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Numerical simulations of premixed cool flames of dimethyl ether/oxygen mixtures

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ABSTRACT

The formation and dynamics of premixed cool flames are numerically investigated by using a detailed kinetic mechanism of dimethyl ether mixtures in both freely-propagating and stretched counterflow flames with and without ozone sensitization. The present study focuses on the dynamics and transitions between cool flames and high temperature flames. The impacts of mixture temperature, inert gas temperature, and ozone concentration on low temperature ignition, cool flame formation, and flammable regions of different flame regimes are investigated. For the freely-propagating flames, three different flame structures (high temperature flames, double flames, and cool flames) are found. The present study shows that the flammability limit of dimethyl ether is significantly extended by the appearance of cool flames and that the conventional concept of the flammability limit of a high temperature flame ought to be reconsidered. Furthermore, the results demonstrate that the cool flame propagation speed can be significantly higher than that of near-limit high temperature flames and that ozone addition dramatically accelerates the formation of cool flames at low temperatures and extends the flammability limit. A schematic of a modified flammability limit diagram including both high temperature flames and cool flames is proposed. For stretched counterflow flames, the results also show that multiple flame regimes exist with and without ozone addition. It is demonstrated that at the same mixture enthalpy, ozone addition kinetically extends the cool flame extinction limit to a higher stretch rate. Moreover, with ozone addition, two different cool flame transition regimes: a low temperature ignition transition and a direct cool flame transition without an ignition limit at higher temperature, are predicted. The present results suggest that cool flames can be an important combustion process in affecting flammability limits and flame regimes as the mixture temperature, turbulent mixing, and radical production/recirculation are increased. The results also provide guidance in observing self-sustaining premixed cool flames in experiments.

1. Introduction

Cool flames have long been considered a key process responsible for engine knock and are also an important phenomenon for fire safety [1–6]. Since the first discovery of cool flames two centuries ago [7,8], extensive efforts have been made to observe cool flames by using various flame geometries including heated surfaces and heated burners [8–11], stirred reactors [12–14], heated flow reactors [1,8,15–17], rapid compression machines [18], counterflow flames [19], droplets [6,20,21], and plasma-assisted flames [22,23]. Despite that many of the observed cool flames were oscillatory, transient, and strongly affected by flame-surface interaction, insights into cool flame spectroscopy, negative temperature coefficient (NTC) chemistry, heat release, and the cool flame peninsula in the temperature/pressure domain were obtained [12,14]. Nevertheless, few studies have been carried out on cool flame dynamics, extinction, and flammability limits. Much of our knowledge today about flame propagation speeds, flame structures, extinction limits, and flammability limits is still limited to high temperature flames [24]. Due to the difficulty in establishing self-sustaining cool flames, a detailed and fundamental understanding of cool flame dynamic behaviors has not been well established.

Recently, a self-sustaining n-heptane cool diffusion flame was experimentally observed for the first time by using ozone sensitization in a counterflow flame over a broad range of flow residence times [19]. The flame structures and extinction limits were quantitatively measured in this study. The results showed that ozone addition extended the flammable region of cool flames and allowed self-sustaining cool flames to be observed on a laboratory flame scale. In other studies, Law and Zhao numerically modeled the NTC effect on n-heptane/air ignition in a diffusion counterflow flame [25]. Their results demonstrated the existence of NTC-affected ignition. In

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n-heptane droplet combustion experiments, Nayagam et al. [6] reported the dual modes of combustion and extinction and presented a hypothesis of cool flame formation in a microgravity environment. In a related n-heptane droplet study, Farouk et al. [21] numerically modeled oscillatory cool flames governed by radiation heat loss and conductive heat loss from flame to droplet. However, the above studies were all limited to diffusion flames.

For premixed cool flames, Maruta and coworkers recently [16,17] studied the stabilization limits of cool flames by using a burner-heated microchannel. Unfortunately, in this geometry the wall temperature gradient and flame-wall coupling strongly dictate the flame stability, making it difficult to address how fast a cool flame can propagate and what the relation is between the flammability limits of high temperature flames and cool flames.

With the expected increases in pressure and initial mixture temperature in future engines, there is a chance that cool flames could not only affect engine knocking [4,5] but also influence heat release rates via turbulence-chemistry interaction. In a previous numerical simulation of spark-assisted homogeneous charge compression ignition (HCCI) [26], unsteady cool flame propagation was observed. In a recent study of low temperature turbulent combustion by using a reactor-assisted turbulent slot (RATS) burner [27], it was demonstrated that low temperature ignition and cool flame chemistry significantly changed turbulent flame speeds and structures.

Unfortunately, the previous studies on flame speeds, extinction limits, and flammability limits for stretched and unstretched flames were often limited to high temperature flames. It was not revealed how fast a cool flame could propagate compared to the high temperature flames, whether it burned leaner than a high temperature flame, or how mixture temperature and radical addition affected its extinction and flammability limits [37].

Motivated by the above discussions, the goal of this study is to simulate numerically the formation of premixed cool flames for both freely-propagating and stretched counterflow flames by using a detailed kinetic mechanism of dimethyl ether/oxygen mixtures with and without ozone sensitization. First, we investigate the propagation speeds, structures, and flammability limits of dimethyl ether/oxygen cool flames and high temperature flames. The effects of mixture temperature and ozone addition on the flammability limits of and transitions between high temperature flames and cool flames are examined, and a schematic of a new flammability diagram including both high temperature flames and cool flames is presented. Flame structures, reaction pathways, and the sensitivity of different flame regimes to transport properties are discussed. Second, we simulate the formation of stretched counterflow cool flames. Different flame regimes are investigated, and the effects of inert gas temperature on the flammable region of cool flames and the transition to cool flames through ignition are examined. Finally, we discuss possibilities for experimental observations of premixed cool flames in the counterflow geometry.

2. Numerical models

In this study, we consider both the one-dimensional freely-propagating premixed flame and the stretched counterflow premixed flame geometries (Fig. 1a and b). The freely-propagating flame is employed to predict the propagation speeds and the flammability limits of cool flames and high temperature flames (HTF). The counterflow flame is computed to understand the flammable region of cool flames in relation to flame stretch and to provide guidance for future experimental studies. Note that for some cool flame computations, the downstream computation domain is changed to 1.5 cm to save computational time.

Dimethyl ether (DME) is one of the simplest hydrocarbon fuels which possesses low temperature chemistry and whose kinetic mechanism has been widely investigated [28–31]. Thus, we have chosen DME as a representative of large hydrocarbon fuels with low temperature chemistry. In our previous diffusion cool flame study [19], it was found that ozone can promote the formation of diffusion cool flames. Therefore, for the purpose of providing experimental guidance and understanding how radical addition in turbulent mixing and plasma discharge affects cool flames, we use a mixture of $(1-x)O_2 + xO_3$ ($x = 0$–0.08) as the oxidizer. This formulation preserves the molar oxidizer/fuel ratio as ozone is added. The mixture temperature and ozone concentration are varied to examine the impact of initial reactant temperature and radical addition on cool flame formation. In the premixed counterflow flames, a heated nitrogen stream is used to stabilize the cool flame.

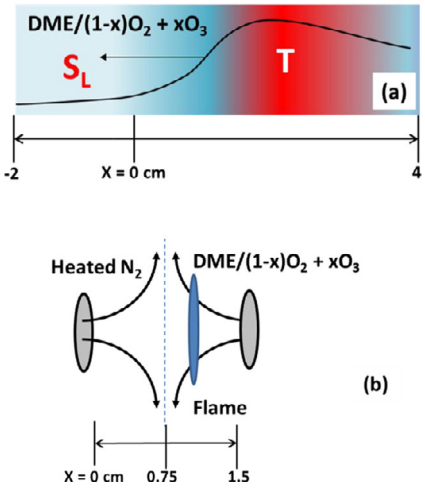

Fig. 1. (a) Schematic of freely propagation flame and (b) schematic of nitrogen stabilized premixed counterflow flame for DME/$(1-x)O_2 + xO_3$ mixtures.

For kinetic modeling of ozone decomposition, the elementary mechanism proposed by Ombrello et al. [32] with an update of the ozone decomposition rate [23] is used. For DME oxidation, the kinetic mechanism of Zhao et al. [31] with the recent update of C_0 and C_1 sub-chemistry as well as the DME decomposition reaction rate [29] is employed. Although this model has some over-prediction of low temperature fuel oxidation, it still able to qualitatively predict the dynamics of cool flames. In the radiation calculation, we used the optically thin radiation model for computational efficiency and simplicity. The Planck mean absorption coefficients are calculated for CH_4, CO_2, H_2O, and CO using the statistical narrow-band model found in [33]. The radiation from CH_2O and other intermediate species is neglected. For all calculations, the pressure is fixed at 1 atm. All steady-state solutions of unstretched freely-propagating flames and stretched counterflow flames are computed by using a revised version of the Chemkin II code [34] with an improved arc-length continuation method [33]. For the convergence criteria, the relative and absolute errors of all species mole fractions and temperature are, respectively, 10^{-4} and 10^{-9}.

3. Numerical results

3.1. Flame structure and flame regimes of freely-propagating premixed cool flames

We first examine the effects of reactant temperature on the flame regimes of freely-propagating premixed DME/O_2 flames. Figure 2a shows the dependence of the maximum flame temperature on the equivalence ratio. At an unburned mixture temperature of $T_0 = 300$ K, the flame temperature decreases with decreases in the equivalence ratio (Φ). At a critical equivalence ratio ($\Phi = 0.0785$), the maximum flame temperature becomes so low ($T_f = 1160$ K) that the important high temperature chain-branching reactions (such as $H + O_2 = OH$