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Numerical study on the transient evolution of a premixed cool flame

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ARTICLE INFO

Article history: Received 25 July 2017 Revised 29 August 2017 Accepted 8 September 2017

Keywords: Premixed cool flame Low-temperature chemistry Propagation speed Dimethyl ether

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 coexistance 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 inverstigate 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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Combustion and Flame

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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

* Corresponding author. E-mail addresses: cz@pku.edu.cn, chenzheng@coe.pku.edu.cn (Z. Chen). 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

http://dx.doi.org/10.1016/j.combustflame.2017.09.009

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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 hightemperature 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 $32 \,\mu$ 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 autoingiton 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 coexistance 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. Finnaly, 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 comparion, the results for single hot flame (correponding to $T_H = 1200$ K) and coexistance of cool and hot flames (correponding 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



Fig. 2. Temporal evolution of (a) temperature, (b) fuel mass fraction, and (c) heat release rate distributions during premixed cool and hot flames propagating in DME/air mixture with $\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm. The time sequence for lines #1–10 is 0, 200, 400, 580, 592, 598, 604, 610, 615, 620 ms.

the hot flame after the cool flame has much larger propagation speed than the single hot flame (i.e., to compare the red line with the black line in Fig. 3b). This is because after the cool flame, fuel is partially oxidized and the temperature increases by about 250 K as shown in Fig. 2. Such decrease of global activation energy and increase of the initial temperature both make the hot flame to propagate faster. After the hot flame catches up the leading cool flame (around point B in Fig. 3), the hot flame deaccelerates and eventually propagates at the same speed as the single hot flame (point C in Fig. 3b).

Figure 4 shows the distributions of temperature and mass fraction of major and minor species in the double-flame structure. At the cool flame front around x = 11 cm, DME is partially oxidized through LTC reactions $\text{CH}_3\text{OCH}_3 + \text{O}_2 = \text{CH}_3\text{OCH}_2 + \text{HO}_2$ and $\text{CH}_3\text{OCH}_3 + \text{HO}_2 = \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O}_2$. Beside the above reaction, hydrogen peroxide can also be produced through reaction $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$. Therefore, large amount of H_2O_2 appears after the cool flame due to LTC. Between the cool and hot flames, there is also large amount of CH_2O , which is another indicator of LTC. HTC reactions happen at the hot flame front around x = 6 cm. Therefore, after the hot flame (i.e., x < 6 cm), DME is completely consumed and the concentrations of HO₂, H₂O₂ and CH₂O decrease quickly, resulting in rapid formation of OH, H₂O and CO₂. Besides, Fig. 4 indicates that the cool flame is much thicker than



Fig. 3. (a) Temporal evolution of flame trajectories and (b) change of flame propagation speed with flame front position for DME/air with ϕ . f = 1, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ or 1200 K, and $x_H = 2$ mm. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article).

the hot flame. This is due to the fact that LTC is much slower than HTC.

3.2. Different factors affecting premixed cool flame evolution

In this section, we study how the premixed cool flame propagation and hot flame initiation are affected by: (1) the temperature and size of the hot spot; and (2) the equivalence ratio, initial temperature, initial pressure, and oxygen concentration of the fresh mixture.

The influence of hot spot temperature, T_H , and hot spot size, x_H , on the initiation and propagation of cool and hot flames is shown in Fig. 5. It is observed that both T_H and x_H have little influence on the propagation speed of cool and hot flames. This is reasonable since the flame propagation speed is the intrinsic property of the mixture. However, as shown in Fig. 3, the cool flame does not appear when the hot spot temperature is high enough (e.g., $T_H = 1200$ K). Therefore, successful cool flame initiation does depend on the temperature of the hot spot. Besides, the time for the appearance of the hot flame is shown to strongly depend on both T_H and x_H . At higher hot spot temperature, the HTC autoignition occurs earlier and so does the hot flame (Fig. 5a). For larger hot



Fig. 4. Distribution of temperature and mass fraction of different species for premixed cool and hot flames propagating in DME/air with $\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm.



Fig. 5. Influence of hot spot temperature (a) and size (b) on the initiation and propagation of cool flame (CF) and hot flame (HF) in DME/air with $\phi = 1$, $T_0 = 500$ K and $P_0 = 1$ atm.



Fig. 6. Influence of the equivalence ratio (a) and initial temperature (b) on initiation and propagation of cool flame (CF) and hot flame (HF) in DME/air with $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm.

spot size, the temperature decrease at the center due to heat conduction to the surrounding cold mixture becomes smaller. Consequently, the HTC autoignition appears earlier and so does the hot flame (Fig. 5b). According to Fig. 5, proper hot spot temperature and hot spot size should be used so that the residence time window for the occurrence of premixed cool flame is long enough for the observation of premixed cool flame in experiments.

Figure 6 shows the influence of equivalence ratio, ϕ , and initial temperature, T_0 , on the evolution of cool and hot flames. With the increase of equivalence ratio, the cool flame speed becomes faster (see Fig. 7a). This is due to the fact that the LTC heat release and cool flame temperature both increase with the equivalence ratio [33]. Moreover, since the HTC autoignition delay time decreases with the increase of equivalence ratio, the hot flame appears much earlier at $\phi = 2$ than $\phi = 1$. At higher initial temperature, the cool flame speed becomes faster (see Figs. 6b and 7b) and the appearance of hot flame also becomes earlier due to the shorter HTC autoignition delay time. Figure 7 shows that the cool flame propagation speed is more sensitive to the initial temperature than to the equivalence ratio. Besides, unlike the hot flame speed which usually peaks around $\phi = 1$, the cool flame speed still monotonically increases with the equivalence ratio for $\phi = 3.5$. As mentioned before, this is due to the increase of LTC heat release with the equivalence ratio [33].

The influence of initial pressure is also examined. Figure 8 compares the results at two pressures of P=1 atm and P=2 atm. It is observed that pressure increase has little influence on the cool flame propagation speed while it greatly reduces the hot flame propagation speed. Moreover, the appearance of hot flame becomes much earlier at higher initial pressure. This is expected since the HTC autoignition delay time decreases with the increase of initial pressure. Consequently, at higher initial pressure, the residence time window for the occurrence of premixed cool flames becomes shorter and thereby it is difficult to observe premixed cool flames in high-pressure experiments. It is noted that though the premixed cool flame speed for DME is nearly the same for



Fig. 7. Change of cool flame propagation speed with the equivalence ratio (a) and initial temperature (b) for DME/air with $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm. The flame propagation speed is evaluated for cool flame at $X_f = 1$ cm.

P=1 atm and P=2 atm, microgravity heptane droplet-burning experiments exhibit very large differences in cool-flame behavior at 1 atm and 2 atm [9,46]. The reasons for such differences remain unclear and deserves further study.

For all the results mentioned above, the oxidizer consists of 21% O_2 and 79% N_2 (in volume). Figure 9 shows the results with different amounts of O_2 in O_2/N_2 mixture. It is observed that the cool flame propagation speed increases greatly with the oxygen concentration. Meanwhile, the hot flame appears earlier at higher oxygen concentration. This is because the HTC autoignition delay becomes shorter at higher oxygen concentration.

3.3. Prediction of premixed cool flame by different chemical mechanisms

Recent study of Zhao et al. [34] showed that there is large discrepancy in the prediction of low temperature DME oxidation by different chemical models. In this section, different chemical mechanisms are used to predict the transient evolution of premixed cool flame. The results are shown in Fig. 10. Besides the mechanism of Zhao et al. [23] (referred to as Mech 1), two recently updated DME mechanisms by Wang et al. (Mech 2) [35] and Kurimoto et al. (Mech 3) [36] are used in simulation. The results predicted by different mechanisms for the same case are compared in Fig. 10.

Figure 10 shows that both the cool flame propagation speed and the onset of hot flame are very sensitive to the DME chemical model. As shown in Fig. 10(b), after the hot flame catches up the cool flame for $x_f > 20$ cm, the hot flame propagation speeds predicted by three mechanisms are nearly the same (the relative difference is within 2%). For cool flame at $x_f = 1$ cm, the propagation speeds predicted by Mech 1, Mech 2 and Mech 3 are 12.8 cm/s, 6.5 cm/s and 5.6 cm/s, respectively. Therefore, though these three mechanisms have nearly the same prediction for hot flame propagation speed, there are very large discrepancy in the prediction of cool flame propagation speed. The San Diego Mechanism [42] and HP Mech [43] were also used and the propagation speeds for cool



Fig. 8. (a) Temporal evolution of flame trajectories and (b) change of flame propagation speed with flame front position for cool flame (CF) and hot flame (HF) in DME/air ($\phi = 1$, $T_0 = 500$ K, $T_H = 800$ K, and $x_H = 2$ mm).

flame at $x_f = 1 \text{ cm}$ (and at the same conditions as those in Fig. 10) are 3.7 cm/s and 5.1 cm/s, respectively. It is noted that the only difference between Mech 1 and Mech 3 is in reaction rate for the QOOH branching reaction, CH₂OCH₂OOH \rightarrow CH₂O + CH₂O + OH [36]. The transport and thermal properties are the same for Mech 1 and Mech 3. Therefore, the cool flame speed is very sensitive to the rates of elementary reactions involved in the LTC. This indicate that measurement of premixed cool flame propagation speed is useful for validating and developing low temperature chemistry of DME. Similarly, cool-flame chemistry was found to be crucial for accurate prediction of droplet diameter at cool flame extinction [44].

It is well known that the propagation of laminar premixed flame is determined by transport processes (i.e., mass diffusion and heat conduction) as well as chemistry. In order to demonstrate the influence of transport on cool flame propagation, in simulation we artificially double the thermal conductivity and mass diffusivities of all specifies. Figure 11 compares the results without and with doubling the transport properties. The cool flame propagation speed is shown to increase by 38% when the diffusivity is doubled. Similar change is also observed for hot flame speed, which is proportional to the square root of the thermal diffusivity. Therefore, the cool flame observed in present simulation is not an autoignition front and it is supported by diffusion as well as LTC.



Fig. 9. (a) Temporal evolution of cool flame trajectories and (b) change of cool flame propagation speed with flame front position for DME/O₂/N₂ ($\phi = 1$, $T_0 = 500$ K, $T_H = 800$ K, and $x_H = 2$ mm) with different amounts of O₂ in O₂/N₂ mixture.

3.4. On the observation of propagating premixed cool flames in experiments

It is difficult to observe cool flames in experiments. In previous experiments [2,18], steady premixed cool flames were observed while the transient initiation and propagation of premixed cool flames were seldom studied. The present simulation results (see Figs. 3, 5 and 6) show that the residence time for the occurrence of premixed cool flame in preheated DME/air mixture is around 0.5 s. Therefore, such kind of premixed cool flame might be achieved in experiments for premixed flames propagating in a tube or channel. Certainly for flame propagation in a tube or channel, there is cool flame-wall interaction due to heat transfer or radical quenching on the wall [37]. Such interaction might affect the residence time for the occurrence of premixed cool flame. This deserves further studies [15,16] and is beyond the scope of the current work.

Besides, we also simulate premixed spherical flame propagation in preheated DME/air mixture. The spherical flame is considered to propagate in a close vessel with the inner radius of 10 cm, which is similar to spherical flame experiments (e.g., [38,39]). A hot spot with radius of $r_H = 3$ mm and termperature of $T_H = 1000$ K is used to initiate the cool flame. Both the temperature and size of the hot spot are much larger than those for the planar case ($T_H = 800$ K and $x_H = 2$ mm) since the tempeature decrease due to heat conduction in spherical geomentry is much faster than that in the planar case.



Fig. 10. (a) Temporal evolution of flame trajectories and (b) change of flame propagation speed with flame front position for DME/air ($\phi = 2$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm) predicted by three mechanisms described in the text.



Fig. 11. Temporal evolution of cool flame (CF) and hot flame (HF) trajectories for DME/air ($\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K, and $x_H = 2$ mm). The same mechanism, Mech 1, is used. The diffusivity is artificially doubled to demonstrate the influence of transport on cool flame propagation.



Fig. 12. (a) Temporal evolution of spherical flame trajectories and (b) change of spherical flame propagation speed with flame radius for DME/air ($\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 1000$ K or 1200 K, and $r_H = 3$ mm).

Figure 12 shows the transient propagation of premixed spherical cool and hot flames. Similar to the planar case shown in Fig. 3, the propagating spherical cool flame is first initiated by the hot spot. The double-flame structure of both cool and hot spherical flames appears after the occurance of the hot flame propagating from the center. Unlike the planar case, Fig. 12(b) shows the propagation speed of spherical hot flame decreases with the flame radius for $R_f > 4$ cm. This is due to the pressure rise in the closed vessel (the so-called confinement effect) [21,40]. Figure 12(a) shows that the propagating spherical cool flame can exist with the duration time above 0.6 s. Therefore, premixed spherical cool flames might also be achieved in experiments. It is noted that the slow propagation of premixed spherical cool flame might be affected by bouyancy and thereby microgravity experiments might be needed. Besides, as shown in Fig. 9(b), increase in the oxygen concentration can make the cool flame propagate faster and thereby diminish the bouyancy effect. However, at higher oxygen concentration, the residence time window for the occurrence of premixed cool flames becomes shorter (see Fig. 9a).

Figure 13 shows the influence of stretch rate (which is defined as $K = 2S/R_f$ for expanding spherical flames) on spherical cool flame propagation. Since the cool flame has very low propagation speed, its stretch rate is much smaller than that of traditional hot flames. When the cool flame radius is less than 4.0 cm, the flame propagation speed changes linearly with the stretch rate.



Fig. 13. Change of spherical flame propagation speed with stretch rate for the cool flame shown in Fig. 12.

Therefore, extrapolation based on the linear model of $S = S^0 - L_b K$ can be conducted to get the unstretched flame speed, $S^0 = 11.1$ cm/s, and burned Markstein length, $L_b = 0.13$ cm, for the cool flame [45]. It is noticed that both *S* and *K* increase after the turning point shown in Fig. 13. This is due to the abrupt increase in cool flame propagation speed for $R_f \approx 7$ cm/s as shown in Fig. 12(b).

It is noted that for all the results presented above, the radiation effect on premixed cool flame propagation [4] is neglected. In simulation we also include radiative loss for the standard case considered in Section 3.1 (i.e., $\phi = 1$, $T_0 = 500$ K, $P_0 = 1$ atm, $T_H = 800$ K and $x_H = 2$ mm). The results show that the radiation effect is negligible. When the propagation speed of premixed cool flame is above 10 cm/s, radiation has little influence on the flame speed. This is similar to the conclusion for hot flames [41].

4. Conclusions

One-dimensional transient simulation is conducted to study the initiation, propagation and disappearance of premixed cool flames in DME/air mixture. Detailed chemistry and temperaturedependent thermal and transport properties are considered in simulation. A well-defined cool flame speed is found. The main conclusions are:

- 1. The premixed cool flame can be initiated by a hot spot with proper temperature only triggering LTC reactions. During the slow propagation of cool flame, HTC autoignition occurs at the center, which results in a hot flame propagating behind the leading cool flame. Therefore, double-flame structure of both cool and hot flames appears. The hot flame has much faster speed than cool flame and it eventually catches up and merges with the leading cool flame. Finially the cool flame disappears and only the hot flame propagation exists. Besdies, due to the partial fuel oxidation and temperature rise after the cool flame, the hot flame after the cool flame has much larger propagation speed than the single hot flame.
- 2. The hot spot temperatue and size affect the appearance of the cool and hot flames. However, they do not affect the propagation speed of cool and hot flames. The cool flame does not appear and only the hot flame occurs when the hot spot temperature is high enough. The cool flame speed is found to increase with the equivalence ratio, the initial temperature, and the oxygen concentration. Moreover, at higher equivalence ratio, higher initial temperature, or higher oxygen concentration, the hot flame appears earlier, indicating that the duration of the double cool/hot flame becomes shorter.

- 3. Though nearly the same hot flame propagation speed is predicted by different DME chemical mechanisms, the cool flame propagation speed is very sensitive to the chemical model used in simulation. Therefore, experimental data of premixed cool flame propagation are needed for the development of low temperature chemistry of DME. Besides, it is shown that the cool flame observed in present simulation is not an autoignition front and it is supported by diffusion as well as LTC.
- 4. The residence time for the occurrence of 1D premixed planar cool flame is around 0.5 s. Therefore, such kind of premixed cool flame might be achieved in experiments for premixed flames propagating in preheated DME/air mixture in a tube or channel. Besides, the present simulation indicates that premixed spherical cool flames might also be achieved in experiments.

It is noted that only the premixed cool flame for DME is investigated here. In future work, it is of interests to study normal alkanes, such as n-heptane.

Acknowledgments

This work is supported by National Natural Science Foundation of China (Nos. 91541204 and 51322602). We appreciate helpful discussion with Professor Sang Hee Won at University of South Carolina and Professor Yiguang Ju at Princeton University. We also thank Mr. Chengyang Huang at Peking University for conducting some simulations.

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