



Numerical study on the transient evolution of a premixed cool flame



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ABSTRACT

Cool flame due to low-temperature chemistry (LTC) has received great attention recently. However, previous studies mainly focused on cool flames in homogenous systems without transport or non-premixed cool flames in droplet combustion or counterflow configuration. There are only a few studies on premixed cool flames, and the transient initiation and propagation of premixed cool flames are still not well understood. In this study, the initiation, propagation and disappearance of one-dimensional premixed cool flames in dimethyl ether (DME)/air mixture is investigated through transient simulation considering detailed chemistry and transport. The premixed cool flame governed by LTC can be initiated by a hot spot. When the hot spot temperature is not high enough to directly trigger the high-temperature chemistry (HTC), only the LTC reactions take place initially and thereby a cool flame is first initiated. During the cool flame propagation, HTC autoignition occurs at the hot spot and it induces a hot flame propagating behind the cool flame. Therefore, double-flame structure for the coexistence of premixed cool and hot flames is observed. Since the hot flame propagates much faster than the cool flame, it eventually catches up and merges with the leading cool flame. A well-defined cool flame speed is found in this study. We investigate different factors affecting the cool flame speed and the appearance of hot flame. It is found that at higher equivalence ratio, higher initial temperature or higher oxygen concentration, the premixed cool flame propagates faster and the hot flame appears earlier. Three chemical mechanisms for DME oxidation are considered. Though these three mechanisms have nearly the same prediction of hot flame propagation speed, there are very large discrepancy in the prediction of cool flame propagation speed. Therefore, experimental data of premixed cool flame speed are useful for developing LTC.

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1. Introduction

Cool flame [1] is controlled by low-temperature chemistry (LTC) and it is closely related to the two-stage ignition behavior for fuels with negative temperature coefficient (NTC). Recently, cool flame has received great attention (e.g., [2–4] and references therein) due to the need for understanding LTC and for developing advanced internal combustion engines [5,6]. For example, for homogeneous charge compression ignition (HCCI) engines, one of the main challenges is the control of ignition timing and combustion rate. Understanding cool flame and LTC is helpful for ignition control in HCCI engines.

Cool flames can be observed in homogenous systems such as jet stirred reactors [7] and HCCI engines [8]. Combustion in homogeneous systems has no mass or heat transport and thereby is purely controlled by chemical kinetics. However, homogeneity

is difficult to be achieved in practice. Therefore, similar to hot flames, chemical reactions and transport might be strongly coupled in cool flames. To investigate the coupling between LTC and transport, previous studies mainly focused on non-premixed cool flames in droplet combustion (e.g., [9,10]) or counterflow configuration (e.g., [11–14]). There are only several studies on premixed cool flames, which are introduced in the following.

In a micro flow reactor with a controlled temperature profile, Oshibe et al. [15] first observed premixed cool flame in dimethyl ether (DME)/air mixture. They found spatially separated flames due to multi-stage oxidations of DME. Using similar type of micro flow reactor, Gao and Nakamura [16] experimentally studied the transition from a premixed cool flame to a hot flame in DME/air mixtures. They identified a limit in reactor temperature, above which cool flame behaviors dominate. Ju et al. [3] numerically investigated premixed cool flames in DME/O₂/O₃ mixtures and found that the existence of cool flames substantially extends the flammability limit. They proposed a modified flammability limit diagram including both hot and cool flames. As an extension of previous work at atmospheric pressure to elevated pressures, Ju [4] numerically

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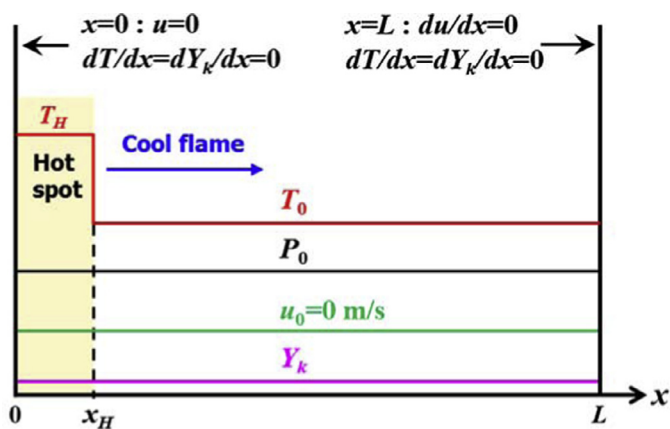


Fig. 1. Schematic of premixed cool flame initiated by a hot spot. The initial and boundary conditions are also shown.

examined the effects of pressure, mixture dilution, and heat loss on premixed cool flames in DME/O₂/N₂ mixtures. It was found that pressure significantly changes cool flame propagation and burning limits. Liang and Law [17] conducted numerical and theoretical investigation on the flammability limits of n-heptane/air mixtures by considering the cool flame chemistry. They also found that the flammability limit of the conventional high-temperature flame is greatly extended by the appearance of cool flames. Hajilou et al. [18] measured the premixed cool flame propagation speed of DME/O₂/Ar/O₃ mixture using a laminar flat flame Hencken burner. They identified two distinct cool flame stabilization modes in experiments: a burner-stabilized mode at low reactant flow rates, and a freely propagating mode at higher flow rates. In their modeling of high pressure spark assisted HCCI, Ju et al. [19] found double-flame structure consisting of a hot flame and a cool flame. Zhao et al. [2] studied the initiation and propagation of premixed cool flames for DME/O₂/N₂ mixtures in the 1D planar configuration and the counterflow configuration. They found that a residence time window exists for the occurrence of cool flames.

Except the studies of Ju et al. [19] and Zhao et al. [2], the transient initiation and propagation of premixed cool flames were not studied before. For the propagating 1D cylindrical [19] and planar [2] premixed cool flames, the residence time window is too narrow to be observed in experiments. The objective of this study is to investigate the transient evolution of a premixed cool flame whose residence time is longer enough to be observed in experiments. The initiation, propagation and disappearance of one-dimensional premixed cool flames in DME/air mixture is investigated through transient simulation considering detailed chemistry and transport. The premixed cool flame is initiated by a hot spot with proper temperature. The residence time for the occurrence of premixed cool flame is around 0.5 s, which is much longer than those reported in [2,19]. Therefore, such cool flame might be achieved in experiments. Different factors (the temperature and size of the hot spot, and the equivalence ratio, temperature and pressure of the fresh mixture, oxygen concentration) affecting the premixed cool flame propagation and the occurrence of hot flame are investigated. Besides, three chemical mechanisms are used to predict the transient evolution of a premixed cool flame, and the sensitivity of cool flame propagation speed to chemical model is demonstrated.

2. Numerical model

As shown in Fig. 1, we consider the one-dimensional premixed cool flame initiated by a hot spot with the temperature of T_H and size of x_H . Initially, static DME/air mixture is at the

specified equivalence ratio of ϕ and pressure of P_0 . The air consists of 21% O₂ and 79% N₂ (in volume) unless otherwise specified as in Section 3.2. The computational domain length is $L = 50$ cm. Reflective and outlet boundary conditions are used at $x = 0$ and $x = L$, respectively. Consequently, the pressure of the system, P_0 , remains to be constant. We set $\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K and $x_H = 2$ mm unless otherwise specified. The hot spot temperature of $T_H = 800$ K is not high enough to directly trigger the high-temperature chemistry (HTC). Consequently, only the LTC reactions take place initially and thereby a cool flame is first initiated.

The transient development of the cool flame is simulated using the code A-SURF (Adaptive Simulation of Unsteady Reactive Flow) [20–22]. Unless otherwise specified, the detailed chemistry for DME oxidation developed by Zhao et al. [23] is used in simulation. CHEMKIN packages [24] are incorporated into A-SURF to calculate chemical reaction rates and temperature-dependent thermal and transport properties. The mixture-averaged model is used to evaluate the mass diffusivities for different species. To accurately and efficiently resolve the propagating flame front, adaptive mesh refinement with the smallest mesh size of $32 \mu\text{m}$ is used. Grid convergence is achieved to ensure numerical accuracy. A-SURF has been successfully used in previous studies on ignition, flame propagation, and detonation development (e.g., [25–32]). The details on numerical schemes and code validation of A-SURF are shown in Refs. [20–22] and thereby are not repeated here.

3. Results and discussion

3.1. Transient development of a premixed cool flame

We first study the transient process of premixed cool flame initiation, propagation and disappearance. Figure 2 shows the distributions of temperature, DME mass fraction and heat release rate during the initiation and propagation of premixed cool and hot flames. At the beginning, the temperature at the center decreases due to heat conduction from the hot spot to the surrounding cold mixture. Meanwhile, LTC autoignition first occurs at the hot spot, which results in a premixed cool flame propagating to the right (lines #2 and 3 in Fig. 2). The fuel passing through the cool flame is only partially oxidized through LTC; and the cool flame temperature is only around 750 K. Then around $t = 580$ ms (line #4), thermal runaway due to HTC autoignition starts to occur at the center, which results in a premixed hot flame propagating from the center. The hot flame propagates behind the leading cool flame. Therefore, double-flame structure for the coexistence of premixed cool and hot flames is observed (lines #5–9). Two reaction zones are shown in Fig. 2(c) for the double-flame structure. The peak heat release rate for the hot flame is about three order larger than that of the cool flame. Since the hot flame is much stronger and faster than the cool flame, the hot flame catches up and merges with the cool flame. Finally, the cool flame disappears and only the single hot flame propagates to the right (line #10).

Figure 3 plots the flame trajectories and speeds of cool and hot flames. When the hot spot temperature is high enough, HTC is directly triggered. Consequently, only hot flame propagation is observed for $T_H = 1200$ K. For comparison, the results for single hot flame (corresponding to $T_H = 1200$ K) and coexistence of cool and hot flames (corresponding to $T_H = 800$ K) are plotted together in Fig. 3. For the double-flame case, the hot flame propagates much faster than the cool flame and thereby it can eventually catch up the leading cool flame. This is because the heat release and temperature rise at the hot flame front are much larger than those at the cool flame front (see Fig. 2). Around point A, the cool flame is accelerated due to the appearance of hot flame which induces large thermal expansion. The cool flame is in fact pushed by the thermal expansion from the hot flame. Besides, it is observed that

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