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Extinction and flame bifurcations of stretched dimethyl ether premixed flames

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Abstract

Extinction limits and flame bifurcation of lean premixed dimethyl ether–air flames are numerically investigated using the counterflow flame with a reduced chemistry. Emphasis is paid to the combined effect of radiation and flame stretch on the extinction and flammability limits. A method based on the reaction front is presented to predict the Markstein length. The predicted positive Markstein length agrees well with the experimental data. The results show that flow stretch significantly reduces the flame speed and narrows the flammability limit of the stretched dimethyl ether–air flame. It is found that the combined effect of radiation and flow stretch results in a new flame bifurcation and multiple flame regimes. At an equivalence ratio slightly higher than the flammability limit of the planar flame, the distant flame regime appears at low stretch rates. With an increase in the equivalence ratio, in addition to the distant flame, a weak flame isola emerges at moderate stretch rates. With a further increase in the equivalence ratio, the distant flame and the weak flame branches merge together, resulting in the splitting of the weak flame branch into two weak flame branches, one at low stretch and the other at high stretch. Flame stability analysis demonstrates that the high stretch weak flame is also stable. Furthermore, a K-shaped flammability limit diagram showing various flame regimes and their extinction limits is obtained.

Keywords: Dimethyl ether; Extinction limit; Radiation; Bifurcation; Stretch

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1. Introduction

Dimethyl ether (DME) has low soot emission, high tolerance to EGR, and causes no contamination of groundwater. In addition, it can be synthesized from natural gas, coal, and bio-fuels, and has been considered as a neat diesel substitute fuel and house cooking fuel. The study of DME combustion attracts great attention [1–5]. Recently, detailed kinetic mechanisms for low and high temperature DME oxidations [6–8] have been established. Applications of DME on diesel engine have been investigated by real engine performance tests and engine CFD simulations [9,10]. One of the key issues to achieve the best performance is to know how lean it can burn and how fast the flame can propagate in a turbulent flow.

The laminar burning velocity of DME–air mixtures was measured by Daly et al. [11] and Zhao et al. [12], respectively, using the spherical bomb and the counterflow flame. However, practical flames are always stretched. Although DME has a mean molecular weight larger than that of air, it decomposes quickly into CH_3 and CH_3O, which have less and comparable mean molecular weights than that of air. As a result, DME and its

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decomposed species play opposite roles in affecting stretched flame burning. As such, it is of great interest to understand how flame stretch affects flame propagation and the flammability limit of DME–air combustion. Furthermore, since DME combustion involves high EGR, radiation impact on flame extinction via CO_2 emission has to be considered. Unfortunately, there is no report available on flame extinction for DME-air combustion.

The effect of radiation on stretched methane–air flames has been extensively investigated using counterflow flames [12–19]. The results showed that radiation flame interaction results in complicated flame bifurcations and radiation extinction. The previous study based on the one-step chemistry [19] demonstrated a transition from G- to K-shaped extinction curve at large Lewis numbers and the existence of a highly stretched weak flame. However, the existence of this flame has not been confirmed using a practical fuel and detailed chemistry.

This study is motivated by the above discussions to numerically investigate the combined effect of stretch and radiation on the extinction limits and flame bifurcations of lean premixed dimethyl ether–air flames using a detailed chemistry. At first, the Markstein length is obtained by linearly extrapolating the flame speeds of weakly stretched lean DME–air flames to zero stretch rate. Several extrapolation methods based on different flame locations are employed and compared. Then, the flammability limit of planar flame is computed. This is followed by the simulation of flame response with stretch rate using the radiative counterflow flame. Different flame regimes, limits, and bifurcations are discussed. Finally, flame stability on highly stretched weak flame is examined, and the flammability diagram is obtained.

2. Numerical models

The axisymmetrical back-to-back counterflow premixed flames are considered in this study. The gaseous mixtures are issued from two opposed burners forming two planar flames near the stagnation plane. The governing equations based on the potential flow assumption were given in [17]. The fuel is DME (CH_3OCH_3), and the oxidizer is air. A reduced chemistry including 39 species (N_2, O_2, H_2, H_2O, H, HO_2, OH, O, H_2O_2, CO, CO_2, HCO, CH_3, CH_3OCH_3, CH_4, CH_2, CH_2O, C_2H_4, CH_3O, C_2H_6, C_2H_5, C_2H_2, C_2H_3, CH_3OH, CH_2OH, CH_3O_2, CH_3O_2H, $CH_3OCH_2O_2$, $CH_2OCH_2O_2H$, $CH_3OCH_2O_2H$, CH_3OCH_2O, $O_2CH_2OCH_2O_2H$, HO_2CH_2OCHO, OCH_2OCHO, CH_2 (S), $HOCH_2OCO$,HOCHO, CH_3OCH_2, and CH_3OCHO) and 168 reactions was developed using the CSP reduced algorithm [20] from the full mechanism [7], which originally has 78 species and more than 300 reactions. As will be shown later, this reduced mechanism can reproduce the experimental data [12] reasonably well and provide much better convergence and efficient computation time than the full chemistry.

In the radiation calculation, we employ the optically thin model. The radiation heat loss is determined by using the Planck mean absorption coefficients, which are calculated for CO_2, H_2O, and CO using the statistical narrow-band model. This is a reasonable and computationally efficient choice for DME–air flames because the CO_2 concentration in thermal diffusion zone is at the same level of CH_4–air flame so that the radiation reabsorption effect can be neglected [21].

The unburned temperature of the mixture is 300 K, and the pressure is 1 atm. Detailed transport properties are computed from the Chemkin database if they are available. For those species whose transport properties are not available, the transport parameters are estimated using the similar molecules. For steady state solutions, the governing equations are solved by a revised version of the Chemkin code [22] with an improved arc-length continuation method [17]. For stability analysis, the initial stretch rate is perturbed by one percent, and the unsteady solution is computed until the flame reaches steady state solution or jumps to any other flame branch. The time step for unsteady computation is between 100 and 10 μs. The computation domain is 10 cm.

3. Results and discussion

3.1. Flammability limit and effect of flame stretch on flame speed

Figure 1 shows the dependence of flame speeds of the one-dimensional (1D) planar DME–air flames (S_{L0}) on the equivalence ratio with and without radiation. It is seen that for the 1D flame, radiation plays a negligible role for equivalence ratio (Φ) larger than 0.6. However, with the decrease in equivalence ratio, radiation increasingly reduces flame speed and causes flame extinction at $\Phi_0 = 0.454$. Hereafter, to differentiate the flammability limit of the stretched flame from that of the planar flame, we will call the extinction limit of the planar flame as the fundamental flammability limit. The experimental data by Zhao et al. [12] are also plotted in Fig. 1. It is seen that the reduced chemistry can reproduce the experimental data reasonably well. In fact, the difference between the full chemistry and the present reduced chemistry is less than 5% for all lean DME–air flames.

For weakly stretched, adiabatic flames, the effect of flame stretch on flame speed (S_L) can be approximately treated as a linear function using