STRUCTURES AND BURNING VELOCITIES OF METHANE/HYDROGEN/AIR PREMIXED FLAMES

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Background

*attractive approach*

- Rich reserve of natural gas
- Feasibility of producing biogas *(main component: CH$_4$)*
- To get energy safety and sustainable development.
- To reduce emissions of carbon dioxide and soot.
- To enhance the burning velocity of methane/natural gas.

*thus*

fully understand
the combustion characteristics under various conditions.
Background

Laminar premixed flames
atmospheric
adiabatic
freely propagating

the flame structures
the laminar burning velocities
peak burning velocity shifting

investigation
carried out
aim

using detailed numerical simulations
accounting for both detailed chemical kinetics and transport properties
Simulation details

an open source code, *Cantera*

1 D freely-propagating flat flames
mechanism: GRI-3.0

Grid independence test
Entire range of hydrogen enrichment ratio $X_{\text{H}_2} = 0 : 0.1 : 1$

a range of $\phi$

pseudo-time stepping
Newton iteration scheme

mass, species, and energy conservation equations

\[
\begin{align*}
\dot{\mathbf{u}} &= \mathbf{S}_u = \dot{\mathbf{m}} = \text{const} \\
\dot{\mathbf{Y}} + \dot{\mathbf{m}} \mathbf{Y} &= \dot{\mathbf{j}} + \mathbf{W} \\
\dot{\mathbf{T}} + \dot{\mathbf{c}} \mathbf{T} &= \left( \begin{array}{c} \mathbf{T} \\ \mathbf{z} \end{array} \right) + \sum_{i=1}^{N} c_{pi} \dot{\mathbf{j}}_{i,z} \mathbf{T} + \sum_{i=1}^{N} h_{i} \cdot \mathbf{W}_i
\end{align*}
\]
Results and discussion

Laminar burning velocity and fuel-rich shifting of peak laminar burning velocities

peaks at phi=1.65

peaks at phi=1.07

$X_{H2}=1$

$X_{H2}=0.2$
the details of the methane/air flames at various \( \phi \)

\[
\begin{align*}
T: & \quad \phi=1 \\
[O]: & \quad \phi=0.9 \\
[OH]: & \quad \phi=1 \\
[H]: & \quad \phi=1.18 \\
D: & \quad \phi=1.36 \\
\text{HRR:} & \\
\text{DxHRR:} & \text{a slightly fuel-rich}
\end{align*}
\]
the details of the hydrogen/air flames at various phi

T: \( \phi = 1.07 \)

[H]: \( \phi = 1.65 \)

D: increases monotonically

DxHRR: \( \phi = 1.7 \)
fuel-rich shifting
peak laminar burning velocities

\[ S_L = 0.3733e^{0.772X_{H_2}} + 0.0021e^{7X_{H_2}} \]

this relation can be approximated by a linear relation

\[ S_L = 0.375 + 0.303X_{H_2} \]

\( X_{H_2} \) below 0.95

Phi@Slmax is nearly identical to phi@HRRmax
Flame structure (methane/air flame)

Oxidation layer

Inner layer: characterized by CH₃
Flame structure (methane/hydrogen/air flame)
Flame structure (hydrogen/air flame)
Local equivalence ratio and heat release rate
Net effect

major consumption:
O + H₂ = H + OH
OH + H₂ = H + H₂O

chain branching reaction:
H + O₂ = O + OH

global reaction:
O₂ + 3H₂ = 2H + 2H₂O

under \( \phi = 1.65 \)
upstream part:
H + HO₂ = 2OH
H + HO₂ = H₂ + O₂
H + O₂ + M = HO₂ + M

fuel consumption:
OH + H₂ = H + H₂O

net effect:
4H + O₂ + 3M = 2H₂O + 3M.
Two-layer flame structure

Radicals recombination layer

Fuel/oxyen consumption layer

[Diagram showing overall production rates of various species over flame coordinate]
Two-layer flame structure
Summary

different mechanisms responsible for the fuel-rich shifting

1. The increased H radical concentration
   The peak $S_L$ is at phi at which the mole fraction of H radicals peak.
   The global reaction $O_2 + 3H_2 = 2H + 2H_2O$ implies that the peak H radical production is in the fuel-rich mixture with the phi = 1.5.

2. The increased heat release rate
   The peak $S_L$ is in the slightly fuel-rich mixture with the phi of the peak HRR. HRR is governed by radicals concentrations and T.
   O and OH peak in mixtures with phi close to 1, whereas the H peaks in fuel-richer mixtures.

3. The enhanced differential diffusion
   Differential diffusion $H_2$ is quickly.
   Local decrease of phi in the reaction zone.
Conclusions

For a given $X_{H2}$ there is a peak $S_L$ in the flames with different phi. With increasing $X_{H2}$ the peak $S_L$ is increasingly shifted to fuel-rich mixtures.

An empirical correlation of the peak $S_L$ with $X_{H2}$ is obtained. At low $X_{H2}$ the peak $S_L$ increases linearly with $X_{H2}$. At high $X_{H2}$ the peak $S_L$ increases with $X_{H2}$ exponentially.

Owing to preferential diffusion the local phi varies across the flame. In the reaction zone the local phi is lower than that in the free stream unburned fuel/air mixture.

This locally decreased phi implies that the fuel/air mixture in the fuel consumption layer of a stoichiometric flame is in fact a fuel-lean mixture, which results in a decreased reactivity in the stoichiometric mixture. Therefore, the laminar burning velocity peaks at a slightly fuel-rich mixture.
Conclusions

In hydrogen enriched methane/air flames the concentration of H radicals is significantly higher than that of O and OH radicals. The peak laminar burning velocity is shown to closely correlate with the concentration of H radicals.

The H production is governed by the global reaction \( \text{O}_2 + 3\text{H}_2 = 2\text{H} + 2\text{H}_2\text{O} \), which implies that the peak H radical production is in the fuel-rich mixture, which is partly responsible for the fuel-rich shift of the peak laminar burning velocity.
Thank you for your attention!