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A composite-fuel additive design method for n-decane low-temperature ignition enhancement

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ABSTRACT

It is challenging to efficiently ignite traditional liquid hydrocarbons when they are applied in extreme combustion conditions, e.g., scramjet combustor. In this study, the low-temperature ignition enhancement performance of fuel additives of various properties and concentrations in n-decane were investigated theoretically and experimentally. The theoretical results indicate that there exists an optimized relationship between the effective activation energy and vaporization rate. Based on the optimization study, a novel design method for composite fuel additives was proposed. With this method, a metallic organic compound blended with a low-boiling-point auxiliary, methoxydiethylborane/tetrahydrofuran (MDEB/THF) solution, was employed to modify the ignition performance of n-decane. Thermogravimetry analysis and droplet-hot plate impinging experiment were performed to characterize the vaporization rate, ignition temperature, and ignition delay time of n-decane-based hybrid fuels. The experimental results suggest that, at a high concentration of MDEB/THF fuel droplets, the minimal ignition surface temperature is reduced to 160 °C, which is approximately 500 °C lower than that of pure n-decane. The ignition delay time of the fuel droplet is diminished from 353 ms to 45 ms at a surface temperature of 500 °C. Moreover, controlling the low-temperature ignition performance of an n-decane-based hybrid fuels by mixing various proportions of the additive was confirmed to be feasible. The results obtained from this study are of great significance in jet propellant design.

1. Introduction

Although hydrogen is a promising fuel for a scramjet engine, liquid hydrocarbon fuels are attractive in terms of their low cost and ease of handling and operation [1]. Reliable ignition remains an outstanding issue in a scramjet combustor owing to the discrepancy between the fuel ignition delay time (τ_{ig}) and the residence time (τ_{res}) for liquid hydrocarbons, especially at a low flight Mach number. Conventional methods to insure τ_{ig} is shorter than τ_{res} include (i) generating a recirculation zone in the high-speed flow by using embedded cavities [2] and incident shock waves [3], and (ii) ignition augmentation such as the use of plasma ignitors [4]. The disadvantages in the use of these approaches, such as drag penalty [5] and complex operation systems, are unavoidable. As a result, highly inflammable fuels with a reduced ignition delay time as well as sufficient burning rate at low temperatures are required. A potential means of further improving the low-temperature ignition and combustion performance of liquid hydrocarbons is using additives.

Metallic oxide powders play a non-fungible position in the low-temperature catalytic combustion of gaseous hydrocarbons [6]. In order to enhance the low-temperature ignition and burning properties of traditional liquid aviation fuels, the addition of metallic nanoparticles is a possible method to achieve a high-energy density and can alter their initial thermophysical properties such as thermal conductivity, mass diffusivity, radiative heat transfer, and surface tension [7]. Moreover, owing to their high specific surface area, metallic nanoparticles display increased catalytic activity, reduced ignition delay times, and higher burning rates than micron-sized particles [8]. The burning characteristics of fuel droplets containing nano-sized aluminum, boron, and iron particles were investigated by Gan et al. [9,10]. Their studies emphasize on the combustion behaviors of the droplets and the corresponding mechanisms while only rarely mentioning the ignition and combustion enhancement obtained by adding metallic particles. Javed et al. [7,11–13] studied the evaporation, auto-ignition, and combustion characteristics of liquid hydrocarbon-based nano-fluid droplets at elevated temperatures. The results indicate that the reduction in the ignition delay time with increasing temperature depended on the loading of nanoparticles in the heptane droplet. The addition of 0.5% Al nanoparticles to heptane result in ignition at 600 °C, which is not observed with stabilized heptane or 2.5% and 5.0%

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nano-Al/heptane droplets. The addition of dilute (0.1%, 0.5% and 1.0%) concentrations of Al nanoparticles lower the minimum ignition temperature of kerosene droplets to 600 °C at which the pure kerosene droplet of same initial diameter is not ignited. Agglomeration and cluster formation due to the high surface energy of the nanoparticles is the major drawback that restricts the applications of liquid hydrocarbon fuels with metallic nanoparticles as additives [7]. In addition, although it is possible to increase the hot-plate ignition probability by using suspended metallic nanoparticles in liquid diesel, the reduction in the minimum ignition temperature is less than 100 °C [14].

Homogeneous initiators are widely used in endothermic hydrocarbon fuels to increase the cracking rate at lower temperatures [15] and improve the heat sink capacity of the jet fuel [16]. Fundamental research on homogeneous fuel additives used to enhance the ignition of traditional liquid hydrocarbons effectively is rarely reported. Metal alkyls used with transition metal polyolefin catalysts are usually highly reactive with air and other oxidants [17]. Thus, triethylaluminum/triethylborane (TEA/TEB) is used in engineering applications as an ignition fuel in both high-speed air-breathing [18] and rocket engines [19] because of its pyrophoricity or hypergolicity. When metal alkyls like TEA/TEB are blended with liquid hydrocarbons, the solution ignites spontaneously when exposed to air if the concentration of the metal alkyls is denser than its nonpyrophoric limit [17]. Ryan et al. [20] had demonstrated that aluminum alkyls significantly reduced the overall ignition delay time and the ignition temperature of JP-10 in a constant-volume combustion apparatus. Therefore, using metallic organic compounds to promote the ignition of fuel is highly efficient and practical. It merits comprehensive fundamental investigations.

Based on these previous research works, the addition of metal alkyls significantly improves the ignition performance of traditional liquid hydrocarbons, which is a promising solution for high-performance supersonic ignition and combustion. Nevertheless, in order to realize satisfactory low-temperature ignition performance, pure metal alkyls are used or a high proportion of metal alkyls is added to the hydrocarbons; however, their practical applications may involve the disadvantages of safety concerns and the excessive generation of metallic oxides after the oxidization or combustion. Composite fuel additives containing metal alkyls and a highly volatile ignition auxiliary, which is more moderate than pure metallic organic compound, is a preferable solution. This is because phase change and ignition are essential procedures in the liquid-fueled combustion configuration. Accelerating the gasification of the liquid fuel contributes to reducing the ignition delay time and promoting the ignition. Theoretically, increasing the chemical reaction rate at a low temperature as well as enhancing the vaporization simultaneously would have synergistic effects on the ignition enhancement under extreme conditions. In the case of composite additives, the hybrid fuel would have superior operability with excellent low-temperature ignition properties. Unfortunately, the selection of the components and the determination of the amount of fuel additive have generally been based on experience to date instead of relevant theories.

The motivation of the present study is to comprehensively understand the essence of the effective activation energy and vaporization rate on low temperature ignition promotion, and thus provide significant evidence for the design and composition optimization of composite fuel additives. With the optimized relationship between the effective activation energy and vaporization rate, a novel homogeneous additive, 1:1 methoxydiethylborane/tetrahydrofuran (MDEB/THF) solution, was proposed. To characterize the effectiveness on low temperature vaporization and ignition enhancement, thermogravimetry analysis and hot-surface ignition experiments with hybrid fuel droplets were performed. The effects of the additive concentration on the vaporization rates, minimum surface temperatures for ignition, ignition probabilities, and ignition delay times are discussed.

2. A composite additive design method

2.1. Optimized relationship between activation energy and vaporization rate

For a liquid-fueled combustion system, oil is injected into the combustor as sprayed droplets. Ignition occurs in the gas phase region where the temperature and stoichiometric ratio are sufficient [21]. The physical and chemical processes both play critical roles in the ignition. A basic mechanism in spray combustion is vaporization rate of a liquid fuel droplet, which must be taken into account in design and optimization [7]. On the other hand, activation energy is also an important kinetic parameter for describing the oxidation and combustion reactivity [22]. Several research works [23,24] have concentrated on the effects of these two parameters on ignition. However, the effects of the interaction between the vaporization rate and activation energy on the low-temperature ignition have rarely been studied. Accordingly, the theoretical analysis described in this section is performed to investigate the mutual effect of the effective activation energy and vaporization rate on the ignition enhancement.

A fuel droplet impacting with a heated surface undergoes typical boiling, vaporization, and subsequent combustion in a matter of seconds [21,25–27]. It is a practical method for investigating the liquid fuel ignition characteristics. This combustion configuration is employed in the present study to fundamentally investigate the effects of the properties of the fuel additive and its concentration on the ignition characteristics of the hybrid fuel. The additive consists two components, each of which is employed to regulate the vaporization rate and activation energy of the hybrid fuel, respectively. In order to simplify the theoretical analysis, the following major assumptions are considered: (i) a constant volume combustor is employed; (ii) the hybrid fuel is completely homogeneous during gasification, and the gasification is independent of chemical reactions; (iii) the diffusion and mixing progress are ignored; (iv) chemical reactions only occur in the gas phase mixture; (v) no reactant depletion occurs until ignition; (vi) a one-step Arrhenius irreversible reaction $F + \nu_o O \rightarrow \nu_p P$ is assumed; (vii) all of the physical parameters, except the effective vaporization rate and activation energy, remain constant with varying temperature and additive concentration. Some of the above assumptions are classical and some need further explanation. For single droplet ignition, vaporization dominates the physical process because fuel vapor contacts sufficiently with air. Thus, only gasification time is taken into account and diffusion and mixing are ignored. Self-heating is one of the main factors for a low-surface-temperature ignition. In this model, the effect of self-oxidation is included in the effective activation energy term, and no gaseous fuel depletion occurs until ignition.

The Van't Hoff ignition criterion ($dT/dx = 0$ at wall), which has been widely used in many applications [28–30], is introduced to evaluate the occurrence of ignition. Some comparisons between the Van't Hoff and Semenov–Frank-Kamenetski criterion have been carried out [31]. To theoretically predict the hot surface ignition, the Van't Hoff criterion is precise enough. In the droplet-hot plate ignition configuration, when considering the gasification behavior, the ambient mole fraction of fuel is a transient value. It is proportional to the vaporization rate and vaporization time, which is not identical to that obtained in Ref. [32]. Focusing on this difference between pre-mixed and diffusion ignition, the steady-state Van't Hoff criterion has been modified in the present study. A transient Van't Hoff ignition criterion is obtained, and the time required for gasification to reach the minimum stoichiometric ratio sufficient