Computational investigation of rod-stabilized laminar premixed hydrogen–methane–air flames

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A computational study of steady, rod-stabilized, inverted, lean, CH₄–air and H₂–CH₄–air flames is conducted. For the CH₄–air flames, either decreasing the inlet equivalence ratio or increasing the mean inflow velocity leads to a larger standoff distance, and below a critical value of the inlet equivalence ratio or above a critical value of the inflow velocity, the flame blows off. For the H₂–CH₄–air flames, decreasing the inlet equivalence ratio has similar effects as those on the CH₄–air flames; however, increasing the inflow velocity reduces the standoff distance. Though counter-intuitive, the predicted behaviour of the flames is consistent with the experimental observations. Both the CH₄–air and H₂–CH₄–air flames exhibit preferential diffusion effects such as superadiabatic temperatures and local equivalence ratio variations, which are more pronounced for the H₂–CH₄–air flames, displaying non-uniform and localized consumption rates of the fuel components. The strong diffusion of H₂ plays an important role to maintain and even strengthen the reaction processes in the anchoring region and the counter-intuitive stabilization/blow-off of the H₂–CH₄–air flames.

I. Introduction

The understanding of stabilization mechanisms of premixed flames at lean conditions is important for the design of more efficient and less polluting combustion devices that can operate safely. Besides, there is a growing interest in the utilization of hydrogen-containing (H₂-containing) fuel blends that can potentially enhance the stability and reduce the pollutant emissions of lean premixed flames.

Inverted conical or V-shaped flames stabilized downstream of the trailing edge of either a cylindrical rod or a thin plate are commonly employed to study the stabilization and blow-off mechanisms of premixed flames. The inverted flame configuration is frequently adopted for such studies because the base of the flame is symmetric and unaffected by the surrounding environment. Moreover, the findings associated with the stabilization mechanisms of inverted flames are applicable to a wider class of flames, for instance those present in multi-slit or multi-hole burners utilized in domestic and industrial heating systems. According to the literature [1–11], heat loss to the flame holder, flame stretch induced by flow straining and local flame curvature, and mixture non-equidiffusive properties at the flame base have been identified as the main factors influencing the stabilization and blow-off of inverted flames, yet no consensus has been achieved on the relative role and importance of each of these factors.

In a study of particular interest, Shoshin et al. [11] reported measurements on stabilization/blow-off limits for CH₄–air and H₂–CH₄–air flames stabilized on metallic rods finding what they referred to as the “anomalous” stabilization and blow-off behaviour of H₂–CH₄–air flames for mixtures with certain H₂ content and described as follows: “Stabilization of such flames was possible only when the mixture velocity exceeded some critical value. Flames were blown off when the mixture velocity was reduced below this value. The stand-off distance above the flame holder for those flames decreased and heat transfer from the flame base to the flame holder became more intense when the mixture velocity was increased. This is opposite to the regular behavior of inverted flames.”

The goal of this work is to provide new insights into the characteristics of inverted flames through high-fidelity simulations and computational singular perturbation analysis (CSP), taking as a reference selected conditions of the

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flames studied by Shoshin et al. [11]. To this end, two-dimensional simulations of steady, rod-stabilized, inverted, lean, CH_4 -air and H_2 - CH_4 -air premixed laminar flames are performed. For the H_2 - CH_4 -air flames, mixtures with a mole fraction of H_2 in the fuel, $\chi = n_{\text{H}_2} / (n_{\text{H}_2} + n_{\text{CH}_4})$, equal to 0.4 are considered.

II. Configuration and solution method

The experimental configuration is described in detail by Shoshin et al. in Reference [11]. Inverted flames were stabilized above the top end of a cylindrical rod. The top end of the rod was approximately 0.5 mm above the top edge of the tube. The configuration is represented schematically in Fig. 1. The present study is restricted to a copper rod having a diameter of 2 mm and mixtures with 40% or 0% H_2 content in the fuel, specified on a molar basis. For the 2 mm diameter rod these two mixtures are representative of the normal blow-off (0% H_2) and the so called anomalous blow-off (40% H_2).

Fig. 1 Schematic of the flame configuration and computational domain.

Six cases for different values of inlet equivalence ratio, ϕ_{in} , and mean inlet velocity, U_{in} , of the premixed mixture are considered for the simulations. The conditions for the various cases under study have been selected such that the influence of an increase in the mean inflow velocity at a reference inlet equivalence ratio and a decrease in the inlet equivalence ratio at a reference mean inflow velocity can both be examined. At the same time, the chosen conditions are representative of the normal and counter-intuitive stabilization behaviour. The conditions for all the cases are summarized in Table 1. The cases B and E are the reference situations for the CH_4 -air and H_2 - CH_4 -air flames, respectively. The cases A and D allow to study the effect of decreasing the inlet equivalence ratio on the characteristics of the CH_4 -air and H_2 - CH_4 -air flames, respectively. Similarly, the cases C and F allow to analyze the influence of increasing the mean inflow velocity.

A rectangular domain with a height, $L = 40$ mm, and width, $R = 8$ mm, is used. The axis of symmetry is aligned with the left boundary of the domain. The right and top boundaries are treated as subsonic outflows. A schematic representation of the computational domain is displayed in Fig. 1. For both outflow boundaries Neumann boundary conditions are applied to all variables except for pressure, which is held constant and has a value of one atmosphere. The bottom is divided into three regions. The innermost region ($r = 0$ mm to $r_1 = 1$ mm) corresponds to the rod and it extends vertically 0.5 mm into the domain. The adjacent region ($r_1 = 1$ mm to $r_2 = 6.2$ mm) is the inlet that feeds the premixed mixture at 298 K with a velocity profile corresponding to the steady flow through an annular tube [12, Ch. 7]. The next region of width 1.8 mm is associated with the tube top edge thickness. Isothermal no-slip boundary conditions are applied to the rod and tube top edge.

To model the flames the conservation equations for mass, momentum, energy and species are solved. The flow is treated as a continuous, multicomponent, compressible, and thermally-perfect mixture of gases that obeys the ideal gas equation of state. The governing equations are solved using a body-fitted, multi-block, adaptive mesh refinement,

Case	Fuel	$\mathcal{X} = \frac{n_{\text{H}_2}}{n_{\text{H}_2} + n_{\text{CH}_4}}$ (—)	ϕ_{in} (—)	U_{in} (m/s)
A	CH ₄	0	0.68	1.85
B	CH ₄	0	0.69	1.85
C	CH ₄	0	0.69	2.5
D	H ₂ -CH ₄	0.4	0.48	1.85
E	H ₂ -CH ₄	0.4	0.49	1.85
F	H ₂ -CH ₄	0.4	0.49	2.5

Table 1 Summary of characteristic conditions for the cases that have been studied.

finite-volume framework that has been originally developed by Groth and co-researchers [13–15], and extended by Hernández Pérez et al. [16–19]. For brevity the governing equations are omitted here, but they are fully described in axisymmetric form in Ref. [17].

Chemical kinetics is described by the GRI-Mech 3.0 reaction mechanism [20], assuming nitrogen (N₂) to be inert (36 species, 219 reactions), while transport is described by the mixture-averaged model. Thermal radiation is accounted for via the optically-thin Planck model, with the Planck mean absorption coefficient of the mixture being evaluated from the major radiating species CO₂, H₂O and CO.

The computational domain is initially discretized with 6 blocks in the radial direction and 12 blocks in the vertical direction and later refined during the computation. Each block contains 10 × 12 quadrilateral cells. The steady state solutions are obtained with four levels of refinement and a minimum cell size of 16.1 μm, providing sufficient resolution of both the flame front and the flow field as well as grid-independent solutions.

III. Computational singular perturbation (CSP) algorithmic tools

Consider the system of species and energy governing equations in the general form of

$$\frac{d\mathbf{z}}{dt} = \mathbf{L}(\mathbf{z}) + \mathbf{g}(\mathbf{z}), \quad (1)$$

where $\mathbf{z}$ is a $(N + 1)$ -dimensional column vector including N species mass fractions and temperature ($\mathbf{z} = [\mathbf{y}, T]^T$), $\mathbf{L}(\mathbf{z})$ represents the spatial operators (convection and diffusion) and $\mathbf{g} = \hat{\mathbf{S}}_1 R^1 + \dots + \hat{\mathbf{S}}_{2K} R^{2K}$ represents the chemical source term, where $\hat{\mathbf{S}}_n$ and R^n are the generalized stoichiometric vector and rate of the n -th unidirectional reaction, respectively, and $2K$ is the total number of unidirectional reactions. According to the CSP theory, Eq. 1 can be cast in the form of

$$\frac{d\mathbf{z}}{dt} = \sum_{n=1}^{N+1} \mathbf{a}_n f^n, \quad f^n = \mathbf{b}^n \cdot [\mathbf{L}(\mathbf{z}) + \mathbf{g}(\mathbf{z})], \quad (2)$$

where $\mathbf{a}_n$ is the $(N + 1)$ -dimensional CSP column basis vector of the n -th mode, f^n is the related amplitude and $\mathbf{b}^n$ is the corresponding $(N + 1)$ -dimensional row dual basis vector ($\mathbf{b}^i \cdot \mathbf{a}_j = \delta_j^i$) [21–23]. In the current analysis, the CSP vectors $\mathbf{a}_n$, $\mathbf{b}^i$ have been approximated, respectively, by the right and left eigenvectors of the Jacobian $\mathbf{J}$ of the chemical source term [24–28]. Each CSP mode is characterized by two components: (i) a timescale, which is approximated by the inverse norm of the related eigenvalue ($\tau_i = \frac{1}{\|\lambda_i\|}$) and sets the timeframe of action of that mode and (ii) an amplitude, which signifies the impact of the mode to the system’s slow evolution. When M timescales become exhausted, the reduced model can be generated [21–23]:

$$f^m \approx 0 \quad (m = 1, \dots, M), \quad \frac{d\mathbf{z}}{dt} \approx \sum_{n=M+1}^{N+1} \mathbf{a}_n f^n. \quad (3)$$

The system of the M algebraic equations ($f^m \approx 0$) defines a low dimensional surface, known as slow invariant manifold (SIM), on which the solution evolves, while the system of ordinary differential equations (ODEs) governs the slow

evolution of the solution on the *SIM* and its dynamics is characterized by the fastest of the slow time scales ($M + 1$), when the solution evolves sufficiently far from the boundaries of the *SIM* [29]. The identification of the slow characteristic CSP mode (i.e., the $M + 1$ mode) can be achieved only in the context of a reduced model, where the fast and slow modes can be well-defined [30–34]. The sign of the real part of the eigenvalue associated with each mode determines the mode’s nature: a positive or negative real part indicates an explosive or dissipative mode, respectively. Previous studies have shown that explosive modes are closely related to flame propagation and ignition phenomena [24, 26, 31, 35–37] and recently to (super)-knock events [27]. It is highlighted, though, that the selection of the system’s explosive mode as a characteristic one is not straightforward and has to be investigated case by case, since its timescale has to be among the fastest of the slow ones (i.e., either the $M + 1$ or close to the $M + 1$ mode) and its amplitude has to be dominant [28, 32, 33, 38]. In the current study, the analysis revealed that an explosive mode, when existent, was indeed the characteristic one, in accordance with previous related studies [26, 27, 32, 33, 35–38]. Therefore, in the following, the analysis will focus on the examination of the system’s fast explosive mode.

The eigenvalue of the n -th mode can be expressed as $\lambda_n = \beta^n \cdot \mathbf{J} \cdot \alpha_n$, where α_n and β^n are the n -th right (column) and left (row) eigenvectors of $\mathbf{J}$, respectively. Since

$$\mathbf{J} = \text{grad}(\mathbf{g}) = \text{grad}(\hat{\mathbf{S}}_1 R^1) + \cdots + \text{grad}(\hat{\mathbf{S}}_{2K} R^{2K}), \quad (4)$$

it follows that

$$\lambda_n = \beta^n \cdot \sum_{k=1}^{2K} \text{grad}(\hat{\mathbf{S}}_k R^k) \cdot \alpha_n. \quad (5)$$

For all the results related to the CSP analysis, the CSPTk package was employed [39], a software employing the TChem package [40] for the thermo-kinetic database management.

IV. Results and discussion

A. Overall features of the flames

Figure 2 shows temperature contours and the blocks associated with the steady-state solutions obtained for all the cases listed in Table 1. Figures 2(a), 2(b) and 2(c) correspond to the cases A, B and C, respectively, for the CH_4 –air mixtures, whereas Fig. 2(d), 2(e) and 2(f) correspond to the cases D, E and F, respectively, for the H_2 – CH_4 –air mixtures. The top end of the rod is represented by the white region at the bottom of each subfigure.

By taking case B as a reference for the CH_4 –air mixtures, it can be seen that a decrease in inlet equivalence ratio (from 0.69 to 0.68) while keeping the same inlet velocity (Fig. 2(a)) leads to an increase in the standoff distance. Likewise, an increase in the mean inlet velocity (from 1.85 m/s to 2.5 m/s) while keeping the same inlet equivalence ratio leads to an increase in the standoff distance (Fig. 2(c)).

By taking case E as a reference for the H_2 – CH_4 –air mixtures, it can be observed that either a reduction in the inlet equivalence ratio (from 0.49 to 0.48) while maintaining the same inlet velocity (Fig. 2(e)) or an increment in the mean inlet velocity (from 1.85 m/s to 2.5 m/s) while maintaining the same inlet equivalence ratio (Fig. 2(f)) gives rise to a smaller change in the standoff distance, as compared to the CH_4 –air flames. Qualitatively this is consistent with the so called anomalous behaviour that was observed and reported by Shoshin et al. [11]. Furthermore, a comparison between the solutions for cases B (Fig. 2(b)) and E (Fig. 2(e)), i.e. the reference cases, shows that the flame corresponding to the H_2 – CH_4 –air mixture stabilizes closer to the rod, despite its lower inlet equivalence ratio.

The inverted flames display superadiabatic temperatures for the H_2 – CH_4 –air flames (the laminar flame speed, s_1 , thermal thickness, δ_{th} , and adiabatic flame temperature, T_{ad} , of 1D unstretched flames as well as maximum temperature, T_{max} , and temperature at the peak-heat-release point, T_r , of the inverted flames are all provided in Table 2).

To compare the flame shape in more detail and determine the standoff distances of the flames, isotherms corresponding to the maximum heat release in the flames are extracted for each case. The flame position is defined as the location of the maximum heat release, which identifies the location of the flame inner layer. The values of the standoff distance, h_f , are given in Table 2. By taking case B as a reference for the CH_4 –air flames, both the increase in the mean inflow velocity of the mixture (case C) and the decrease in the inlet equivalence ratio (case A) increase the standoff distance, which is larger for the former, and decrease the aperture of the conical flame front.

By taking case E as reference for the H_2 – CH_4 –air flames, both the increment in the mean inflow velocity of the mixture (case F) and the reduction in the inlet equivalence ratio (case D) reduce the aperture of the conical flame front. However, in terms of the standoff distance, the reduction in inlet equivalence ratio results in a slight increment in

Fig. 2 Temperature (K) distribution and computational blocks of the adaptively refined mesh corresponding to each steady-state numerical solution. (a) CH₄-air flame, $\phi_{in} = 0.68$ and $U_{in} = 1.85$ m/s. (b) CH₄-air flame, $\phi_{in} = 0.69$ and $U_{in} = 1.85$ m/s. (c) CH₄-air flame, $\phi_{in} = 0.69$ and $U_{in} = 2.5$ m/s. (d) H₂-CH₄-air flame, $\phi_{in} = 0.48$ and $U_{in} = 1.85$ m/s. (e) H₂-CH₄-air flame, $\phi_{in} = 0.49$ and $U_{in} = 1.85$ m/s. (f) H₂-CH₄-air flame, $\phi_{in} = 0.49$ and $U_{in} = 2.5$ m/s. The top end of the rod is represented by the white region at the bottom of each subfigure.

Case	1D flames			Inverted flames (centerline)				
	s_l (cm/s)	δ_{th} (mm)	T_{ad} (K)	T_{max} (K)	T_r (K)	h_f (mm)	h_0 (mm)	s_d (cm/s)
A	17.6	0.71	1810	1812	1507	3.78	3.58	10.9
B	18.3	0.69	1827	1827	1499	2.06	1.91	8.62
C	18.3	0.69	1827	1828	1497	3.85	3.9	-2.64
D	6.3	1.55	1469	1600	1361	2.69	2.52	8.52
E	7.0	1.42	1488	1614	1352	1.01	0.97	1.33
F	7.0	1.42	1488	1615	1347	0.82	1.09	-9.32

Table 2 Summary of flame speeds (s_l), thermal thicknesses (δ_{th}) and adiabatic temperatures (T_{ad}) of one-dimensional (1D) unstretched flames, along with the centerline peak temperatures (T_{max}), temperatures at the peak-heat-release point (T_r), standoff distances (h_f), distances from the rod end to the flow stagnation point (h_0), and flame displacement speeds (s_d) of the predicted inverted flames, for all the cases studied.

Fig. 3 Net consumption rate ($\text{kg m}^{-3} \text{s}^{-1}$) of CH_4 for the CH_4 -air flames in the near-rod region. (a) Case A: $\phi_{\text{in}} = 0.68$ and $U_{\text{in}} = 1.85$ m/s. (b) Case B: $\phi_{\text{in}} = 0.69$ and $U_{\text{in}} = 1.85$ m/s. (c) Case C: $\phi_{\text{in}} = 0.69$ and $U_{\text{in}} = 2.5$ m/s. The top end of the rod is represented by the white region at the bottom of each subfigure.

Fig. 4 Net consumption rates ($\text{kg m}^{-3} \text{s}^{-1}$) of CH_4 (top) and H_2 (bottom) for the H_2 - CH_4 -air flames in the near-rod region. (a) Case D: $\phi_{\text{in}} = 0.48$ and $U_{\text{in}} = 1.85$ m/s. (b) Case E: $\phi_{\text{in}} = 0.49$ and $U_{\text{in}} = 1.85$ m/s. (c) Case F: $\phi_{\text{in}} = 0.49$ and $U_{\text{in}} = 2.5$ m/s. The top end of the rod is represented by the white region at the bottom of each subfigure.

standoff distance (case D, $h_f = 2.69$ mm), whereas the increment in the mean inflow velocity results in a reduction of the standoff distance (case F, $h_f = 0.82$ mm). Though counter-intuitive, this response agrees with the anomalous behaviour observed by Shoshin et al. [11]. Compared to the CH_4 -air flames, the H_2 - CH_4 -air flames stabilize closer to the rod and the changes in the standoff distance are smaller. While the decrease in inlet equivalence ratio leads to an increase in standoff distance for both the CH_4 -air and H_2 - CH_4 -air flames, the effect is more pronounced for the CH_4 -air flames.

B. Fuel consumption

To further investigate the opposed behaviour displayed by the CH_4 -air and H_2 - CH_4 -air inverted flames, magnified contour plots of the fuel consumption rates near the rod, as shown in Fig. 3 for the CH_4 -air flames and in Fig. 4 for the H_2 - CH_4 -air flames, are examined. In all of these plots the flow streamlines are also displayed. The net consumption rates of fuel exhibit significant differences when H_2 is added to CH_4 . For the CH_4 -air flames the consumption rate of CH_4 is more uniform along the flame front, whereas for the H_2 - CH_4 -air flames the CH_4 and H_2 consumption rates are

more intense close to the rod. In particular, for the $\text{H}_2\text{-CH}_4\text{-air}$ flames the consumption rate of H_2 is more notably intensified in the anchoring region, while that of CH_4 is more intensified at the base-wing juncture of the flame and along the lower part of the flame wing. This non-uniformity of the consumption rates of the fuel components indicates important changes in the local composition of the reactant mixture which can be ascribed to preferential diffusion of H_2 .

Fig. 5 The spatial distribution of the fast explosive eigenvalue $\lambda_{e,f}$ [1/s] for the six cases under study.

Fig. 6 The spatial distribution of scalar dissipation χ [1/s] on top (Figs. (a)-(f)) and the Da number on bottom (Figs. (g)-(l)) for the six cases under study.

C. CSP analysis

As highlighted in Section III, in reacting flows the fast explosive mode has been associated with the characterization of flame fronts and ignition events. The CSP analysis of the cases A to F, confirms this expectation. Firstly, since the explosive character of the fast explosive mode results from the existence of a fast explosive eigenvalue $\lambda_{e,f}$, the spatial evolution of $\lambda_{e,f}$ for all six cases is depicted in Fig. 5. It is shown that in all cases, $\lambda_{e,f}$ exists in a small portion of the computational domain and takes on high values in a very thin region in the back end of the highlighted region. It is noted that with the addition of H_2 (cases D, E, F), the maximum values of $\lambda_{e,f}$ drop significantly compared to the pure CH_4 -related cases (cases A, B, C). This is an indication that the reactivity of the system in cases D, E, F is decreased compared to cases A, B, C. Moreover, $\lambda_{e,f}$ obtains higher values in the neighborhood of the anchoring region, a finding which is more pronounced in cases D, E, F.

To further examine the effects of transport and chemistry on the flame's anchoring region, the scalar dissipation rate based on a progress of reaction variable, Y_C , is computed as follows:

$$\chi = 2\alpha |\nabla Y_C|^2, \quad (6)$$

where α is the thermal diffusivity and Y_C is the sum of the mass fractions of the species H_2O_2 , CO , CO_2 , and H_2O . Figure 6 shows that in the anchoring region of the flame, χ is significantly decreased and takes on higher values in a sector of the flame wing. Having available χ , the calculation of the local Damköhler number (Da) using $\lambda_{e,f}$ as the characteristic chemical timescale is straightforward: $Da = \lambda_{e,f} \cdot \chi^{-1}$. As Fig. 6 shows, in all cases the Da number obtains locally its maximum values in the neighborhood of the anchoring region of the flame, suggesting that the effect of chemistry becomes dominant there, with a minimal effect of transport as was also highlighted by the spatial distribution of the χ .

V. Conclusion

Simulations of steady, rod-stabilized, inverted, lean, CH_4 -air and H_2 - CH_4 -air premixed laminar flames were performed. For the CH_4 -air flames, either decreasing the inlet equivalence ratio or increasing the mean inflow velocity leads to a larger standoff distance. Below a critical value of the inlet equivalence ratio or above a critical value of the mean inflow velocity the flame blows off. For the H_2 - CH_4 -air flames, decreasing the inlet equivalence ratio leads to a larger standoff distance, and below a critical value of the inlet equivalence ratio, the flame blows off, while increasing the mean inflow velocity leads to a reduction in the standoff distance, with the flame remaining stable. The predicted behaviour of the flames for the conditions studied is fully consistent with the experimental observations of Shoshin et al. [11]. Although both the CH_4 -air and H_2 - CH_4 -air flames exhibit preferential diffusion effects such as variations in the local equivalence ratio and superadiabatic peak temperatures, the effects are much more pronounced for the H_2 - CH_4 -air flames, which display non-uniform and remarkably localized consumption rates of the two fuel components.

Acknowledgments

This work was supported by King Abdullah University of Science and Technology (KAUST). Computational resources were provided by the KAUST Supercomputing Laboratory (KSL).

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