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Propagation and stability characteristics of laminar lifted diffusion flame base

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ABSTRACT

Numerical calculations of the flame propagation speed and the Damköhler number (Da) at laminar lifted flame base were carried out. The results are intended for further understanding the propagation and the Damköhler mechanisms for flame stabilization, with the former based on a tribrachial flame propagating against the local flow velocity and the latter based on the competition between the reaction time and local residence time of the peak reaction zone. Propane fuel without and with dilution (40% helium and argon, by volume) was used, while the reaction scheme adopted was the one-step irreversible Arrhenius kinetics (see Li et al., *Combust. Flame* 157 (2010) 1484–1495) which proved successful in predicting the flame lift-off height and effects of thermal expansion and multi-component diffusion. The results reported in this paper show that the flame base propagation speed is up to approximately four times of the one-dimensional stoichiometric flame speed of the fuels used, depending on where the propagation front is defined. These results are compared with previously published experimental and theoretical results from laminar and turbulent diffusion flames. It is found that the flame base propagation speed (V_p) increases in the downstream direction as a result of increasing jet velocity (V_o) under most flame conditions, providing a stabilizing mechanism. However, there exist conditions where V_p decreases while the flame stabilizes. The flame base Damköhler number (Da) always increases as the flame liftoff height increases (resulting from increasing jet velocity). Da is here defined as ratio of peak reaction rate of the reaction kernel (RR) to the flame stretch rate (k) determined at the intersection of the reaction kernel (approximately coinciding with the 2000 K isotherm) and the stoichiometric contour. The value of Da appears to be of the order of 10^{-3} for the three fuels studied, and the increasing trend of Da with the lift-off height also helps to explain the flame stabilization.

1. Introduction

The flame base propagation speed in both laminar and turbulent diffusion flames has been a topic of investigation because of its relevance to the stabilization mechanism of these flames. For laminar jet diffusion flames of fuels such as C_3H_8 and C_4H_{10}, stable liftoff is achieved prior to flame blowoff as the jet exit velocity (V_o) is increased [1–3]. At the lifted flame base, a tribrachial (or triple) structure exists, as first observed and studied by Phillips [4] for a stratified fuel–air mixing layer. A triple flame is thought to result from the premixing of fuel and air and in general may consist of a diffusion flame, a lean premixed flame, and a rich premixed flame [3,4]. It exists not only in gaseous diffusion flames in a free jet or near quenching walls but also in flame spread across liquid fuel pools or combustible solids [5–7]. The evolution and relevance of the triple flame structure in jet diffusion flame blow-off was investigated in an earlier study [8]. Recent reviews can be found [9–12] that summarize the findings related to laminar lifted flames through experimental, theoretical, and numerical studies.

Theoretical analyses of gaseous lifted flames often assumed the flame base to be located at the intersection of the stoichiometric fuel–air contour and the iso-velocity contour that has a local axial velocity component (V_x) equal to the one-dimensional stoichiometric flame speed S_L^0 [1], defined as the speed of the cold reactant flow in the direction normal to the planar flame front. Using the cold flow similarity, the flame liftoff height (H_L) is equal to the distance between the burner exit and the flame base [1,2]. H_L thus predicted was in agreement with experimental results, which increased with V_o [1,2]. Later theoretical studies considered effects of curvature of the flame base, the flow redirection and heat release on the local tribrachial flame speed (V_p) [13–17]. Because of these effects, V_p in general exceeds S_L^0 [13,14,18–20]. The combined effect of curvature and the flow redirection causes the flame to be stretched. These effects on the flame base propagation speed should more closely resemble those in turbulent flames than those in the counter-flow configuration, which are one-dimensional. Xue and Ju [21] further argued that, in laminar diffusion flames,

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the stabilization mechanism for a lifted flame requires that V_p be increasing/decreasing in the downstream/upstream direction along the stoichiometric contour, so that perturbation from the stabilization point would always return the flame base to that point. In lifted flames, the value of V_p increases as the flame stretch decreases, which occurs as the flame base moves in the downstream direction. Because the flame base needs to propagate against the incoming flow for flame stabilization, the stabilization mechanism can be called the "propagation mechanism" and it requires premixing to yield combustible mixture for the propagation to take place.

For laminar flames the flame base propagation speed V_p has been predicted to be in the range of up to approximately 3.5 S_L^0 [18–20] while in turbulent diffusion flames the average value has been reported to be in the range of 1.8–3.5 S_L^0 with instantaneous values approaching 8.0 S_L^0 [15,22]. The value of V_p varies with the flame base location (and thus with the flame stretch rate, k) in a laminar jet diffusion flame. For stable liftoff V_p was found to increase as the lift-off height increases to a downstream location associated with a decreased value of k [9,23]. In turbulent flames, the value of k varies not only with location but also with time. As noted by some researchers [9,10,24], the experimental determinations of V_p in turbulent flames have been rather limited.

Differing from the propagation mechanism, Takahashi and coworkers reported the stability of a laminar *attached* flame based on the concept of "reaction kernel (i.e., the peak reactivity spot)" without invoking the tribrachial flame or the flame base propagation speed. When the coflowing air surrounding the fuel jet was perturbed by changing its velocity, the reaction kernel shifted to locations where reactivity increased [25–27]. They obtained the reaction kernel at an equivalence ratio (ϕ) substantially lower than 1.0. It was noted that the locally $\phi = 1$ mixture existed within the quenching distance, not allowing a triple flame to propagate through it. Such results suggest that a diffusion flame base may propagate in regions away from the stoichiometric contour. Furthermore, the reaction kernel may have a lower temperature than at other locations where richer conditions existed. These authors further found that the ratio of the heat release rate to the flow velocity ($\dot{q}/u$) at the flame kernel under nearly-lifting (but not lifted) conditions remained relatively constant, albeit slightly increasing, as the flame base moved to different locations [25]. Lifted flames in these studies [25–27] were achieved only after the transition to turbulent flow. Since ($\dot{q}/u$) ratio is essentially a Damköhler number (Da), such a stabilization mechanism is here called the "Damköhler mechanism" for convenience. As reported by the present authors [28], the flame base region in a *lifted* laminar flame is situated around the stoichiometric region and not necessarily at the intersection of the stoichiometric and iso-velocity contours. The appropriate Damköhler number can be based on the thermal and fluid mechanical parameters in that region – for example V_p can be used instead of S_L^0. In laminar jet diffusion flames, velocity and concentration gradients decrease in the downstream direction, and the value of Da is expected to increase. Because the flame base in a turbulent flame exists in an environment having wide ranges of velocity and length scales and curvatures, it is more appropriate to adopt k (the inverse of the local flame residence time) instead of u for the calculation of Da. For generality, such a definition of Da should also be used for laminar lifted flames.

In some theoretical studies [6,7,12], both V_p (reflecting the wave-like nature of the flame base) and Da were invoked in treating lifted flames, with V_p determined through a balance of convection, diffusion, and reaction and as a result V_p was a function of Da. When the Da is greater/smaller than a critical value, V_p can be positive/negative, which is different from premixed flame front that has only positive propagation speeds [12]. Therefore, an increase, not just a constant, in Da (i.e., a decrease in flame stretch rate) in the flow direction is necessary for flame stabilization.

In summary, for both the propagation and Damköhler mechanisms both k and V_p are essential. This study examines how k affects V_p and Da of the reaction kernel. The reaction rate needed is difficult to obtain experimentally. Furthermore, the flame base location, used to experimentally determine V_p, may be separated by as far as 2 mm using the temperature isotherm and the CH radical concentration contour [10,22]. Such an experimental difficulty can be circumvented by adopting a numerical approach. A recent combined numerical (using FLUENT) and experimental study [28] on flame lift-off and stabilization demonstrated the capability of FLUENT coupled with a one-step irreversible reaction and multi-component gas diffusion to (1) accurately predict lift-off height, (2) determine whether an inert-diluted flame will lift or not, (3) reveal that Schmidt number may not be the criterion for flame lift-off, and (4) that flame base is not necessarily located at the intersection of the stoichiometric and flame velocity contours. In this study, a similar approach is used to obtain results for comparing and accessing the propagation and the Damköhler mechanisms. The implication of the one-step mechanism vs. the detailed multi-step mechanism is noted when appropriate.

2. Numerical

Details of the numerical procedure using FLUENT can be found in [28]. The reaction was one-step Arrhenius irreversible reaction with heat release. Species diffusion including the Soret and multi-component effects were included. The boundary conditions used were the pressure outlet type except at the base of the fuel tube, where the wall condition was adopted. Typical results obtained contain the contours of axial velocity (including the one equal to S_L^0), mixture fraction (Y_F), stoichiometric mixture fraction (Y_{st}), temperature (T), and reaction rate (RR). Here the Y_{st} contour is replaced by that of $[C_3H_8]$:$[O_2] = 1{:}5$, as different diluents (helium and argon) result in different values of Y_{st}, not only because of different molecular weights of the diluents but also because of their different diffusivities [28]. The boundary conditions and solution method were described in Ref. [28]. Attention was also paid to the grid independence of the calculated results. To test such independence, 4×4 refined meshes with grid size of 0.5 mm $\times$ 0.5 mm, 8×8 refined meshes with gird size of 0.25 mm $\times$ 0.25 mm, and 16×16 refined mesh with mesh size of 0.125 mm $\times$ 0.125 mm were investigated. The simulation results show that the 8×8 refined meshes have the same accuracy as 16×16 refined meshes. For some cases, even more refined 32×32 or 64×64 meshes for the flame base zone were used to confirm their grid-independence.

The one-dimensional value of flame propagation speed, S_L^0, was calculated both using CHEMKIN, with C3 mechanism and a one-step mechanism was used for the flow field calculations using FLUENT for C_3H_8 (reactants at 1 atm and 298.15 K). The value of the flow velocity across the flame can be obtained from the results shown in Figs. 1a and 1b. The interpretation of the flow field calculations may differ when the one-step mechanism is used as opposed to the C3 mechanism. It can be seen that the one-step mechanism produces a wider heat release reaction zone, with a smaller peak reaction rate. The one-step mechanism also produces smaller value of S_L^0, approximately 0.33 m/s vs. 0.41 m/s when C3 chemistry is used. Flame speeds were also obtained for diluted flames using one-step kinetics, and they were recorded in Table 1 that is to be discussed along with the flow field predictions. This is done to be consistent with the fact that flow fields in this study were predicted using one-step chemical kinetic model contained along with the FLUENT code, as was done in a previous article [28] of which the present article is a continuation.