Propagation Speeds and Kinetic Analysis of Premixed Heptane/Air Cool Flames at Large Ignition Damköhler Numbers

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1 Introduction

Cool flame and low temperature chemistry (LTC) have been considered as a key process to realize engine knock control in novel engines, such as homogeneous charge compression ignition engine (HCCI)[1], reactivity controlled compression ignition engine (RCCI)[2] and so on. Cool flames have been studied in various flame geometries including heated burners[3][4], stirred reactors[5][6][7], counter flow flames[8], droplets[9], rapid compression machine[10] and so on. The main efforts were focused on the heat release, low temperature chemistry, negative temperature coefficient (NTC) without considering the effects of pre-ignition. However, in advanced internal combustion engines and detonation engines, the mixtures are compressed to high temperature and pressure, and the auto-ignition timescale is comparable to the burning time of cool flames themselves. As a result, the ignition Damköhler number is high and combustion occurs in a manner of auto-ignition assisted flame propagation[11]. For example, knocking formation in gasoline engines is an outcome of auto-ignition induced deflagration to detonation transition[12].

Unfortunately, few studies have been conducted to understand how auto-ignition affects the propagation speeds of a cool flame. In addition, cool flame exists in both fuel lean and fuel rich conditions and they have different flame structures. However, it is not clear how auto-ignition affects the propagation of lean and rich cool flames differently. Furthermore, as reported in a recent study, with the increase of pressure or initiation temperature, a lean cool flame can transfer into a warm flame with a double flame structure[13]. It is therefore interesting to understand how auto-ignition affects warm flame and its transition to a hot flame. As such, the goal of the current study is to understand the effects of auto-ignition and ignition Damköhler number on the structure and propagation speeds of lean and rich premixed cool flames, warm flame and hot flame at different temperatures and pressures. First, the cool flame speed is studied within a wide range of ignition Damköhler numbers. Then, the effects of pressure, initial temperature, and equivalence ratio on auto-ignition assisted flame propagation are investigated at different ignition Damköhler numbers. Furthermore, the key reactions for auto-ignition assisted cool flames, warm flame, and hot flame are analyzed using computational singularity perturbation (CSP) method under G-scheme framework[14]. Finally, the conclusions are made.

2 Numerical modeling

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In this study, n-heptane is chosen as the fuel because it has strong low temperature chemistry and it is one of the major components of the Primary Reference Fuel (PRF). A comprehensively reduced n-heptane/air mechanism with 170 species and 962 reactions is produced by the multi-generation path flux analysis (PFA)[15] method from HP-Mech.

Both steady-state flame and transient flame are considered for the. For the one-dimensional, steady-state, freely-propagating premixed flames, the initial temperature and species concentrations are fixed in the upstream. The upstream domain length will be adjusted to study the effect of the ignition Damköhler number and the consequent inlet boundary is varied from -30 to 1 cm depending on the case. The downstream size is varied from 1 to 15 cm. The arc-length method[16] is used to accelerate computation.

The transient simulations are performed using the ASURF+[17][18], which solves the compressible Navier-Stokes, conservation of species mass fraction, conservation of energy equations using 3rd order weighted essentially non-oscillatory (WENO) scheme[19] and multi-level dynamically adaptive mesh refinement. In order to improve simulation efficiency, the correlated dynamic adaptive chemistry and transport (CO-DACT) method[20] and the hybrid multi-timescale (HMTS) method[21] are used. In addition, to study the ignition Damköhler number effect, the preheat zone length is fixed. The schematic of the calculation domain is shown in Fig. 1. The flame propagates to the right and on the right-hand side, the shadow part is the 'cold boundary', the length between flame front and the cold boundary is L_f which is fixed in each case. The temperature T_0, equivalence ratio φ_0 and pressure P_0 are given as the boundary conditions. The ignition Damköhler number is calculated by $Da = \frac{L_f/u}{\tau(T_0,P_0,\varphi_0)}$ where τ is the ignition delay time and u is the flame propagation speed. Both lean and rich cool flames are simulated, where the steady-state solver and the transient simulation show satisfying agreement.

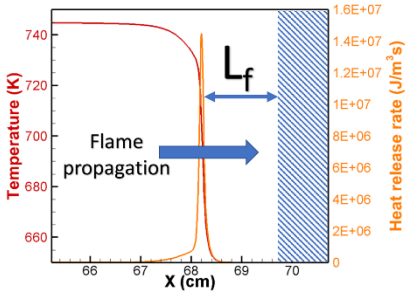

Fig.1. The schematic of the calculation domain for the transient simulation.

3 Results and discussion

Fig.2. shows the results for the lean cool flames at $T = 650\ K, \varphi = 0.2, P = 1\ and\ 20\ atm$. In both atmospheric and high pressure conditions, flame speed increases with ignition Damköhler number Da. when Da is low (Da<0.6), the flame propagation speed change is relatively small, since the preheat zone is so short that there is little radicals and heat accumulated in the upstream. When Da>0.6, the propagation speed grows exponentially with Da. At this stage, the unburned mixture in the preheat zone undergoes further autoignition process, thus significantly strengthens the reaction at the flame front and accelerates the flame propagation due to the richer radical pools and higher temperature of the unburned mixture. Da=1 is a singularity point and the flame speed will asymptotically go to infinity since the residence time is long enough for mixtures to auto-ignite. It is worth noticing that under engine condition, the ignition delay time for the 1st stage low temperature autoignition can be very short, comparable to the characteristic time of the cool flame propagation. As such, the cool flame propagation speed can be at high ignition Damköhler number and behaves differently from typical laminar flame speed.

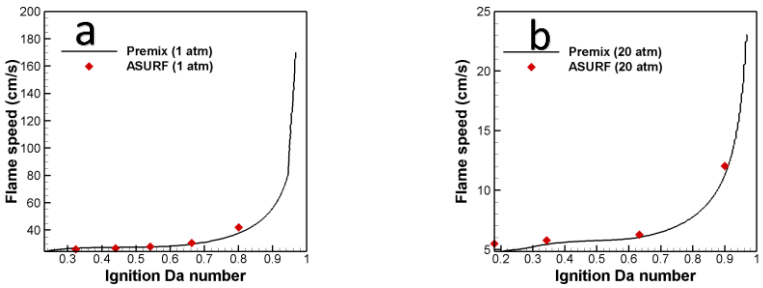

Fig.2. The flame speed for the cool flame at $T = 650\ K, P = 1\ and\ 20\ atm, \varphi = 0.2$. Left: a). $P = 1\ atm$. Right: b). $P = 20\ atm$. The black curves are from the steady-state solver, the red dots are transient simulation results.

Fig.3. shows the results for lean cool flame at $Da = 0.4, P = 1\ or\ 20\ atm, \varphi = 0.2$ with a wide range of initial temperature. Results at different pressures show strong non-monotonic trends. Basically, before reaching the turnover temperature of the NTC region, the flame speed increases with the temperature and reaches its peak value around the turnover temperature. After entering NTC region, the flame speed drops down dramatically due to the inhibited reactivity of the low temperature chemistry. Finally, when initial temperature high enough to exceed low temperature chemistry domain, the cool flame transits to the hot flames and the flame speed increases again with the temperature.

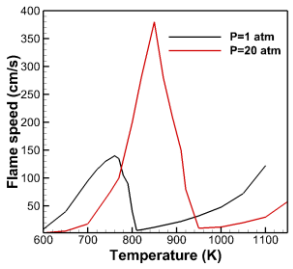

Fig.3. The flame speed for the cool flame at $Da = 0.4, P = 1\ and\ 20\ atm, \varphi = 0.2$. Black curve: $P = 1\ atm$, red curve: $P = 20\ atm$.

Fig.4. shows the results for rich cool flame at $T = 650\ K, P = 1\ and\ 20\ atm, \varphi = 20$. Comparing with cool flames at the lean side, both lean and rich cool flame exhibits monotonic trend with the ignition Damköhler number which agrees with the Arrhenius law. It can be seen that similarly, before Da=0.6, there is little change in flame speed both in low and high pressures. After Da>0.6, the flame speed increases significantly with the ignition Damköhler number. In addition, it is noticed that the high pressure curves is smaller in terms of absolute values, but it starts to rise at a much earlier stage in terms of the ignition Damköhler number compared with atmospheric condition, since the low temperature autoignition is more sensitive with increased residence time in high pressure conditions.

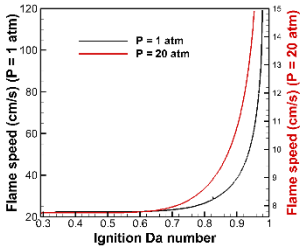

Fig.4. The flame speed for the cool flame at $T = 650\ K, P = 1\ and\ 20\ atm, \varphi = 20$. Black: $P = 1\ atm$. Red: $P = 20\ atm$.

In addition, CSP analysis is performed for cool flame cases. For the lean cool flame case $T = 650\ K, P = 1\ atm, \varphi = 0.2, Da = 0.3$. Fig.5. shows the flame structure. CSP analysis identifies the key reaction in the preheat zone (x=12.6 cm, T=650 K) is C7H16+O2=C7H15+HO2 reaction, which is the typical H abstraction reaction from the fuel. The normalized G-scheme Participation Index (GPI) is calculated which shows the importance of the reactions. For the H abstraction reaction in the preheat zone, the GPI is 0.95 which is dominant compared with other reactions. Thus, H abstraction from the fuel is the main chain initiation reaction in the preheat zone. At the cool flame front (x=12.2 cm, T=725 K), the key reaction with the largest GPI becomes isomerization reaction C7H15O2=C7H14OOH whose GPI is 0.24. Since there are much more active reactions at the flame front, the absolute GPI for the key reaction decreases but is still much larger than other reactions. This isomerization reaction generates weakly bound QOOH which is further decomposed to generate OH radicals and dominates the low temperature chemistry.

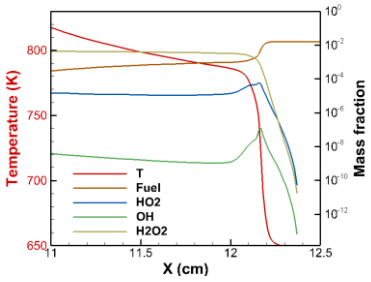

Fig.5. Cool flame structure at $T = 650\ K, P = 1\ atm, \varphi = 0.25, Da = 0.3$.

4 Conclusions

The auto-ignition assisted laminar cool flame speeds at different ignition Damköhler numbers under elevated temperatures and pressures are numerically modeled in a broad range of equivalence ratios with detailed chemistry. The results show both fuel lean and fuel rich cool flame speeds increase dramatically with the increase of the ignition Damköhler number. At higher pressure, the flame speed becomes smaller but more sensitive to the ignition Damköhler number change. Furthermore, the results show that at the same ignition Damköhler number, with the increase of the initial mixture temperature, there is a strong non-monotonic dependence of flame speeds on temperature due to the Negative Temperature Coefficient (NTC) effect. The peak speed appears around the turnover temperature. The results show that flame speed decreases immediately once a cool flame transits to a hot flame after the NTC region. A comprehensive analysis of the controlling reaction modes for cool flame propagation is performed using the CSP based on G-scheme. It identifies H abstraction reaction from the fuel in the preheat zone and the isomerization reaction at the flame front dominates the chemistry reaction system respectively.

Acknowledgement

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