The effect of mixture composition on stabilized flames in a meso-scale channel with a wall temperature gradient

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The characteristics of stable premixed combustion are studied in a heated tube with a fixed wall temperature gradient. These flames are examined experimentally and with a 1-D, volumetrically-averaged computational model with detailed chemistry. The heated tube concept is a simple, quasi one-dimensional burner configuration which has relevance to new burner technologies that utilize small channels to support stable combustion. Flames in these devices have reaction zone thicknesses that are on the same order as the tube diameter, therefore heat transfer to and from the walls is an important phenomenon that governs burning rate and stabilization position.

Two parameters of considerable importance in scaling this problem are the flame speed, S_{L}, and flame thickness, δ_{f}, given by the classic Thermal Theory [2] as

$$S_{\mathrm{L}} \propto \sqrt{\frac{\alpha_{\mathrm{eff}}}{\tau_{\mathrm{c}}}}, \qquad \delta_{\mathrm{f}} \propto \sqrt{\alpha_{\mathrm{eff}} \tau_{\mathrm{c}}}, \tag{1}$$

where α_{eff} is the effective thermal diffusivity and τ_{c} is the combustion time. In a standard flame, the system is defined by flame speed by setting the burning rate. However, as the tube becomes smaller heat losses become more important and the flame thickness becomes a controlling parameter. These parameters are thought to scale the burning rate and heat loss, respectively. The large activation energy model of Minaev et al. [4] is particularly successful in using these parameters to describe the approximate features of flame stabilization over a wide inlet velocity, S_{u}, range. These fundamental parameters are a function of mixture composition only. Therefore, it is necessary verify that flame speed and flame thickness are able to scale the flame stabilization phenomenon over a wide range of mixture composition.

This work is an extension of that by Maruta et al. [3] who studied the flame characteristics of a fuel lean premixed methane-air mixture in a similar experimental configuration. The present study extends this work by carrying out measurements for stoichiometric and rich mixture compositions.

1 Apparatus and method

A vertical, cylindrical tube with an inner diameter of $D = 2\ \mathrm{mm}$ is used as the flow channel. This tube is made of transparent quartz for direct visual observation of combustion inside the tube. The downstream portion of the tube is circumferentially heated by radiant heaters to set up a steady, smooth, monotonically increasing wall temperature gradient along the tube surface. The highest downstream

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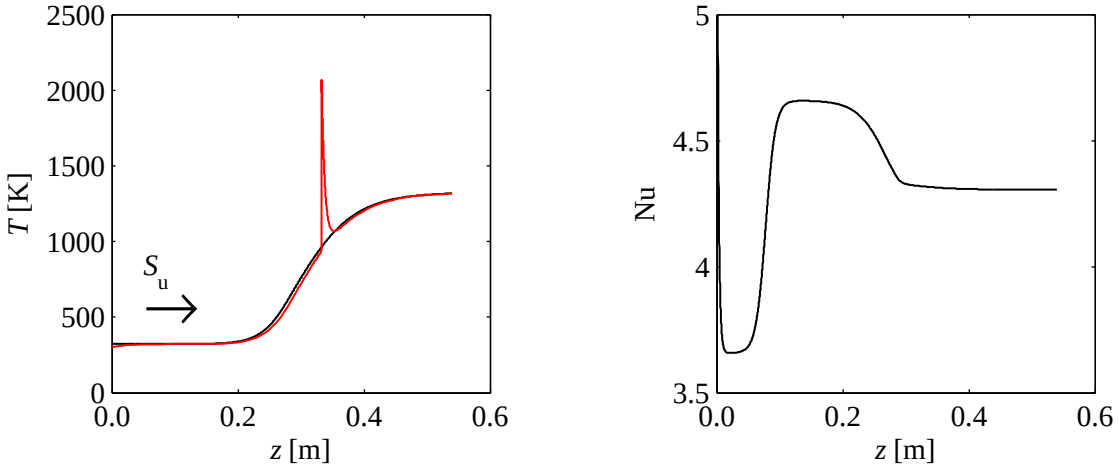

Figure 1: Computationally obtained flame profiles. (a) Gas (red) and wall (black) temperature. (b) Nusselt number calculated from the cold boundary layer. $\phi = 1.0$, $S_\mathrm{u} = 1.00$ m/s, $T_\mathrm{u} = 300$ K, $T_\mathrm{af} = 2223$ K.

wall temperature used in the experiments is $T_\mathrm{w} = 1320$ K which is sufficient to induce auto ignition, but is lower than the adiabatic flame temperatures of the mixtures. It should be noted that the length of the temperature gradient used in these experiments is 0.54 m, which is quite long when compared to similar reactors used in other studies [3]. The length allows for the study of a wider range of mixture compositions, especially fuel-rich mixtures, with a high sensitivity apparatus in the respect that small changes in heat release cause large changes in flame position.

Metered methane/air mixtures at fuel lean, stoichiometric and rich equivalence ratios and variable total flow rates are supplied at the inlet of the burner to create the stabilized flame front within the temperature gradient zone of the tube. The parameters for these mixtures are shown in Table 1. To test the effect of composition, nitrogen diluent and oxygen concentrations are chosen to tailor the adiabatic flame speed and thickness of the mixtures.

Modeling the effects of lean and rich chemistry on these flames requires that the conservation equations be solved with detailed chemical kinetics mechanisms and variable transport properties. With the assumption of a 1-D flame, the model for a stable combustion wave reduces to calculation of the steady state solution for a system of coupled differential equations described by the conservation of mass, energy, and the mass transfer of the chemical species:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho U) = 0 \tag{2}$$

$$\rho c_p U \frac{\mathrm{d}T}{\mathrm{d}z} = \frac{\mathrm{d}}{\mathrm{d}z}\left(\lambda \frac{\mathrm{d}T}{\mathrm{d}z}\right) - \sum_i Y_i V_i (\rho c_p)_i \frac{\mathrm{d}T}{\mathrm{d}z} - \sum_i \dot{\omega}_i h_i W_i - \frac{4\lambda \mathrm{Nu_z}}{D^2}(T_\mathrm{g} - T_\mathrm{w}) \tag{3}$$

$$\rho U \frac{\mathrm{d}Y_i}{\mathrm{d}z} = -\frac{\mathrm{d}}{\mathrm{d}z}\left(\rho Y_i V_i\right) + \dot{\omega}_i W_i \tag{4}$$

The numerical algorithms needed to solve these equations are well established and are readily available in premixed laminar flame codes. Models in this study are solved with the CANTERA software package [1] and the GRI-Mech 3.0 kinetics mechanism [5].

Figure 1(a) shows the wall temperature and a typical gas temperature profile obtained from the computation. The flame is marked by the sharp temperature peak. In Equation 3, Newton's Law of Cooling and

Table 1: Mixture parameters. Normalized equivalence ratio, $\Phi = \phi/(1+\phi)$. Flame thickness, $\delta_f = (T_{af} - T_u)/(\mathrm{dT/dz}|_{max})$. All parameters are calculated from an adiabatic free flame with the GRI-Mech 3.0 kinetics mechanism.

Mixture	ϕ (Φ)	%O_2	%N_2	T_u [K]	T_{af} [K]	S_L [m/s]	δ_f [mm]
A	1.0 (0.50)	21.0	79.0	300	2230	0.372	0.436
B	0.7 (0.41)	21.0	79.0	300	1843	0.190	0.655
C	1.4 (0.58)	21.0	79.0	300	1978	0.137	1.000
D	1.0 (0.50)	17.2	82.8	300	2015	0.204	0.677
E	1.0 (0.50)	15.4	84.6	300	1888	0.136	0.918
F	0.7 (0.41)	25.8	74.2	300	2087	0.369	0.407
G	1.4 (0.58)	26.9	73.1	300	2253	0.372	0.447

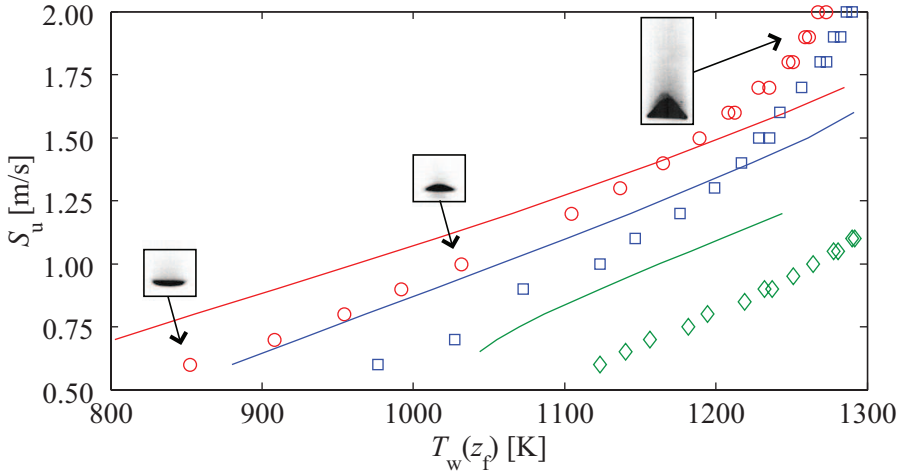

Figure 2: Experimental (symbols) and simulated (lines) trends in flame stabilization wall temperature, $T_w(z_f)$, due to flame speed, S_L. Stoichiometric mixture A (red, ○, —), lean mixture B (blue, □, —), rich mixture C (green, ◇, —).

a varying, local Nusselt number profile is used to model interfacial heat transfer between the gas and the channel walls. This Nusselt number is determined by numerically solving the thermal boundary layer equation neglecting a source term for the effect of chemical heat release. Figure 1(b) shows the resulting Nusselt number profile used for this case. This "cold" boundary layer approximation is accurate outside the reaction zone where there is no appreciable chemical heat source, however the model under-predicts heat loss inside the flame not resolving steep radial wall temperature gradients caused by non-linear heat release [6].

2 Results and discussion

Figure 2 shows a summary of flame position data obtained experimentally and numerically for mixtures A, B and C. This figure shows inlet flow velocity, S_u, verses the wall temperature at the flame stabilization position, $T_w(z_f)$. These are strongly burning, stable, symmetric flames that have a unique stabilization position within the wall temperature profile. For each mixture, the flame position progressively moves upstream to lower wall temperatures with decreasing inlet flow velocity. Below the lower velocity limit shown in Figure 2, unstable "flames with repetitive extinction and ignition" (FREI) were observed [3]. It is not possible to reproduce FREI with the present numerical model due to the highly

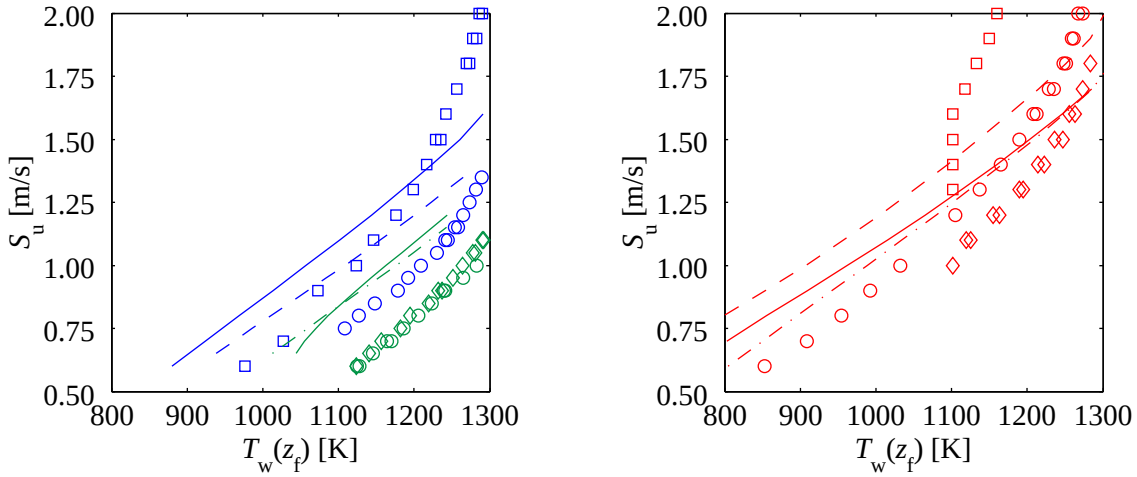

Figure 3: Experimental (symbols) and simulated (lines) trends in flame stabilization wall temperature, $T_w(z_f)$, with flame speeds, S_L, matched via nitrogen-to-oxygen ratio. (a) Lean mixture B (blue, —, □) is matched with stoichiometric, diluted mixture D (blue, – –,○). Rich mixture C (green, ◇, —) is matched with stoichiometric, diluted mixture E (green, ○, – · –). (b) Stoichiometric mixture A (red, ○, —) is matched with lean, enriched mixture F (red, □, – –) and rich, enriched mixture G (red, ◇, – · –).

unsteady flame conditions, therefore flames in this regime are not considered.

The general trends for flame position can be extracted from the experimental and numerical data in Figure 2. It is clear from the figure that flame speed is a leading-order effect for these flames. Flames with higher flame speeds (see Table 1) have faster burning rates resulting in stabilization positions at lower wall temperatures.

The discrepancies in simulated and experimental flame stabilization position result from two-dimensional interfacial heat transfer and curvature. This is apparent when looking at the relative position and shape of the stoichiometric flames (mixture A). At low inlet velocities simulated flames with the cold boundary layer predict positions which are consistently upstream of those obtained experimentally. These simulations neglect the effect of heat release on interfacial heat transfer and, thus, underestimate heat loss inside the reaction zone. Flame position is also affected by an increase in flame area perpendicular to the reactant stream caused by curvature which results in an increase in burning rate. Flames at the lowest velocities are relatively flat, however they become quite curved due to hydrodynamic stretch. This effect is quite strong at the highest velocities where curved experimental flames are upstream of predicted stabilization positions even with an underestimate of heat loss inside the reaction zone provided by the cold boundary layer model.

To clarify the effects of flame thickness, δ_f, mixtures are also tuned to have the same flame speed by modification of nitrogen-to-oxygen ratio. In Figure 3(a), mixture D and E have stoichiometric equivalence ratios, but are made to have similar flame speeds to mixtures B and C, respectively. Similarly, lean and rich mixtures F and G are tuned to match the flame speed of mixture A in Figure 3(b). However, matching S_L through the ratio of α_{eff} and τ_c does not ensure that the product of these variables will give equivalent flame thicknesses (see Equation 1). Figure 4 gives stabilization positions which are close to, but do not exactly match corresponding mixtures at the same inlet flow velocity, but these mixtures do capture the second-order dependence of flame thickness. Flame location and thickness are correlated in that thinner flames have lower heat loss and, therefore, sit upstream of thicker flames.

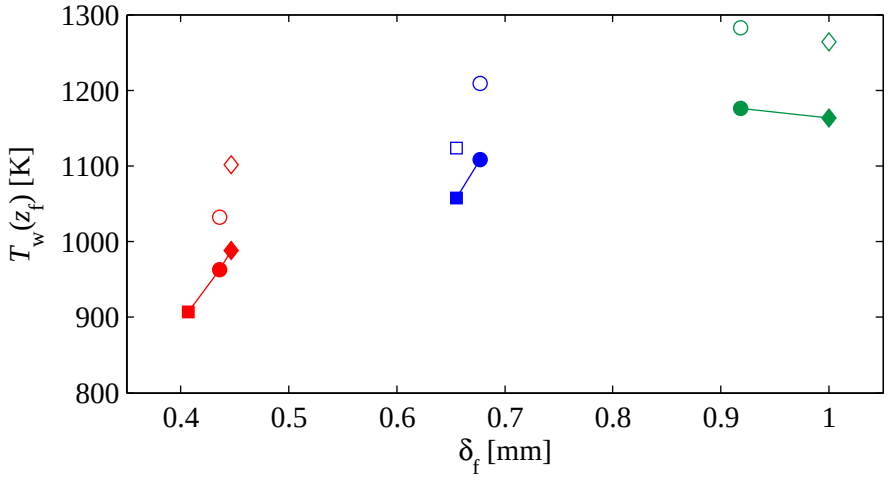

Figure 4: Experimental (symbols) and simulated (lines) flame stabilization wall temperature, $T_{\rm w}(z_{\rm f})$, verses flame thickness, $\delta_{\rm f}$ for an inlet flow velocity of $S_{\rm u} = 1.00$ m/s. Legend as in Figure 3.

3 Acknowledgements

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References

[1] Goodwin, D. (2003). An open-source, extensible software suite for CVD process simulation. In *Proceedings of CVD XVI and EuroCVD Fourteen*, pages 155–62. Electrochemical Society.

[2] Mallard, E. and LeChatelier, H. (1883). Combustion des melanges gazeux explosifs. *Ann. Mines*, 4:274–381.

[3] Maruta, K., Kataoka, T., Kima, N., Minaev, S., and Fursenko, R. (2005). Characteristics of combustion in a narrow channel with a temperature gradient. *Proc. Combust. Inst.*, 30:2429–36.

[4] Minaev, S., Maruta, K., and Fursenko, R. (2007). Nonlinear dynamics of flame in a narrow channel with a temperature gradient. *Combust. Theor. Model.*, 11(2):187–203.

[5] Smith, G. P., Golden, D. M., Frenklach, M., Moriarty, N. W., Eiteneer, B., Goldenberg, M., Bowman, C. T., Hanson, R. K., Song, S., Gardiner, W. C., Lissianski, V. V., and Qin, Z. (2000). GRI-Mech 3.0. http://www.me.berkeley.edu/gri_mech/.

[6] Watson, G. and Bergthorson, J. (2011). The effect of chemical energy release on heat transfer from flames in small channels. *Combust. Flame*. submitted.