Two-Dimensional Effects in Counterflow Methane Flames

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Abstract

The effect of flowfield geometry on flame propagation and extinction of atmospheric $\text{CH}_4/\text{N}_2/\text{air}$ flames was studied in the counterflow configuration. Laminar flame speeds and extinction strain rates for lean premixed and non-premixed flames were measured in axisymmetric burners producing either uniform or non-uniform axial velocity exit profiles. Particle image velocimetry was used to characterize the two-dimensional flowfield between the burners. The experiments were modeled with a one-dimensional code and a detailed C_2 hydrocarbon kinetic model. Laminar flame speeds were found to be insensitive to the burner exit velocity profile shape but extinction measurements were strongly affected. In non-uniform flows, two-dimensional flow field measurements revealed significant radial dependence of flow quantities and high-speed video captured off-center initiation of extinction. Thus, centerline measurements did not represent the extinction state properly, given the direct contradiction to one-dimensional modeling assumptions, and the data was deemed unreliable for kinetic model validation. Flames in uniform flows were found to exhibit minimal radial dependence with extinction initiating at near-centerline locations.

Keywords:

Laminar flames; premixed flames; non-premixed flames; flame propagation; flame extinction

1. Introduction

The counterflow configuration was developed in the 1950s and it has been an invaluable tool for experimental study of laminar flames (e.g., [1]) along with one-dimensional (1D) models (e.g., [2]-[5]) that were subsequently developed. At the same time, computational efficiency afforded by 1D models comes at the expense of generality; only carefully designed counterflow experiments are suitable for comparison. When properly implemented, counterflow flames may provide high quality flame data over a wide range of thermodynamic conditions [1], and such data contain important physical and chemical information.

Data from two classes of experimental burner design are widely compared to 1D modeling results; straight tube burners with flow conditioning screens (e.g., [6] and [7]) and high-contraction-ratio contoured burners (e.g., [8] – [11]). Both designs are idealized to produce plug-flow conditions and the data are modeled using 1D codes by imposing zero velocity gradient boundary conditions. Flows that generate sufficiently strong stagnation pressure fields deviate from plug-flow conditions and are characterized by velocity gradients at the burner exit, which should be included as boundary conditions in modeling. A strong stagnation pressure field is often suggested from observation of a “dimple” on the flame surface that is convex on the upstream side and indicates velocity non-uniformity at the burner exit.

Early studies seeking experimental verification of 1D modeling assumptions include that of Chelliah et al. [12], who identified plug flow boundary conditions in counterflow experiments, and Rolon and coworkers [13] who concluded that realistic flow fields could fail to reproduce plug flow conditions. Frouzakis et al. [14] and Park and Hamins [15] determined that results derived from 1D and axisymmetric two-dimensional (2D) simulations closely agree when uniform axial velocity exit profiles are implemented at the burner exit. Bergthorson and coworkers [16] investigated the accuracy of 1D modeling in contoured-nozzle-generated premixed flames and found agreements provided, in part, that

the velocity boundary conditions were measured and implemented in the simulations. Oh et al. [6] used straight-tube burners with flow conditioning screens and found 1D-compatible centerline extinction for high strain rates but 2D effects for lower strain rates. Ji et al. [8] quantified the effect of boundary velocity gradients in contoured-nozzle extinction measurements. Sarnacki et al. [10] identified a stagnation pressure field of ellipsoidal geometry to be the physical mechanism causing departure from plug flow assumptions. Mittal et al. [17] attributed the departure from 1D behavior in non-uniform exit velocity profiles to the presence of temperature curvature at the system centerline as a result of flow non-uniformity. Bouvet et al. [11] studied contour-nozzle generated premixed flames and traced inconsistencies with 1D modeling to the assumption of constant pressure derivative eigenvalue. Niemann et al. [7] determined that straight tube burners with flow conditioning screens can reproduce 1D plug flow assumptions to within an accuracy of 5% in unreacting flows, allowing the use a one-parameter analytical description of the effective (global) strain rate [18] in lieu of local flow measurements. Johnson et al. [19] corroborated the assertion of Ref. 7 and further confirmed that contour-type burners are sufficiently modeled with 1D codes when appropriate boundary conditions are included.

In the present study, experiments and computations were performed to quantify the sensitivity of **measured** laminar flame speeds, S_u^0 s, and extinction strain rates, K_{ext} , in lean premixed CH₄/air and K_{ext} in non-premixed CH₄-N₂/air flames to the velocity boundary conditions in straight-tube **counterflow** burners. **The data were compared with 1D modeling results in order to assess their compatibility with 1D assumptions and highlight pitfalls** for kinetic model validation.

2. Experimental approach

The measurements were carried out in the counterflow configuration using straight-tube burners at atmospheric pressure and unburned reactant temperature $T_u = 298$ K. Burner diameter, $D = 21$ mm, and burner separation distance, $L = 15.3$ mm, were chosen to mimic the geometry of Ref. 7 and allow for well-resolved velocity measurements. Flow conditioning screens were placed within the burner tubes and two configurations studied; burners with screens $\sim 5D$ upstream from the exit, hereafter called Type A, and burners with an additional set of screens at the exit, called Type B. Flow velocities were measured using particle image velocimetry (PIV) and micron-size silicone oil as flow tracers produced by a pneumatic nebulizer (Meinhard HEN-170-A0.2). Direct flame imaging was obtained with a CMOS monochrome high-speed camera (Phantom v710). A system schematic is shown in Fig. 1.

The premixed flames studies were carried out in the symmetric twin-flame configuration (e.g. [20]) for lean CH_4/air mixtures. Non-premixed flames were established by counterflowing fuel/inert mixtures against air. S_u^0 and K_{ext} were determined using flow velocity measurements along the stagnation streamline. A reference velocity, $S_{u,ref}$, and a reference strain rate, K_{ref} , were defined as the minimum axial velocity and maximum norm of the axial velocity gradient in the axial direction, respectively, ahead of the flame front (e.g., [1], [8], and [20]). Velocity and velocity gradient boundary conditions were measured and included in 1D simulations. S_u^0 was derived using a numerically-assisted, non-linear extrapolation approach (e.g., [8] and [21]-[24]). K_{ext} was measured in both premixed and non-premixed flames by first establishing a near-limit flame and then gently reducing the fuel flow rate by up to 0.5% to achieve extinction (e.g., [8] and [21]-[24]). The uncertainty of the reported data was quantified based on repeated trials and is reported as $\pm 1\sigma$ standard deviation from the mean value. Uncertainty in flow composition has been shown to be less than 0.5% [23].

3. Modeling approach

Detailed 1D modeling was based on the Sandia CHEMKIN [25] and Transport [26] subroutine libraries. Freely propagating flames were computed with the PREMIX code [3], while the counterflow flames were simulated using an opposed-jet code [4, 24]. Both codes include radiation at the optically thin limit, Soret diffusion, and an updated description of H and H₂ diffusion coefficients [27]. The stretched flame simulations accounted for the experimental boundary velocity gradients and for a finite spatial domain of 15.3 mm. The extinction states were computed by first establishing a vigorously burning flame and subsequently increasing the boundary velocity until flame extinction was approached. Near extinction, a two-point approach was employed whereby the problem is solved with exit velocity, and thus strain rate, as a dependent variable (e.g., [8]). All simulations employed the multicomponent transport formulation. The USC Mech II kinetic mechanism [28] was reduced to include only H₂/CO/C₁-C₂ species resulting in 38 species and 249 reactions.

4. Results and discussion

4.1 Flow fields

Representative radial, v_r , and axial, v_x , velocity profiles for Type A and Type B burners were measured about 1 mm from the burner exit for an equivalence ratio $\phi = 0.542$, normalized by $|v_x|_{max}$, and are compared in Fig. 2. It can be seen that, compared to Type B, Type A burners produce strong radial nonuniformity of v_x as well as greater radial gradients of v_r , which due to continuity implies greater axial gradients of v_x . Neither configuration produces strictly plug-flow conditions but existing literature suggests that this may be accounted for in 1D modeling by including the experimental axial velocity gradients at the boundary.

Many details of the experimental flow field cannot be captured by centerline and boundary measurements, for example the distribution of v_r and its radial gradient, as well as v_x and its axial gradient as shown in Fig. 3. For the Type A burners shown in Fig. 3 (a-d), all flow quantities exhibit a radial dependence. Among those, v_x and both velocity gradients are greatest in magnitude towards the outer edges of the flow field, although the radial variation of v_x appears to diminish at x/D locations downstream. Type B burners, Fig. 3 (e-h), exhibit notably less radial dependence; v_x and both velocity gradients at the flame front are maximum in magnitude and nearly uniform over the central 50% of the radial domain. The radial non-uniformity of v_x is an explicit violation of 1D modeling assumptions in which only v_r is permitted to vary linearly with radius.

4.2 Laminar flame speeds

Experimental and computed S_u^0 s for lean CH₄/air flames are shown in Fig. 4 along with select data from Ref. 29. The computations over-predict the measurements across the whole range of conditions studied while the measured S_u^0 s using either burner type and those reported in Ref. 29 are in agreement. Given combustion theory that suggests $S_u^0 \sim \sqrt{\omega}$, where ω the overall reactivity, the results in Fig. 4 suggest that for the present conditions the experimentally observed reactivity is overpredicted by the computations. The kinetic model is known to overpredict the reactivity of lean CH₄/air flames (e.g., [29]), explaining thus the difference between computed and measured values.

As both Type A and Type B data are the same, the experimentally determined S_u^0 was found to be insensitive to the exit velocity profile shape, in apparent contradiction with the observations of Ref. 17. However, in Ref. 17 the differences between uniform and non-uniform exit velocity profiles were 3-5% in $S_{u,ref}$, which are within the experimental uncertainties, and up to 8% in K_{ref} . For CH₄/air flames the Lewis number, Le , is slightly less than one and strain rate only weakly affects flame intensity. Thus the sensitivity of S_u^0 to variations in K_{ref} is small for low strain rate values [30, 31] and the overall uncertainty is dominated by $S_{u,ref}$. These observations may not apply to flames with sufficiently large Le due to greater sensitivity of flame intensity to strain rate.

4.3 Premixed flame extinction

Experimental and computed K_{ext} for lean, premixed CH₄/air flames are shown in Fig. 5(a). The simulation results again overpredict the data, which is consistent with the propagation results. Direct comparison of experimental results between different burner types is inappropriate because K_{ext} increases with increasing boundary velocity gradient [8]. This effect is demonstrated in the modeling results of Fig. 5(a) where the increased boundary velocity gradients measured in Type A burners result in greater K_{ext} values relative to Type B that exhibits milder exit velocity gradients.

The K_{ext} data obtained with different burner types were compared indirectly through 1D simulations. As $K_{ext} \sim \omega$ (e.g., [23]), the notable sensitivity of K_{ext} to kinetics means that any uncertainties in its measurement could impact the validation of various rate constants in detailed kinetic models. The quantity $\frac{K_{ext,sim}}{K_{ext,exp}}$ can be interpreted as a comparison of the overall reactivity suggested by simulations to that measured reactivity; it approaches unity when simulations and experiments agree.

Figure 5(b) depicts the variation of $\frac{K_{ext,sim}}{K_{ext,exp}}$ with ϕ and it can be seen that the predicted values exceed the measured ones, in Type A burners non-monotonically up to a factor of 2.4 and in Type B burners monotonically up to a factor of 1.7. The interpretation of the global reactivity based on the data derived in Type A and Type B burners differ, which suggests that at least one data set is incompatible with the 1D modeling results.

Given the sub-unity Le for CH_4/air mixtures, the flames are strengthened by increasing strain rate, merge at the stagnation plane, and become restrained from further movement whereupon insufficient chemical residence time leads to extinction [32]. It is also known that the flame surface follows the shape of the incoming flow field (e.g. [33]). Therefore, in nonuniform v_x profiles generated by Type A burners (Figs. 2(a) and 3(b)), the flames will first approach the stagnation plane at locations away from the centerline where extinction then initiates. These flames can appear visually planar near extinction because symmetry and conservation of momentum dictate that axial flow velocity must approach zero close to the stagnation plane.

The dynamic behavior of the extinction process was captured with a high-speed camera and images are shown in Fig. 6. Time $t = 0$ ms corresponds to the moment the extinction process initiates. Extinction in Type A burners was found to initiate at a location away from the centerline, followed by transition to a propagating edge flame which momentarily surrounded the still-burning flame core, and eventually resulting in global extinction around $t = 70$ ms; note that unavoidable minor asymmetry in

the burner alignment caused the initiation of extinction on the right edge of the images. For Type B burners on the other hand, extinction initiates near the centerline before transitioning to an outwardly propagating edge flame followed by global extinction at $t = 30$ ms. It should be noted that both burners produced apparently flat flame shapes, suggesting that a visual inspection of flame geometry is not sufficient to ensure flow field quality.

When extinction initiates on the centerline, the direction of edge flame propagation coincides with that of v_r while for off-center extinction the edge flame propagates opposite to v_r . This resulted in the different time scales from initiation to completion of the extinction process, e.g. 30 vs. 70 ms, of Fig. 6; discussion on edge flame dynamics may be found in, e.g., Ref. 34.

Several physical mechanisms result in the trends observed in premixed flame extinction. Locally off-center extinction transitioning to global extinction in Type A burners produces K_{ext} values that are systematically lower because the measured centerline velocity profiles are not representative of the extinction state. Additionally, the magnitude of flow non-uniformity has been shown [7] to scale with flow momentum and burner separation distance as $\rho v_x^2 \left(\frac{D}{L}\right)^2$. For a fixed L/D , extinction of stronger flames (higher ϕ) necessitates greater v_x . As isocontours of the stagnation pressure in counterflow are ellipsoidal in shape [10], the centerline velocity is preferentially decelerated compared to the edges, enhancing the exit velocity non-uniformity with increasing flow rate. There is also a buoyancy effect, which is typically negligible along the system centerline for all but the lowest strain rates. However, buoyancy can play an important role in the flame periphery even before the centerline is affected (e.g., [35]).

Based on this analysis, the differences of K_{ext} values measured along the centerline of Type A and Type B burners is attributed to the non-uniformity of the incoming flow that causes off-center extinction initiation for the Type A burners. The difference between the data measured using Type B burners and computed K_{ext} values is attributed to kinetic effects, as demonstrated in previous studies for lean

CH₄/air flames (e.g., [29]). Consequently, the non-monotonic behavior for Type A flames shown in Fig. 5(b) may be explained by buoyancy for the lower ϕ s, which more directly affects the fluid mechanics of the jet outer edges. For higher ϕ s, the boundary flow non-uniformity increases with the flow rate as discussed earlier and the off-center extinction propensity is magnified. The conclusions derived for the near-unity Le CH₄/air flames are expected to hold for mixtures in which differential diffusion plays a more profound role.

4.4 Non-premixed flame extinction

Experimental and computed K_{ext} for non-premixed CH₄-N₂/air flames are shown in Fig. 7. As with premixed flame extinction, a direct comparison of the experimental results is inappropriate due to different boundary velocity gradients. As with premixed extinction, the notable sensitivity of non-premixed K_{ext} to kinetics [23] dictates that any uncertainties in its measurement could impact the validation of reaction rate parameters.

Data derived with Type B burners are within 30% of the modeling predictions for all cases and the agreement is improved with increasing fuel mole fractions, X_{CH_4} . In contrast, the agreement between data derived in the Type A burners and predictions becomes notably less with increasing X_{CH_4} , up to a factor of 2.6. Similar to premixed flame extinction, the extinction of non-premixed flames initiates at off-center locations for Type A burners and at the center for Type B burners. The velocity gradients and strain rate distributions were determined to be similar to those shown in Fig 3. The relatively close agreement between the computed and measured K_{ext} values in Type B burners does not contradict the results of Fig. 5(a) as the kinetic regimes are different.

5. Concluding remarks

Laminar flame speeds and extinction rate rates of premixed CH_4/air flames and extinction strain rates of non-premixed $\text{CH}_4\text{-N}_2/\text{air}$ flames were measured in the counterflow configuration with burners producing at their exits either uniform or non-uniform axial velocity profiles. Experimental data were simulated with a one-dimensional code and a detailed C_2 kinetic model. Inconsistencies were observed between one-dimensional modeling results and centerline extinction measurements in burners with non-uniform exit axial velocity profiles, leading to large disagreements between computed values and data. In burners with uniform exit axial velocity profiles, one-dimensional modeling was found to be appropriate for centerline extinction measurements and these measurements were in substantially better agreement with the computed values. The flame speed measurements were found to be insensitive to the burner exit axial velocity shape. Thus, the impact of flow field shape on the presently studied flame properties was demonstrated and the implication for validation of kinetic rate parameters was evaluated. Though analysis was limited to straight-tube burners, it is likely that the effects of flow non-uniformity could appear in any counterflow configuration where both the stagnation pressure gradients are sufficiently high and the location of flow-conditioning screens sufficiently far upstream from the burner exit.

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Figure Captions:

Figure 1: Schematic of the experimental system as configured for symmetric, premixed flames.

Figure 2: Flow velocity profiles measured 1 mm from the burner exit near extinction for $\phi = 0.542$: (a) Type A and (b) Type B burners.

Figure 3: Comparison of normalized flow field structure near extinction for $\phi = 0.542$ Type A burner (a-d) and Type B burners (e-h). Lightest (darkest) color corresponds to maximum (minimum) value.

Figure 5: Extinction strain rates of premixed CH₄/air mixtures: (a) measured and computed results and (b) ratio of computed to measured values.

Figure 6: Evolution of the extinction process for lean CH₄/air flames produced by Type A (a-d) and Type B (e-h) burners.

Figure 7: Extinction strain rates of non-premixed CH₄-N₂/air flames. (a) measured and computed results and (b) ratio of computed to measured values.

Figure 1: Schematic of the experimental system as configured for symmetric, premixed flames.

Figure 2: Reacting flow velocity profiles measured 1 mm from the burner exit near extinction for $\phi = 0.542$: (a) Type A and (b) Type B burners.

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Figure 4: Experimental and computed laminar flame speeds of CH_4/air mixtures.

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