Chemiluminescence from Hydrogen-Methane Laminar Premixed Flames: Experiments and Numerical Comparison

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Abstract

The chemiluminescence signals from laminar premixed hydrogen blended methane/air flames are analyzed using a flat and conical flame burner. The results show that with increasing H_2 premixture, there is a reduction in chemiluminescent markers, which is corroborated by numerical models.

Body

Blending fossil fuels, such as methane, with hydrogen is gaining attention as a strategy to reduce emissions. However, due to the change of fuel properties, continuous monitoring is required to avoid situations such as flame flashback. Measuring chemiluminescence of excited radical species (OH*, CH*, etc.) is a diagnostic tool for monitoring flame parameters such as heat release rate and equivalence ratio [1]. Although extensive data is available for methane, the database is limited for fuel blends.

The objective of this study is to characterize the chemiluminescence behavior of hydrogen blended methane-air unstretched laminar flat flames and to compare the experimental measurements with available sub-mechanisms using 1D simulations. This is then extended to a conical flame burner for a 60% H_2 mixture at different equivalence ratios and compared to 2D CFD simulations.

The chemiluminescence was recorded using two facilities, a downfired McKenna burner producing an unstretched laminar flame, and a conical flame burner with a 4mm square port. The flame spectra were captured using a UV-enhanced optical fiber connected to a OceanOptics HR2000 spectrometer. The equivalence ratio was varied from 0.7 to 1.25 for different level of H_2 blending (0-60% by volume) in the flat flame burner, while for the conical flame burner the equivalence ratio was varied between 0.83 and 1.67 for a 60% H_2 blend.

The numerical simulations for the flat flame burner were conducted in Cantera. The baseline chemistry model is an analytically reduced model derived from GRI-Mech 3.0 [2] and is augmented by chemiluminescence sub-mechanisms. These include Mechanism-1, 2 [1], 3 [3], as well as the baseline and a slightly modified FFCM1 [4] model. CFD simulations using OpenFOAM were also performed to study the conical flame burner with the chemiluminescent species calculated in post processing using the quasi-steadystate assumption.

Figure 1 presents the variation of OH*, CH*, and OH*/CH* with equivalence ratio for different levels of H_2 premixture, compared to 1D flame calculations (only the modified FFCM1 model shown for brevity). The data is normalized with respect to the maximum value for the 0% H_2 case to capture the change in trends produced by changing equivalence ratio and levels of hydrogen premixture. It can be observed from the experimental and numerical data that blending with H_2 results in an overall reduction in both OH* and CH* emissions. This can be attributed to an overall reduction of CH and C_2H, which is important in the production of both chemiluminescent species. CH* and OH*/CH* display monotonic trends increasing and decreasing respectively with equivalence ratio while OH* peaks at around ϕ=1.1 for all levels of H_2 injection. The modified FFCM1 model produces good results for OH* across the range of equivalence ratios and H_2 levels, while Mechanisms 1 and 2 (not shown for brevity) match well at ϕ>0.9 but overpredict the rate of reduction of OH* in the lean zone. The ratio OH*/CH* is well captured by the modified FFCM1 model across the whole range of data while other models predicted a greater deviation.

The same models were applied to the chemiluminescence signals captured from the conical burner with 60% H_2 premixture and equivalence ratio between 0.8 and 1.67. Figure 2 shows the variation of OH*, CH*, and OH*/CH* with equivalence ratio, normalized with respect to the value at ϕ=1. As in the case with the flat flame burner, the trend of CH* is captured relatively accurately for

all the mechanisms, whereas the trends in OH*/CH* are similar across all models as well. On the other hand, the experimental peak OH* shifts to ϕ=1.4; which is likely due to flame tip curvature which was absent in the planar flame case. This shift in peak is captured by Mech. 1, 2, and modified FFCM1 model whereas the baseline FFCM1 predicts a peak at $\phi = 1.25$ while Mech. 3 predicts the correct peak but at a lower relative value compared to experiments. This suggests that chemiluminescece of OH* radical is affected by flame stretch which is predicted reasonably well by the current selection of chemiluminescence sub-mechanisms.

Conclusion

Overall, the modified FFCM1 mechanism produces reasonable results when compared to experimental data. It should be noted that the chemiluminescence sub-mechanisms, despite sharing the baseline chemistry model, produce results with significant differences for both the flat flame and the conical flame burners. The study shows the need for the development and validation of mechanisms that can capture the qualitative trends and absolute emission characteristics of chemiluminescent species of alternative fuels. These mechanisms can be used to validate numerical models with experimental observables and to leverage these simulations to better understand the characteristics of the measured flames. Furthermore, the experimental results confirm the potential of chemiluminescence-based monitoring methods for the development of advanced diagnostic techniques for CH_4/H_2 flames.

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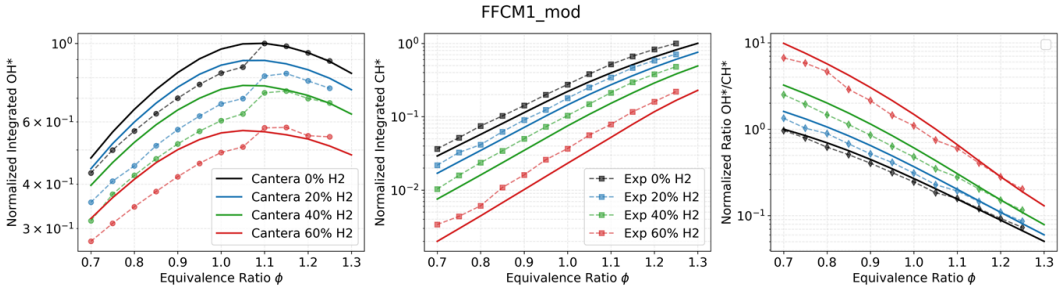

Figure 1 Comparison of OH*, CH*, and OH*/CH* from the flat flame burner with 1D simulations using modified FFCM1 mechanism

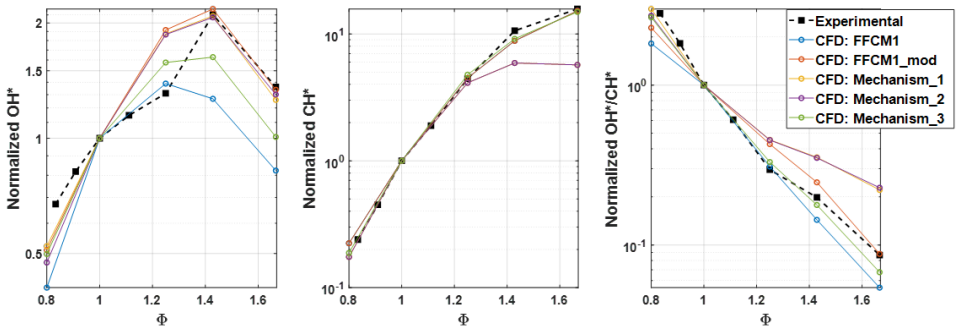

Figure 2 Comparison of OH*, CH*, and OH*/CH* obtained from the conical flame burner with CFD simulations using Mechanisms 1, 3, and modified FFCM1 mechanism for 60%H2/CH4-Air mixture