



HAL
open science

Exploring viability of OH* radicals as flame markers in H₂ combustion

Keerthana Gudemaranahalli Subramanya, Guillaume Dayma, Christian Chauveau, Fabien Halter

► **To cite this version:**

Keerthana Gudemaranahalli Subramanya, Guillaume Dayma, Christian Chauveau, Fabien Halter. Exploring viability of OH* radicals as flame markers in H₂ combustion. 26th International Conference of the Theoretical and Applied Mechanics (ICTAM 2024), IUTAM, Aug 2024, Daegu, South Korea. hal-04677485

HAL Id: hal-04677485

<https://cnrs.hal.science/hal-04677485v1>

Submitted on 26 Aug 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

EXPLORING VIABILITY OF OH* RADICALS AS FLAME MARKERS IN H₂ COMBUSTION

Keerthana Gudemaranahalli Subramanya^{1*}, Guillaume Dayma^{1,2}, Christian Chauveau¹, Fabien Halter^{1,2}

¹CNRS ICARE, Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2 France,

²Université d'Orléans, Orléans, France

Summary The current study focuses on the measurement of OH* radicals for a laminar premixed hydrogen flame and the interpretation of their intensities and assessment of their use as a plausible flame marker. A spherically expanding flame is studied in a constant volume chamber with the application of high-speed chemiluminescence to identify OH* radicals. The temporal evolution of OH* was investigated as a function of pressures and temperatures, thereby providing insights in their dynamic evolution under varied thermodynamic conditions.

INTRODUCTION

Chemiluminescence from OH* has been a focal point in combustion research, serving as a flame marker in pre-mixed hydrocarbon flames to ascertain local equivalence ratios and heat release rates [1], [2], thereby marking the reaction zone. However, certain investigations have indicated the existence of OH* radicals not only in the flame front but also in post-combustion gases [3], [4]. It is therefore imperative to scrutinize the dependability of employing OH* chemiluminescence for marking the heat release rate in a hydrogen flame.

The objective of this work is to evaluate the feasibility of using OH* radical as a prospective flame marker for a hydrogen flame. To attain this, a detailed measurement of OH* has been carried out and the morphology of its evolution is evaluated by interpreting the intensity distribution across all the regions of flame. This work presents a new investigation of OH* chemiluminescence, studying its evolution at elevated pressures and temperatures. The findings from this research have the potential to offer valuable insights for industrial applications.

EXPERIMENTAL FACILITY AND TEST CONDITIONS

The experiments were carried out on the OPTIPRIME facility at ICARE-CNRS, Orleans, France. The OPTIPRIME facility can be used both as a constant pressure chamber and as a constant volume chamber. It consists of a 0.9 L combustion chamber with an internal diameter of 12 cm and is placed inside a furnace. The combustion chamber consists of two stainless steel rings assembled together with a 360 degree fused silica ring with spherical inner and outer surfaces, to ensure the sphericity of the chamber [5]. The optical access helps us to fully visualise the flame, from ignition to extinction and track its radial evolution. OPTIPRIME is designed to operate up to a maximum final pressure of 100 bar and a maximum initial temperature of 473 K. A K-type thermocouple is used to measure the initial temperature and the onboard pressure sensing is done through two AVL GU21D sensors, of high sensitivity and frequency. The mixture is prepared in a high pressure buffer tank. The fuel and oxidizer are mixed using principle of partial pressure law. The large volume of the buffer tank helps in ensuring repeatability of tests with the same mixture conditions. The mixture is introduced into the combustion chamber through a 1/6 inch inlet tube. Spark ignition is provided by two electrodes connected to a capacitance coil and energy deposition can be further controlled by charging time. The imaging system consists of a high speed UV back-illuminated camera coupled with a UV lens of focal length 105 mm and is equipped with a high transmission narrow band OH* filter centred at 310 nm.

OH* measurements were performed on hydrogen flames with air as oxidant. To further reduce the reactivity of the mixtures, different test cases were evaluated by adjusting the oxygen content. Thermodiffusive instabilities were attenuated by the addition of helium and argon. Experiments were carried out at 3 equivalence ratios: a stoichiometric case ($\phi = 1.0$), a fuel rich case ($\phi = 1.4$) and a fuel lean case ($\phi = 0.6$). For each of these configurations inlet pressures of 1, 2 and 3 bar were tested.

RESULTS AND ANALYSES

A comprehensive dataset of OH* chemiluminescence measurements was generated for various test conditions, including changes in equivalence ratios and inlet pressures. The recorded OH* chemiluminescence signals were reconstructed using an Abel inverse technique. The temporal evolution of the flame is shown in Fig.1, the flame front is outlined in red and the inner region of the sphere consists of the burnt gas. From the analysis of the flame images, it can be seen that the OH* intensity is distributed throughout the flame, at the flame front where the heat release occurs and an afterglow observed in the post combustion gases. The OH* signal distribution observed in the experiments is therefore divided into two zones and the emission characterisation is made separately.

* Corresponding author. E-mail: keerthana.gudemaranahalli@cnrs-orleans.fr

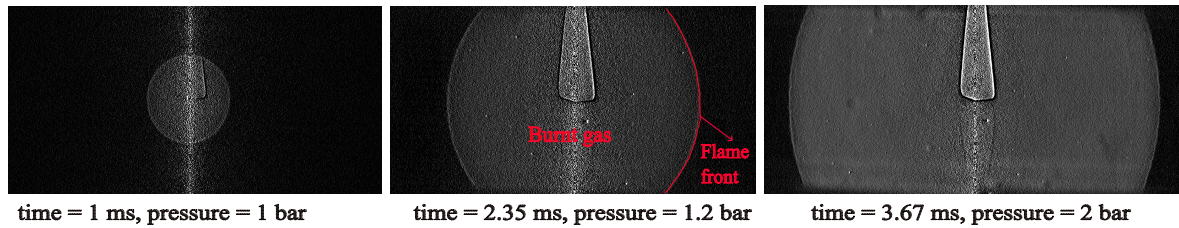


Figure 1. Abel inverted spatial and temporal distribution of OH* for a H₂ / air flame at $\phi = 1.0$

Fig.2 depicts the intensity evolution for hydrogen flame with an oxidizer mixture containing O₂, He and Ar for an equivalence ratio of $\phi = 1.0$ at 3 inlet pressures of 1,2 and 3 bar. An increase of evolving pressure can be seen as indicated by the arrow for an advancing flame radii. There is also an increase of the temperature of unburnt gas due to isentropic compression. By isolating the effects of pressure and temperature from the experiments, it was found that the OH* intensities decrease with increasing pressure due to collisional quenching. During flame propagation, although there is an increase in pressure, there is an increase in the adiabatic flame temperature which outweighs the effect of pressure changes, thereby promoting the production of OH* radicals in the flame front. At the same time, there is a higher temperature in the burnt gas compared to the reaction zone, resulting in increase of OH* formation.

A sensitivity analysis and rate of production evaluation was carried out to identify the reactions leading to OH* formation in both zones and to gain a better understanding of the dependence of these reactions on pressures and temperatures. It was observed that the pathway for OH* formation in the flame front is via chemical excitation, whereas in the burnt gas it is mainly due to thermal excitation. H₂O dissociation occurs at elevated temperatures, leading to the formation of ground OH radicals in the burnt gas, which are further excited by collision with other radicals in this region.

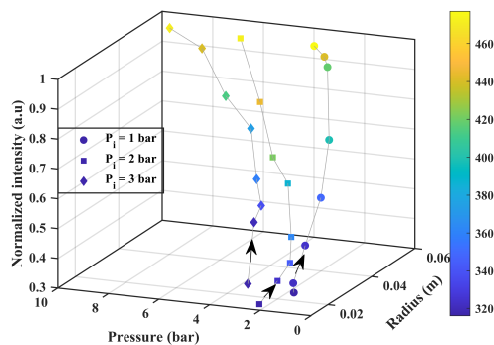


Figure 2. Intensity evolution at flame front

To support our findings, our study is extended to numerically simulate an unsteady 1D spherical flame using FlameMaster [6], which would bridge the gap between experiments and simulations. The numerical database includes the evolution of radius, pressure and OH* mole fraction and other essential flame parameters. An additional helium collision reaction was added to the existing OH* sub-mechanism developed by Kathrotia et al. [7] to account for collisions with helium, as a major part of our oxidant mixture consisted of helium.

CONCLUSIONS

Our experimental analysis shows that the intensity distribution in the burnt gas is more pronounced than in the flame front. Thus, on the separation of the reaction zone, it casts doubt on the indication of the OH* radical as a flame marker for hydrogen flames.

References

- [1] Y. Hardalupas, M. Orain.: Local measurements of the time-dependent heat release rate and equivalence ratio using chemiluminescent emission from a flame. *Combustion and Flame*, 2004.
- [2] T. García-Armingol, Y. Hardalupas, A. Taylor, J. Ballester.: Effect of local flame properties on chemiluminescence-based stoichiometry measurement. *Experimental Thermal and Fluid Science*, 2013.
- [3] M. Richter, R. Schultheis, J.R. Dawson, A. Gruber, R.S. Barlow, A. Dreizler, D. Geyer.: Extinction strain rates of premixed ammonia/hydrogen/nitrogen-air counterflow flames, *Proceedings of the Combustion Institute*, 2023.
- [4] Venkata N. Nori.: Modeling and analysis of chemiluminescence sensing for syngas, methane and Jet-A combustion, *PhD Thesis*, Georgia Institute of Technology, Atlanta, 2008.
- [5] Fabien Halter, Zheng Chen, Guillaume Dayma, Chaimae Bariki, Yong Wang, Philippe Dagaut, Christian Chauveau.: Development of an optically accessible apparatus to characterize the evolution of spherically expanding flames under constant volume conditions. *Combustion and Flame*, 2020.
- [6] Heinz Pitsch.: Flamemaster: A C++ computer program for 0d combustion and 1d laminar flame calculations, <https://www.itv.rwth-aachen.de/en/downloads/flamemaster/>, 1998
- [7] T. Kathrotia, M. Fikri, M. Bozkurt, M. Hartmann, U. Riedel, C. Schulz.: Study of the H+O+M reaction forming OH*: Kinetics of OH* chemiluminescence in hydrogen combustion systems, *Combustion and Flame*, 2010.