K, the ignition time of gasoline can be effectively shortened with the addition of methanol and ethanol. Currently, promoting gasoline ignition becomes increasingly prominent as the proportion of methanol and ethanol increases. In addition, it is found that ethanol has a more remarkable effect on gasoline than methanol, and this law is present at different equivalence ratios and pressures. As the pressure increases to 5 and 10 atm, although auto-ignition of the fuel can be achieved at lower temperatures, it is found that there is an opposite result at higher temperatures. At 800 K, the positive effect of ethanol on gasoline self-ignition begins to weaken, while methanol begins to have a negative impact on gasoline ignition. When the temperature drops to 700 K, the ignition time of pure gasoline is the shortest. The more methanol and ethanol are blended, the more pronounced the inhibitive effect on gasoline self-ignition is, as shown in Figure 4b,c,e,f,h,i. This phenomenon is more evident as the initial pressure increases.

Adiabatic flame temperature is an essential property in fuel combustion characteristics. The adiabatic flame temperature significantly affects chemical reaction rates, and a higher adiabatic flame temperature indicates that the fuel can do more work externally. In addition, adiabatic flame temperature plays a vital role in studies on combustion efficiency and heat transfer. The high heating values of gasoline, methanol, and ethanol are about 44, 21, and 28 MJ/kg, respectively.[44] Since the combustion heat of methanol and ethanol with the same moles is significantly lower than that of gasoline, it is reasonable to believe that, after blending methanol and ethanol in gasoline, the adiabatic flame temperature of fuel blends is lower than the combustion temperature of pure gasoline under the same conditions. To better present the extent of the effect of blending components on the combustion temperature of the gasoline, Figure 5 presents the effect by the relative change rate of temperature, $R_T = (T_b - T_o)/T_o$, where T_b is the adiabatic

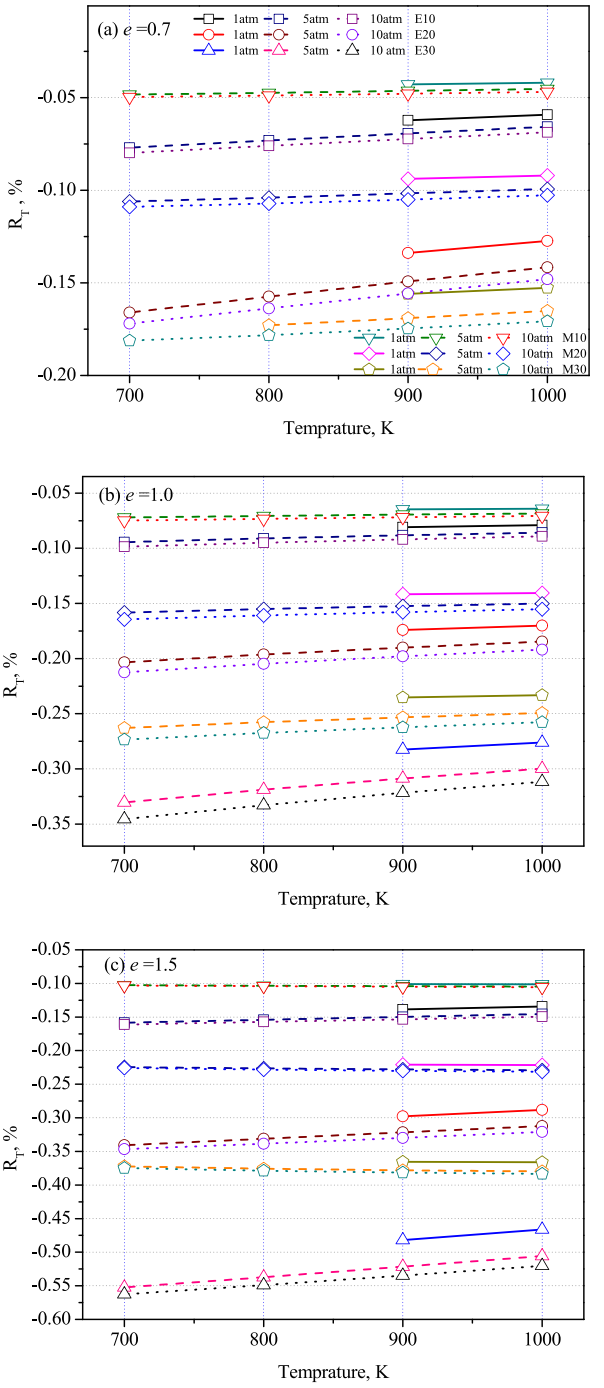

Figure 5. Comparison of adiabatic flame temperatures of different fuels at (a) e = 0.5, (b) e = 1.0, and (c) e = 1.5.

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flame temperature of alcohol-blended gasoline fuels, and T_o is the combustion temperature of pure gasoline. As shown in Figure 5, the values of R_T are all negative and decrease as the proportion of alcohol-blended gasoline fuels increases. Based on the value, it is possible to judge that methanol has a weaker effect on the combustion temperature of gasoline than ethanol when blended with gasoline. The main reason is that the mass of gasoline in methanol−gasoline is greater than that in ethanol−gasoline under the same blending ratio. Therefore, under the same conditions, the combustion temperature of methanol−gasoline is higher than that of ethanol−gasoline. Methanol has less effect on gasoline combustion temperature by comparing with pure gasoline. Similar results were obtained in ref 17. With the increase in blending proportion and initial pressure, it is more unfavorable for the adiabatic flame temperature of fuel combustion. In addition, it is found that the effects of methanol and ethanol on the adiabatic flame temperature of the gasoline are more evident in rich fuel states than in lean fuel states. Similar results were found in previous studies.[44,45]

The OH radical is a crucial intermediate component in the combustion of hydrocarbon fuels. It is closely related to the two key reactions H + O_2 = OH + O and CO + OH = CO_2 + H that control the combustion rate and combustion heat release rate of fuels. Since OH is involved in both reactions, the effect of OH concentration on the combustion process and the performance of fuels is crucial. The result of OH on gasoline combustion can be known by analyzing the concentration of OH radicals during the combustion of different fuels. In this paper, the maximum concentration of OH during fuel combustion is selected as the object of research. It is analyzed in the same way using the relative change value of alcohol−gasoline and pure gasoline, $R_{OH} = (c_b - c_o)/c_o$. It can be seen from Figure 6 that most R_{OH} values are positive, indicating that blending methanol and ethanol is conducive to the formation of OH radicals during gasoline combustion overall, and the concentration of OH increases as the blending proportion of methanol and ethanol increases. At the same time, it is found that OH can be formed more efficiently in a lean fuel state, and an increase in initial temperature also contributes to the formation of OH when the fuel blends is burned. With the rise in pressure and equivalence ratio, the increase rate of OH slows down; however, in the state of high pressure, low temperature, and rich fuel, it is found that methanol and ethanol inhibit the formation of OH with a relatively low effect, as shown in Figure 6c.

The flame speed can guarantee combustion stability and ensure that the engine can output higher power. This paper presents the effects of alcohols by the difference in flame speed between six kinds of alcohol-blended gasoline fuels and gasoline, $\Delta S = S_b - S_o$. At pressures of 1, 5, and 10 atm, temperatures of 298 and 400 K, and an equivalence ratio of 0.7−1.5, the laminar flame speed and CO emission of different fuels are simulated with the results being shown in Figures 7 and 8. Detailed simulation results are provided in Table S4 of the Supporting Information. It is found that the effects of alcohol fuels on the combustion rate of gasoline are also affected by factors such as pressure and equivalence ratio. As can be seen from Figure 7a,b, when the initial pressure is low, the blending of methanol and ethanol can increase the flame speed of gasoline. This effect is more evident in the vicinity of the stoichiometric ratio of fuels. Figure 7c−f shows that, with the increase in pressure, the blending of methanol and ethanol

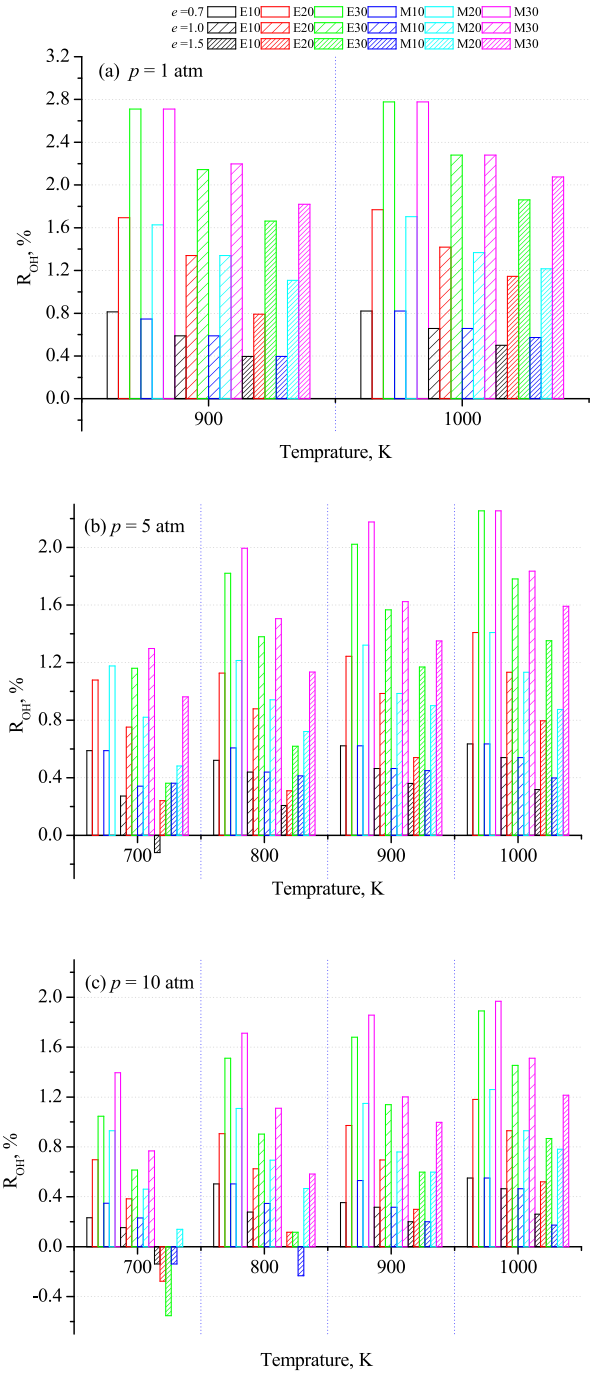

Figure 6. Comparison of OH concentration during combustion of different fuels at (a) p = 1 atm, (b) p = 5 atm, and (c) p = 10 atm.

reduces the flame speed of gasoline, and this effect is more obvious with the increase in blending proportion. It is also found that, when the equivalent ratio of fuel blends is large, methanol still has a positive effect on the combustion rate of gasoline. Generally speaking, ethanol has a more significant inhibitive effect on the combustion rate of gasoline than methanol. The main reason is that the laminar flame velocities of ethanol and methanol show diametrically opposite trends with different equivalence ratios. When the fuel is lean, the laminar flame speed of ethanol is slightly higher than that of methanol as a whole, and values are basically the same when approaching the equivalent ratio. However, when the fuel is rich, the combustion speed of methanol is significantly higher

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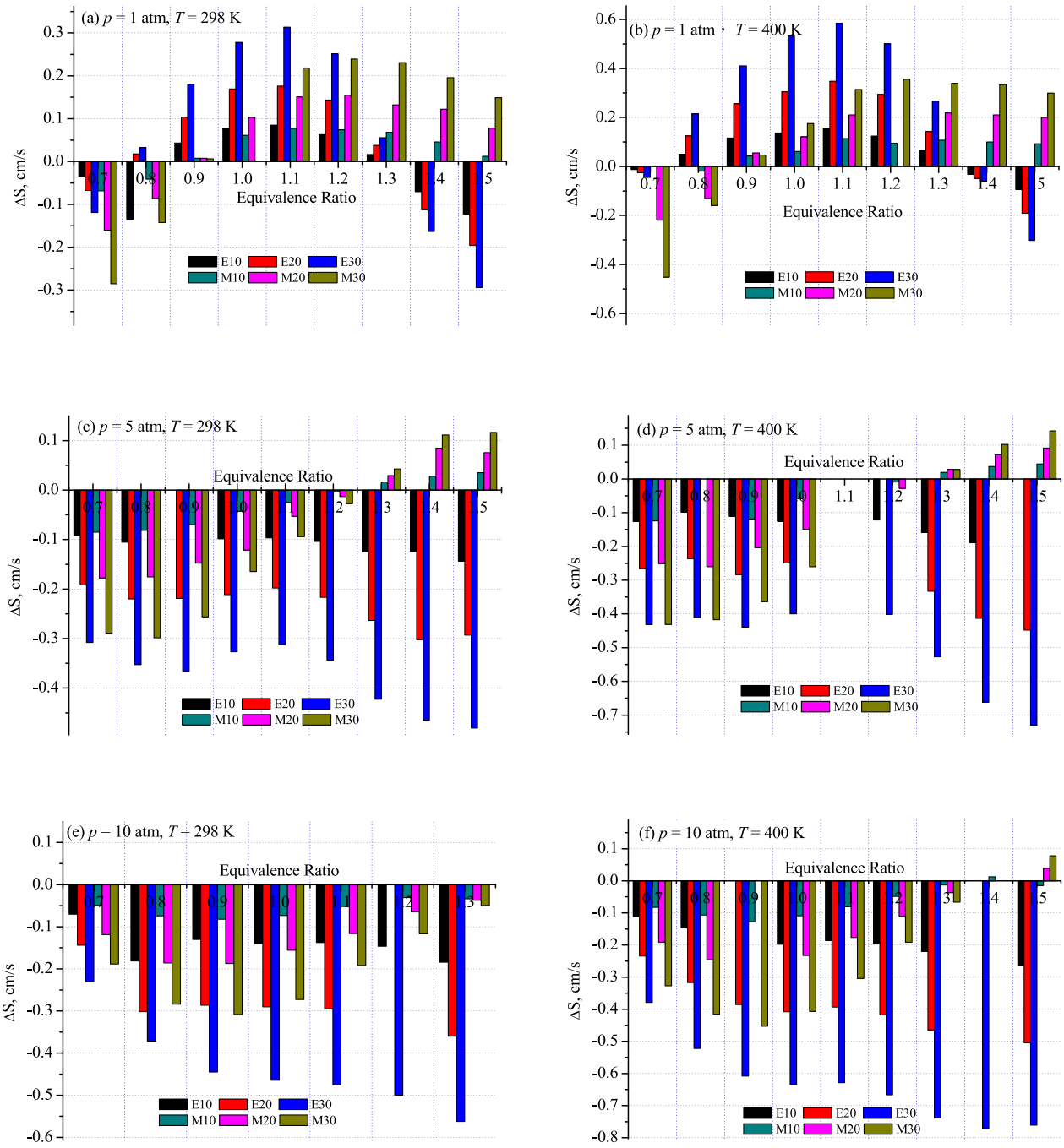

Figure 7. Comparison of laminar flame speed of different fuels at (a) p = 1 atm and T = 298 K, (b) p = 1 atm and T = 400 K, (c) p = 5 atm and T = 298 K, (d) p = 5 atm and T = 400 K, (e) p = 10 atm and T = 298 K, and (f) p = 10 atm and T = 400 K.

than that of ethanol. Because of the negative correlation of laminar flame speed and pressure, the inhibitory effect of ethanol on gasoline combustion rate is more obvious at 5 and 10 atm. Therefore, methanol can still accelerate the combustion rate of gasoline under rich fuel states. So overall, ethanol is inferior to methanol in terms of flame speed, which is similarly described in a previous study.[40]

3.2. Emission of Combustion Pollutants. Pollutant emission is also an important characteristic of fuel combustion and a relatively demanding standard for utilizing fossil fuels. In this paper, the CO emission in the premixed laminar combustion process of seven fuels, including gasoline and alcohol−gasoline, is selected as the target. Simulation results are provided in Table S5 of the Supporting Information. The relative variation of CO, R_{CO} = $(EICO_b - EICI_o)/EICO_o$, is also used to analyze the effect of blending of methanol and ethanol on CO emission from gasoline combustion. The results are shown in Figure 8. As can be seen from Figure 8, most of the R_{CO} values are negative, indicating that the blending of methanol and ethanol effectively inhibits the CO generation during gasoline combustion and reduces the CO emission from fuel combustion. Especially in the rich fuel state, the inhibitive effect of methanol and ethanol on CO emission is the most prominent. In addition, by comparing the R_{CO} at each equivalence ratio, it is found that ethanol has a stronger ability to reduce the CO emission from gasoline combustion

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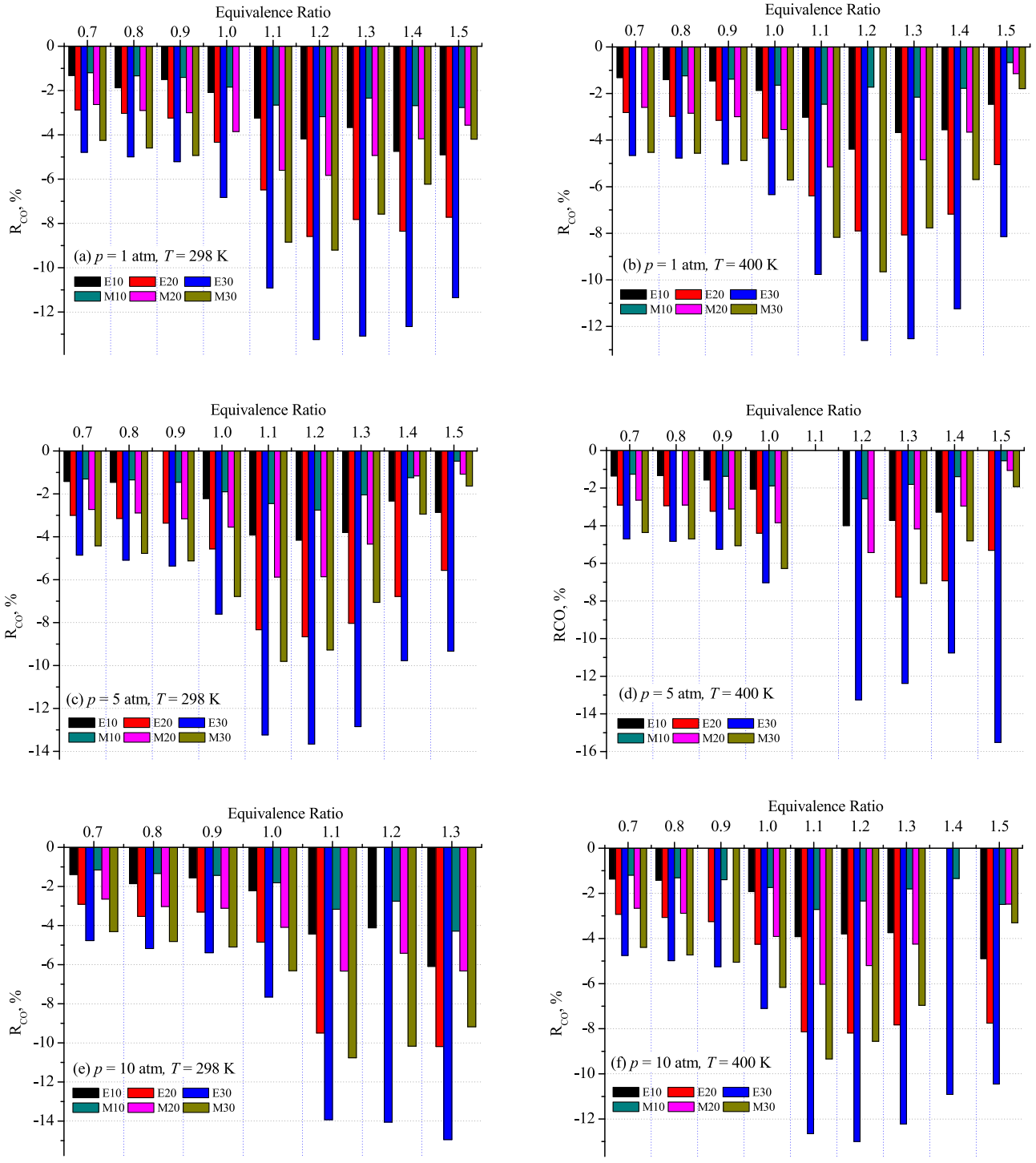

Figure 8. Comparison of CO emissions during combustion of different fuels at (a) p = 1 atm and T = 298 K, (b) p = 1 atm and T = 400 K, (c) p = 5 atm and T = 298 K, (d) p = 5 atm and T = 400 K, (e) p = 10 atm and T = 298 K, and (f) p = 10 atm and T = 400 K.

than methanol. With the increase in equivalence ratio, the ability of ethanol to inhibit the CO emission is more advantageous than that of methanol. The main reason is that the laminar flame speed of methanol is significantly higher than that of ethanol under the oil-rich state; therefore, the combustion rate of methanol−gasoline will be significantly higher than that of ethanol−gasoline under rich fuel states. However, due to the serious lack of oxygen, the accumulation of CO during the combustion of methanol−gasoline will be greater than that of ethanol−gasoline. It can thus be concluded that ethanol is superior to methanol in suppressing gasoline CO emissions. Similar results are also shown in refs 45 and 46.

3.3. Combustion Stability. The extinction strain rate is an important parameter to characterize the combustion stability of fuels. The extinction strain rate indicates the extent to which the flame is stretched; a higher extinction strain rate shows stronger tensile capacity and is most resistant to extinction,[47,48] which leads to better combustion stability of fuels. Therefore, a higher extinction strain rate leads to better combustion stability of fuels. In this paper, a systematic simulation of the diffusion

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combustion of seven fuels is conducted at 1 atm and 10 cm/s as well as 10 atm and 1 cm/s at the temperature of 300 K, where 10 and 1 cm/s represent the injection velocities of fuel and oxidant in a diffusion opposed-flow flame. The results are shown in Figure 9a,b, respectively. In general, the blending of

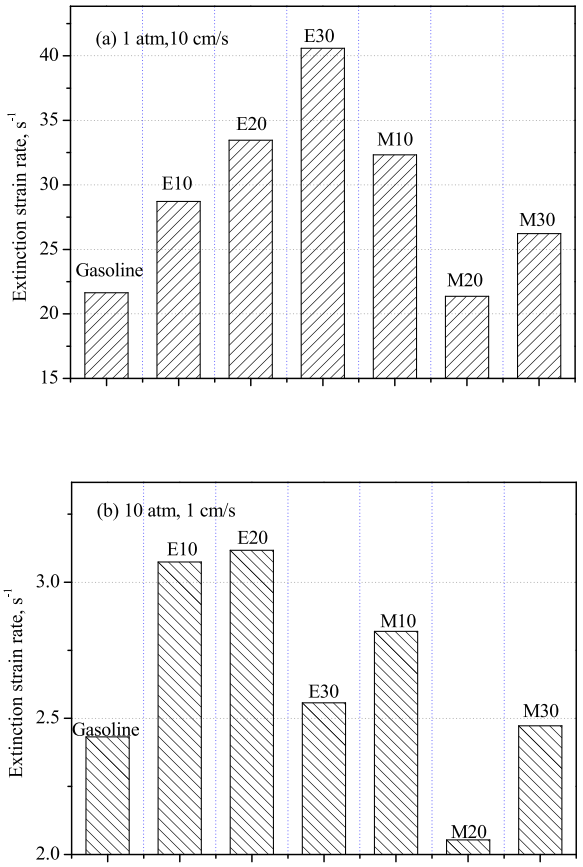

Figure 9. Comparison of extinction strain rates of different fuels at (a) 1 atm and 10 cm/s and (b) 10 atm and 1 cm/s.

methanol and ethanol can improve the extinction strain rate of gasoline and increase the stability of fuels. The effect of ethanol on gasoline is more potent than that of methanol. The increase of ethanol in the blended mixture is more favorable for the combustion stability of fuels; however, methanol shows an opposite result, and when the blending proportion of methanol is 20%, it is more unfavorable for the combustion stability of gasoline.

4. QUANTITATIVE CHARACTERIZATION AND VERIFICATION OF THE EXTENT OF EFFECTS OF METHANOL AND ETHANOL

4.1. Quantitative Characterization Based on the Variation Disturbance Method. The return value of the δ function defined in this paper is mainly judged based on the S_i value under different operating conditions. The correspondence between them is determined based on the combustion characteristics of fuels and the requirements of combustion engineering. If the ignition delay of fuel is as short as possible and the emission during combustion is as low as possible, and if the corresponding S_i value is less than 0, the effect at this time is positive, and the δ function returns to +1; if the S_i value is greater than or equal to 0, the δ function is −1 or 0, respectively. Similarly, for the adiabatic flame temperature of the fuel, if a blending component can increase the flame temperature, the effect is considered to be positive, and the corresponding S_i should be greater than 0. In this case, the δ function is +1. In general, the δ value will not be 0 because, if other fuels or blending agents are added to the primary fuel, these blending agents will generate a disturbance to the combustion characteristics of the primary fuel under the effect of their heat, kinetics, or only dilution capability so that the S_i value is not 0. In this paper, the relationship of δ function when it is +1 at each combustion characteristic S_i is shown in Table 2, and δ is −1 when it is contrary to its constraint conditions.

Table 2. Constraint Conditions When the Return Value of the δ Function Is +1 at Different Combustion Characteristics

combustion performance	δ_i	S_i
ignition delay time	+1	<0
adiabatic flame temperature	+1	>0
component concentration	+1	>0
laminar flame speed	+1	>0
emission index (CO)	+1	<0
extinction strain rate	+1	>0

After the δ function is determined, the weight ω_i and disturbance d_i in the extent of effects of methanol and ethanol on gasoline combustion performance at the i-th combustion characteristic are calculated respectively based on all the simulation data of the six fuel characteristics simulated by this working system and as per formulas 3 and 4 in this paper, and the total disturbance ratio D of ethanol and methanol is calculated in combination with formula 1. The results are shown in Table 3. It can be seen from the table that the overall effects of ethanol and methanol on the combustion characteristics of gasoline are positive. Besides some adverse effects on the ignition temperature and flame speed, other combustion characteristics of gasoline are obviously promoted. For the ignition delay, the performance disturbance value of ethanol on gasoline self-ignition reaches 0.5443, indicating that ethanol can accelerate the rapid ignition of gasoline overall; the disturbance value of methanol is −0.073, reflecting that methanol is disadvantageous to gasoline self-ignition, but its effect is not apparent. The effects of ethanol and methanol on promoting the formation of OH are similar and very positive, with disturbance values above 0.32. In addition, the effect on the emission of ethanol combustion pollutants is significant, and the disturbance values of the two are 0.3780 and 0.2390, respectively. This indicates that the CO emission during combustion is significantly reduced by the blending of the two. At the same time, the extinction strain rate also increases along with the mixing of ethanol and methanol, and the disturbance values of the two reach 0.5592 and 0.2351, respectively, indicating that the blending of ethanol and methanol enhances the combustion stability of gasoline. It should be noted that the blending of ethanol and methanol is unfavorable for the adiabatic flame temperature and laminar combustion rate of alcohol−gasoline, and the disturbance values of the two are negative. Ethanol especially has a noticeable inhibitive effect on the combustion rate of gasoline, and its disturbance value reaches −0.6158. The total disturbance value of ethanol to gasoline is 0.8493, while the disturbance value of methanol is 0.2605. The former is 3.26 times higher than the latter.

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Table 3. Variation Disturbance Values of Ethanol and Methanol

	ethanol				methanol			
combustion performance	δ_i	ω_i	d_i	D_i	δ_i	ω_i	d_i	D_i
ignition delay time	+1	0.9300	0.5853	0.5443	−1	0.0700	1.0426	−0.0730
adiabatic flame temperature	−1	0.5777	0.5966	−0.3447	−1	0.4223	0.5977	−0.2524
component concentration (OH)	+1	0.4676	0.7020	0.3283	+1	0.5324	0.6226	0.3315
laminar flame speed	−1	0.7674	0.8025	−0.6158	−1	0.2326	0.9441	−0.2196
emission index (CO)	+1	0.6066	0.6233	0.3780	+1	0.3934	0.6075	0.2390
extinction strain rate	+1	0.7666	0.7294	0.5592	+1	0.2334	1.0075	0.2351
total (D)				0.8493				0.2605

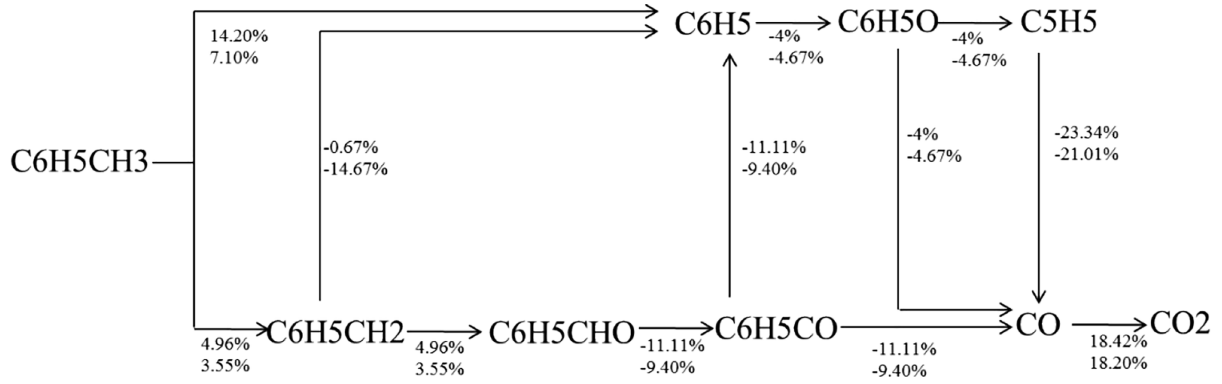

Figure 10. Combustion reaction path of toluene.

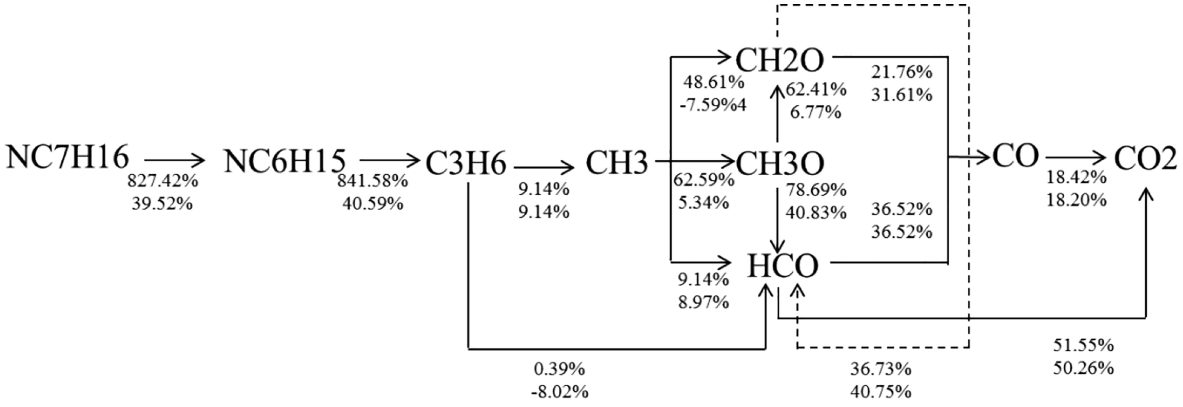

Figure 11. Combustion reaction path of *n*-heptane.

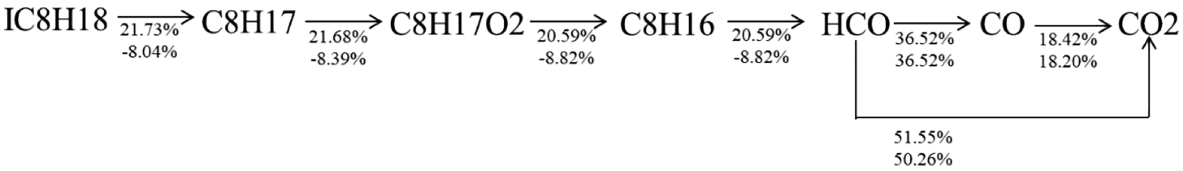

Figure 12. Combustion reaction path of iso-octane.

Therefore, the results show that ethanol is more favorable for gasoline combustion.

4.2. Chemical Hierarchy and Verification of Fuel Combustion. The combustion reaction path can intuitively reveal the fuel consumption path and critical reaction paths. It can be combined with the absolute rate of production (mol·cm^{-3}·s^{-1}) between components to provide a clear understanding of critical reactions that determine the change of component concentration. To better present the effects of ethanol and methanol blending on the combustion path, the ignition time of gasoline, E20, and M20 is selected as sampling points at 10 atm, the temperature of 1000 K, and the equivalence ratio of 1.0, and the reaction paths of three alternative components of gasoline, $C_6H_5CH_3$, NC_7H_{16}, and IC_8H_{18}, are analyzed based on C element tracing. To reveal the extent of effects of ethanol and methanol on the reaction paths of important components of gasoline more directly, the ROP of these components is quantitatively characterized based on the relative change rate of the rate of production of alcohol−gasoline components (ROP_b) and the rate of production of pure gasoline components (ROP_o). The calculation formula is $R = [(ROP_b - ROP_o)/ROP_o] \times 100\%$. If the value is greater

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than 0, it indicates that the blending of ethanol and methanol into gasoline promotes the reaction path of gasoline. The two percentage values between the alternative components of gasoline in Figures 10−12 represent the change rates of E20 and M20 relative to gasoline, respectively.

As can be seen from Figure 10, there are mainly two reaction channels for the consumption of toluene in this condition: In the first channel, toluene generates $C_6H_5CH_2$ through reactions $C_6H_5CH_3 + O_2 = C_6H_5CH_2 + HO_2$ and $C_6H_5CH_3 + OH = C_6H_5CH_2 + H_2O$, while in the other channel, the methyl group in toluene breaks off directly with the benzene ring to form C_6H_5 and CH_3; the first reaction channel occupies a more significant proportion. The addition of ethanol and methanol has a positive effect on both reaction channels of toluene, and the relative change rate of production is positive, especially for $C_6H_5CH_3 = C_6H_5 + CH_3$. However, methanol and ethanol show negative increments to their reaction channels in the following hierarchical structure, and their effects are almost the same. Still, in the last channel for CO to generate CO_2, the two have a positive impact again.

Figure 11 shows the combustion reaction path of *n*-heptane. The results also show that ethanol has a more prominent effect than methanol. Ethanol contributes 827.42 and 841.58% to $NC_7H_{16} \rightarrow NC_7H_{15}$ (mainly based on the reaction $NC_7H_{16} + OH = NC_7H_{15} + H_2O$) and $NC_7H_{15} \rightarrow C_3H_6$ (mainly based on the reaction $NC_7H_{15} = C_3H_6 + C_2H_5 + C_2H_4$), respectively, in the reaction path of *n*-heptane, about 20 times higher than that of methanol. In the following reaction paths, ethanol also exhibits a positive effect on each reaction channel better than methanol, indicating that ethanol blending can effectively accelerate the reaction rate of straight-chain p in gasoline.

Figure 12 shows the relative variation of the effects of ethanol and methanol on the reaction path of iso-octane during gasoline combustion. It is also found that ethanol blending is favorable for iso-octane consumption, while methanol inhibits the early reaction channel of iso-octane. This is contrary to the effect of methanol on the combustion of toluene and *n*-heptane. Moreover, the same phenomenon is present in multiple reaction channels, including $IC_8H_{18} \rightarrow C_8H_{17} \rightarrow C_8H_{17}O_2 \rightarrow C_8H_{16}$. Ethanol promotes the reaction channels above by more than 20%, while methanol slows down the reaction channels with an obvious inhibitive effect and an average relative change rate below −8.0%.

By analyzing the combustion reaction paths of the three alternative components above, the effects of methanol and ethanol on the reaction paths of important components in gasoline are positive, but ethanol is more superior. This is in accordance with the disturbance values of ethanol and methanol to gasoline combustion in Section 4.1 of this paper, indicating that the quantitative characterization of the effects of combustion characteristics on fuel blends is effective.

5. CONCLUSIONS

This paper proposes a new variation disturbance method to provide a practical approach and evaluation method for combustion design and quantitative characterization of the effects of blending agents on fuel combustion performance. With this method, it is more convenient to quantify the extent of effects and compare the effects of different blending agents on the combustion of primary fuels. The effects of methanol and ethanol on gasoline combustion performance are systematically studied in a wide range of operating conditions. It is found that alcohol−gasoline formed by blending methanol and ethanol has a slightly lower adiabatic flame temperature than pure gasoline, and the maximum value of its temperature sacrifice is less than 0.6% in all operating conditions; however, alcohol−gasoline is obviously superior to gasoline in terms of self-ignition time, fuel combustion rate, extinction strain rate, and CO emission and contributes to rapid, stable, and clean combustion of gasoline, especially to CO emission reduction. Based on the calculation of the variation disturbance method, the total disturbance values of ethanol and methanol to the gasoline combustion process are 0.8493 and 0.2605, respectively. This indicates that ethanol has a more significant comprehensive effect on gasoline combustion performance than methanol. Also, according to the definition and calculation results of the variation disturbance method, ethanol plays a more active role in gasoline combustion. With the increase of ethanol added to the mixture, a more significant role in improving combustion performance and reducing emissions is played—it can reduce CO emission by nearly 16% during gasoline combustion. In addition, the combustion reaction paths of alternative gasoline components are traced based on C elements. It is also found that the blending of ethanol enlarges the combustion reaction channels of these alternative components and accelerates their reaction process. This also demonstrates the rationality of the method proposed in this paper. Next, relevant experimental studies will be carried out, and expanded validation of the method will be conducted based on the experimental data of the system. In conclusion, ethanol is more suitable for blending with gasoline to produce ethanol−gasoline to solve the problems of energy crisis and environmental protection caused by fossil fuels and can provide support for the sustainable application and promotion of alcohol−gasoline. The research in this paper enriches the analytical methods of chemical kinetics. Applying the new variation disturbance method can also provide comprehensive and valuable guidance for fuel design and combustion chamber optimization.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.2c00991.

Simulation results of gasoline and blended fuel combustion (PDF)

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Author Contributions

S.-h. Li carried out the conceptualization, provided the methodology, and wrote the original draft of the manuscript. P. Fang, X. Guo, and Z. Wang provided the resources. S. Xi, S. Li, and Y. Li provided the software. J. Hou and Z. Wen carried out the conceptualization.

Notes

The authors declare no competing financial interest.

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