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Ignition of methane with hydrogen and dimethyl ether addition

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HIGHLIGHTS

- Ignition enhancement of CH_4 by H_2 and DME addition is studied.
- Different ignition enhancement trends are found for H_2 and DME addition.
- The kinetic effects and transport effects on the ignition enhancement are examined.
- The non-premix ignition is greatly affected by the mass diffusivity of each fuel.

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ABSTRACT

Premixed and non-premixed ignition of methane/hydrogen and methane/dimethyl ether (DME) binary fuel blends with hot air is studied through numerical simulation with detailed chemistry and variable thermodynamic and transport properties. The emphasis is spent on assessing the kinetic and transport effects involved in CH_4 ignition enhancement caused by H_2 and DME addition. Two configurations are considered: a premixed homogeneous configuration to examine the chemical kinetics and a non-premixed counterflow configuration to assess the transport effects. For the homogeneous ignition process, small amount of DME addition is found to be more effective than H_2 addition in terms of promoting the ignition of CH_4/air mixture. Sensitivity analysis and reaction path analysis are conducted and key elementary reactions involved in CH_4 ignition enhancement by H_2 and DME addition are identified. For the non-premixed ignition process, H_2 addition is shown to be always more effective than DME addition in terms of CH_4 ignition enhancement. It is found that the preferential mass diffusion of H_2 over CH_4 and that of CH_4 over DME have great influence on the local blending ratio at the ignition kernel, which controls the non-premixed ignition process. Therefore, non-premixed ignition of binary fuel blends is significantly affected by the mass diffusivity of each fuel component. Moreover, the effects of strain rate on the non-premixed ignition of CH_4/H_2 and CH_4/DME binary fuel blends with hot air are discussed.

1. Introduction

Due to the rapid increase in energy consumption and increasingly stringent emission regulations, it has become imperative to develop alternative fuels and high-efficiency, low-emission combustion devices [1]. As the cleanest fossil fuel, natural gas (NG) has huge reserves around the world [2]. Recently, natural gas has become one of the most promising alternative fuels because of its favorable chemical characteristics, such as high H/C ratio, large octane number [3], excellent knock resistance [4], and low emissions. However, due to its stable molecular structure, methane (the main component of natural gas) has some unfavorable burning properties such as long ignition delay time, low flame speed, low ignitability, and narrow flammability limit range, which pose great challenges for its utilization in combustion engines. An effective way to solve this problem is to add more reactive fuels such as hydrogen or dimethyl ether (DME) into natural gas to promote its ignition and combustion performance. Therefore, a thorough understanding of fundamental combustion properties of natural gas with hydrogen-like fuel addition is important for developing advanced NG-based combustion engines and corresponding operating strategies.

In the literature, there are many studies on the fundamental combustion properties of CH_4/H_2 or CH_4/DME binary fuel blends, including their ignition delay time [5–8], internal combustion engine (ICE) performance [9–12], laminar flame speed [13–19] and so on. For examples on ignition, Zhang et al. [7] conducted shock-tube experiments to measure the ignition delay time of lean $CH_4/H_2/Ar$ mixtures and they found that the ignition delay time of CH_4/H_2 binary fuel blends has complex dependence on

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pressure and there exists two-step transition in the global activation energy; Tang et al. [8] measured the ignition delay time of CH_4/DME over a wide range of temperature and pressure and the nonlinear effect of DME addition in ignition promotion was observed and interpreted through kinetic analysis. All the previous studies showed that both H_2 and DME addition can greatly promote the ignition of CH_4. Since the DME oxidation mechanism is totally different from that of H_2, it is expected that the ignition enhancement by adding DME to CH_4 is different from that by adding H_2 to CH_4. Moreover, the kinetics involved in the ignition enhancement should be different for H_2 and DME addition. Therefore, the first objective of this study is to compare different ignition enhancement behavior and identify the kinetics involved in ignition enhancement caused by H_2 and DME addition to CH_4.

Most of previous studies on the transient ignition process of CH_4/H_2 or CH_4/DME were conducted in a homogeneous system, in which only the chemical kinetics during ignition can be thoroughly examined. However, in practical combustion process, ignition usually takes place in non-homogeneous zones due to a lack of time for fully mixing of fuel and air. A laminar non-premixed counterflow configuration can provide a well-defined flow field in which the influence of strain rate, diffusive and convective transports, and their coupling effects with chemical kinetics on ignition can be examined [5,20–24]. For examples, Fotache et al. [22] investigated the forced ignition of CH_4/H_2 blends by hot counter-flowing air and three ignition regimes in terms of H_2 blending ratio were identified; Chen et al. [5] studied the transient ignition of CH_4/DME blends in non-premixed counterflow configuration and they found that the ignition enhancement by DME addition to CH_4 is strongly affected by the strain rate. Other studies using counterflow configuration include premixed ignition of H_2/air by Zheng et al. [23], non-premixed ignition of n-decane/toluene binary fuel blends by Dai et al. [20], and non-premixed ignition of methane with pulsed discharge by Sun et al. [24]. The non-premixed ignition is controlled not only by the chemical kinetics but also the transport of heat and mass. The ratio among the mass diffusivities of H_2, CH_4, and DME is about 6:2:1. Consequently, it is expected that due to the different transport properties, the non-premixed ignition of CH_4 is differently affected by H_2 addition and DME addition. As shown later, the preferential mass diffusion between different fuels in fact plays a very import role in non-premixed ignition. Therefore, the second objective of this study is to compare different ignition enhancement behavior and analyze the transport effects on non-premixed ignition enhancement caused by H_2 and DME addition to CH_4.

Premixed and non-premixed ignition of CH_4/H_2 and CH_4/DME binary fuel blends with hot air is numerically studied in the present work and the chemical kinetics and transport effects involved in the ignition are examined. In order to assess the kinetic effects involved in CH_4 ignition enhancement by H_2 and DME addition, we study the homogeneous ignition process of CH_4/H_2/air and CH_4/DME/air mixtures which is purely controlled by chemical kinetics. In order to examine the transport effects on the ignition of these binary fuel blends, the non-premixed counterflow configuration is employed to study the transient ignition process of CH_4/H_2 and CH_4/DME binary fuel blends with hot air. The rest of the paper is organized as follows. The numerical models and chemical mechanism are introduced in the next section. In Section 3, the homogeneous ignition process of CH_4/H_2 and CH_4/DME binary fuel blends is studied and the kinetic effects involved in CH_4 ignition enhancement by H_2 and DME addition are assessed. In Section 4, the non-premixed ignition process is investigated and the transport effects involved in ignition enhancement are examined using the non-premixed counterflow configuration. Finally, the conclusions are presented in Section 5.

2. Numerical models and chemical mechanism

Since the homogenous ignition process does not have mass or heat transport and is purely controlled by chemical kinetics, we study the adiabatic homogeneous ignition process at constant pressure so that the kinetics involved in CH_4 ignition enhancement by H_2 and DME addition can be revealed. Stoichiometric CH_4/H_2/air and CH_4/DME/air mixtures initially at $T_0 = 1400$ K and atmospheric pressure are considered and detailed chemistry is employed in simulation. The blending ratio, c, defined as the molar fraction of H_2 or DME in the binary fuel blends, changes from 0 (pure CH_4) to 1.0 (pure H_2 or DME).

In order to examine the transport effects, we study the non-premixed ignition in a counterflow configuration. The transient non-premixed ignition process is simulated using the code for unsteady counterflow flame [25]. The counter-flowing fuel jet is at 300 K and it consists of CH_4/H_2 or CH_4/DME binary fuel blends with the blending ratio of H_2 or DME in the range of $0 \leqslant c \leqslant 1$. The hot air jet is at 1400 K. The pressure is fixed to be $P = 1$ atm. The distance between the fuel and oxidizer exits is fixed at $L = 10$ cm. The initial temperature and species distributions are determined under a frozen flow constraint with all the reaction terms suppressed. At the beginning (i.e. $t = 0$ s), chemical reactions are allowed in the precalculated frozen flow field and the afterwards evolution of the reactive counterflow system is simulated. Potential counterflow is considered and thereby the strain rate, a, is given as input parameter in the initial frozen flow, defined as the global gradient of the axial velocity, namely $a = (u_L - u_R)/L$, with the subscripts L and R denoting the fuel (left) and oxidizer (right) jets, respectively. It is noted that increasing strain rate leads to the decrease of flow residence time within ignition kernel, which influences the ignition process in counterflow configuration. Similar procedures were used in previous studies [5,20,26].

In the literature there are few mechanisms that can accurately predict the ignition of both CH_4/H_2 and CH_4/DME binary fuel blends. Here we use the detailed chemical mechanism for DME oxidation developed by Zhao et al. [27]. It consists of 55 species and 290 elementary reactions and was validated against experimental data of ignition delay time from shock-tube, species profiles from flow-reactor, and laminar flame speeds from spherical- and stagnation-flame experiments for DME [27]. Since this DME mechanism contains the H_2 oxidation sub-mechanism developed by Li et al. [28], the ignition process of H_2 as well as DME can be well predicted by this mechanism. In the Supplementary Material we demonstrate that this mechanism against experiments can well predict the ignition delay time of CH_4/DME/air mixtures [8] and CH_4/H_2/air mixtures [7].

3. The homogeneous ignition process

The homogeneous ignition process is studied in order to compare different ignition enhancement behavior and to identify the kinetics involved in ignition enhancement caused by H_2 and DME addition to CH_4. Fig. 1 shows the ignition delay time, τ, of stoichiometric CH_4/H_2/air and CH_4/DME/air mixtures as a function of the blending ratio, c. The ignition delay time is defined as the time when the temperature exceeds its initial value by 400 K (i.e. $T = T_u + 400$ K = 1800 K). Other definitions based on the maximum temperature changing rate and the sudden rise in OH concentration are checked and the ignition delay times defined in different ways are nearly the same (the relative difference is within 2%, see Fig. 1 of Zhao et al. [29]). Fig. 1 indicates that both H_2 and DME addition can greatly reduce the ignition delay time of CH_4/air mixture. However, different enhancing trends are observed for these two additives: the logarithmic ignition delay time of