Computational study on the stability of lean CH4-air and H2-CH4-air laminar premixed flames
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Introduction

Recently, Shoshin et al. [1] reported measurements on blow-off limits for methane-air and hydrogen-methane-air flames stabilized on metallic rods finding a so-called “anomalous” blow-off behaviour of hydrogen-methane-air flames with certain hydrogen content. It is well known that lean methane-air and hydrogen-methane-air flames have characteristics that differ substantially owing to preferential diffusion effects. In this study, two-dimensional simulations of steady, rod-stabilized, inverted, lean, methane-air and hydrogen-methane-air premixed laminar flames are performed to further investigate the stability and blow-off characteristics of such flames. The simulations are carried out with complex chemistry and non-unity Lewis transport. For the hydrogen-methane-air flames, mixtures with a 40% (molar based) hydrogen content in the fuel are considered. Six cases for different values of equivalence ratio, \( \phi \), and mean inlet velocity, \( \bar{V} \), of the premixed mixture are studied. The conditions for all the cases are summarized in Table 1. In what follows, the governing equations are provided, the burner and computational setup are described and the numerical results are discussed.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fuel</th>
<th>( \frac{n_{H_2}}{n_{H_2} + n_{CH_4}} )</th>
<th>( \phi )</th>
<th>( \bar{V} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>CH(_4)</td>
<td>0</td>
<td>0.665</td>
<td>1.85</td>
</tr>
<tr>
<td>B</td>
<td>CH(_4)</td>
<td>0</td>
<td>0.68</td>
<td>1.85</td>
</tr>
<tr>
<td>C</td>
<td>CH(_4)</td>
<td>0</td>
<td>0.68</td>
<td>2.5</td>
</tr>
<tr>
<td>D</td>
<td>H(_2)-CH(_4)</td>
<td>0.4</td>
<td>0.47</td>
<td>1.85</td>
</tr>
<tr>
<td>E</td>
<td>H(_2)-CH(_4)</td>
<td>0.4</td>
<td>0.48</td>
<td>1.85</td>
</tr>
<tr>
<td>F</td>
<td>H(_2)-CH(_4)</td>
<td>0.4</td>
<td>0.48</td>
<td>2.5</td>
</tr>
</tbody>
</table>

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

Governing Equations

The inverted laminar flames are mathematically described by conservation equations for mass, momentum, energy and species in a cylindrical coordinate system. The flow is treated as a continuous, multi-component, compressible, and thermally-perfect mixture of gases. A Newtonian flow is assumed and Soret and Dufour effects are neglected. Although the equations are solved in axi-symmetric form, they are presented here in Cartesian coordinates for the sake of simplicity. The conservation equations for a thermally perfect reactive mixture of \( N \) chemical species evolving in time, \( t \), and space, \( x \), can then be written using tensor notation as

\[
\frac{\partial p}{\partial t} + \nabla \cdot (pu) = 0, \quad (1)
\]

\[
\frac{\partial (pu_i)}{\partial t} + \nabla \cdot (pu_iu_j + \delta_{ij}p) \frac{\partial \tau_{ij}}{\partial x_j} = \rho g_i, \quad (2)
\]

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot ((\rho E + p)u_j) - \nabla \cdot (\tau_{ij} u_i) + \frac{\partial \dot{q}_l}{\partial x_j} = \rho g_i u_i, \quad (3)
\]

\[
\frac{\partial (\rho Y_\alpha)}{\partial t} + \nabla \cdot (\rho Y_\alpha(u_j + V_{j,\alpha})) = \dot{\omega}_\alpha, \quad (4)
\]

where

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_l}{\partial x_l}, \quad (5)
\]

\[
\dot{q}_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{\alpha=1}^{N} h_\alpha Y_\alpha V_{j,\alpha}, \quad (6)
\]

with the indices \( i, j, l = 1, 2, 3 \) and \( \alpha = 1, \ldots, N \). Einstein summation convention applies to the indices \( i, j, \) and \( l \).

In the expressions above, \( \rho \) is the mixture density, \( u_i \) is the mixture velocity, \( p \) is the mixture pressure, \( T \) is the mixture temperature, \( E \) is the total mixture energy (including chemical energy or heat of formation), \( Y_\alpha \) is the mass fraction of species \( \alpha \), \( \dot{\omega}_\alpha \) is the net reaction rate of species \( \alpha \), \( g_i \) is the acceleration due to gravity, \( \tau_{ij} \) is the viscous stress tensor, \( q_j \) is the heat flux vector (energy flux due to thermal conduction and energy flux due to the diffusion of species), and \( V_{j,\alpha} \) is the diffusion velocity of the species \( \alpha \). The coefficients \( \mu, \lambda \) and \( h_\alpha \) are the mixture viscosity, mixture thermal conductivity and enthalpy of species \( \alpha \), respectively. Additionally, \( \delta_{ij} \) is the Kronecker delta. The mixture is assumed to obey the ideal gas equation of state, which has the form

\[
p = \rho RT / M = \rho RT, \quad (7)
\]

where \( R \) is the universal gas constant (8.314 J · mol\(^{-1} \) · K\(^{-1} \)) and \( \rho R \) is the mixture gas constant given by \( R = R \sum_{\alpha=1}^{N} Y_\alpha / M_\alpha = \sum_{\alpha=1}^{N} Y_\alpha R_\alpha \).

Burner Setup

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The experimental setup is described in detail in [1]. Inverted flames corresponding to premixed $\text{H}_2$-$\text{CH}_4$-air mixtures were stabilized above the top end of a vertical rod, which was inserted in a 35 cm long Pyrex tube of 12.4 mm inner diameter. The top end of the rod was approximately 0.5 mm above the top edge of the tube. Although inverted flames for rods having different diameters and mixtures with different hydrogen content were studied in the experiments, the present study is limited to the 2 mm rod and mixtures containing 40% or 0% (on a molar basis) hydrogen content in the fuel.

In the simulations, a rectangular domain with a height, $H = 40$ 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. 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.
Figure 3: Magnification of the near-rod region for the CH$_4$-air flames with $\phi = 0.68$ and $V = 1.85$ m/s (top) and $V = 2.5$ m/s (bottom). (a) Temperature distribution, $\bar{V} = 1.85$ m/s. (b) Heat release, $\bar{V} = 1.85$ m/s. (c) Net consumption rate of CH$_4$, $\bar{V} = 1.85$ m/s. (d) Temperature distribution, $\bar{V} = 2.5$ m/s. (e) Heat release, $\bar{V} = 2.5$ m/s. (f) Net consumption rate of CH$_4$, $\bar{V} = 2.5$ m/s.

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. The next region of width 1.8 mm is associated with the tube top edge thickness. Isothermal non-slip boundary conditions are applied to the rod and tube top edge. 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 $10 \times 12$ quadrilateral cells. The steady state solutions are obtained with three levels of refinement.

Numerical Solution Method

The set of governing equations is solved using a body-fitted, multi-block, adaptive mesh refinement (AMR), finite-volume framework that has been originally developed by Groth and co-researchers [2, 3, 4, 5, 6, 7], which has been extended and modified to model the configurations under study. Applications of this framework to reacting flows have included laminar atmospheric [3, 6] and high-pressure sooting [5, 8] flames, as well as turbulent premixed [7] and non-premixed [4, 6] flames, among others.

The DRM22 [9] reduced reaction mechanism, which is based on GRI 1.2 [10] and consists of 24 species and 104 reactions, is used to obtain the formation and destruction rates of chemical species. Wilke’s formula [11] and a combination-averaging formula [12] are employed to compute the mixture viscosity and thermal conductivity, respectively. The diffusion velocity of each species is calculated assuming Fickian diffusion and the Lewis numbers for each species are prescribed based on steady-state solutions of one-dimensional premixed flames. Thermo-dynamic properties, transport properties and species net production/destruction rates are all evaluated utilizing the open-source package Cantera [13].

The transport equations were solved on multi-block quadrilateral meshes employing a second-order spatial discretization. The inviscid flux at each cell face was evaluated using limited linear reconstruction. Particularly, the Roe [14] flux function along with the Venkatakrishnan [15] limiter were utilized. The viscous fluxes were evaluated utilizing a diamond-path reconstruction [16]. Moreover, the low-Mach number preconditioner described by Weiss & Smith [17] and the explicit multi-stage optimally-smoothing time marching scheme of van Leer et al. [18] were used to achieve steady-state solutions.

Results and Discussion

Figure 1 shows temperature contours and the blocks associated with steady-state solutions obtained for all the cases in Table 1. Figures 1(a), 1(b) and 1(c) correspond to the cases A, B and C, respectively, for CH$_4$-air mix-
Figure 4: Magnification of the near-rod region for the H$_2$-CH$_4$-air (40% H$_2$) flames with $\phi = 0.48$ and $V = 1.85$ m/s (top) and $V = 2.5$ m/s (bottom). (a) Temperature distribution, $\bar{V} = 1.85$ m/s. (b) Heat release, $\bar{V} = 1.85$ m/s. (c) Net consumption rate of CH$_4$, $\bar{V} = 1.85$ m/s. (d) Net consumption rate of H$_2$, $\bar{V} = 1.85$ m/s. (e) Temperature distribution, $\bar{V} = 2.5$ m/s. (f) Heat release, $\bar{V} = 2.5$ m/s. (g) Net consumption rate of CH$_4$, $\bar{V} = 2.5$ m/s. (h) Net consumption rate of H$_2$, $\bar{V} = 2.5$ m/s.

Figures 1(d), 1(e) and 1(f) correspond to the cases D, E and F, respectively, for H$_2$-CH$_4$-air mixtures. By taking case E as reference, it can be observed that a decrease in equivalence ratio (from 0.68 to 0.655) while keeping the same inlet velocity (Figure 1(a)) leads to an increase in the stand-off distance. Similarly, an increase in the mean inlet velocity (from 1.85 m/s to 2.5 m/s) while keeping the same equivalence ratio leads to an increase in the stand-off distance (Figure 1(c)). It should be noted that the conditions for cases A and C are very close to the blow-off limits reported by Shoshin et al. [1]. A further decrease in equivalence ratio for case A or a increase in the mean inlet velocity for case C would result in the eventual blow-off of the flame. For qualitative comparison, experimental images of CH$_4$-air flames at conditions close to the blow-off limits are displayed in Figure 2. The numerical predictions for the CH$_4$-air flames are able to reproduce, at least qualitatively, the behaviour observed in the experiments.

Figures 1(d), 1(e) and 1(f) correspond to the cases D, E and F, respectively, for H$_2$-CH$_4$-air mixtures. By taking case E as reference, it can be observed that a decrease in equivalence ratio (from 0.48 to 0.47) while keeping the same inlet velocity (Figure 1(e)) or an increase in the mean inlet velocity (from 1.85 m/s to 2.5 m/s) while keeping the same equivalence ratio (Figure 1(e)) does not lead to a significant change in the stand-off distance. This is consistent with the so called “anomalous” behaviour that was observed and reported by Shoshin et al. [1]. Furthermore, a comparison between the solutions for cases B (Figure 1(b)) and E (Figure 1(e)) shows that the flame corresponding to the H$_2$-CH$_4$-air mixture stabilizes closer to the rod, despite its lower equivalence ratio. It is worth noting that the unstretched laminar flame speed associated with this H$_2$-CH$_4$-air flame is approximately three times lower than that of the CH$_4$-air flame under consideration in this comparison.

To further investigate the opposed behaviour displayed by the CH$_4$-air and H$_2$-CH$_4$-air inverted flames, magnified contour plots of temperature, heat release, and fuel consumption rates near the rod are shown in Figure 3 for cases B and C and in Figure 4 for cases E and F. In all these plots the flow streamlines are also displayed. The presence of a recirculation zone is apparent in all the cases. For the CH$_4$-air flames, the increase in mean inlet velocity (from 1.85 m/s to 2.5 m/s) results in a larger stand-off distance and an elongated recirculation zone. In contrast, for the H$_2$-CH$_4$-air flames, the same increase in mean inlet velocity results in a slightly shorter stand-off distance and a minor change in the recirculation zone. Additionally, the heat release contours of Figures 3(b), 3(e), 4(b), and 4(f) reveal a different qualitative distribution for the CH$_4$-air and H$_2$-CH$_4$-air flames. The heat release is more uniform for CH$_4$-air flames whereas for
the H₂-CH₄-air flames it is more localized in the near rod region. Moreover, the net consumption rates of fuel (Figures 3(c), 3(f), 4(c), 4(g), 4(d), and 4(h)) exhibit significant differences when hydrogen is added to methane. For CH₄-air flames, the methane consumption rate is more uniform, whereas for H₂-CH₄-air flames the methane and hydrogen consumption rates are more intense near the rod. In particular, the hydrogen consumption rate is intensified at the anchoring point. This can be attributed to preferential diffusion of hydrogen to the flame leading edge, which in turn enhances the local burning rate and leads to an improved stability of the flame. It should also be pointed out that the H₂-CH₄-air flames displayed superadiabatic peak temperatures.

Conclusions
For the methane-air flames, increasing the mean inflow velocity at a fixed equivalence ratio leads to larger stand-off distances and above a critical value the flame blows-off. In contrast, for the hydrogen-methane-air flames, above a critical value of inflow velocity, the stand-off distance decreases and the flame remains stable. The hydrogen-methane-air flames display superadiabatic temperatures and intensification of the hydrogen consumption rate and heat release in the vicinity of the stabilization point due to preferential diffusion. Future work will involve the extension of the set of numerical simulations for a larger range of equivalence ratios, mean inflow velocities and hydrogen content in the fuel and detailed comparisons of the numerical predictions with experimental measurements.

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