HAL open science

EXPERIMENTAL AND NUMERICAL STUDY OF LAMINAR FLAME SPEED OF AMMONIA/METHANOL AND AMMONIA AT HIGH PRESSURE AND TEMPERATURE

Ronan Pelé, Guillaume Dayma, Christine Mounaïm-Rousselle, Pierre Brequigny, Fabien Halter

To cite this version:

Ronan Pelé, Guillaume Dayma, Christine Mounaïm-Rousselle, Pierre Brequigny, Fabien Halter. EXPERIMENTAL AND NUMERICAL STUDY OF LAMINAR FLAME SPEED OF AMMONIA/METHANOL AND AMMONIA AT HIGH PRESSURE AND TEMPERATURE. 1st Symposium on Ammonia Energy, Sep 2022, Cardiff (Wales), United Kingdom. hal-04050086

HAL Id: hal-04050086

https://hal.science/hal-04050086v1

Submitted on 31 Mar 2023

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.

Distributed under a Creative Commons Attribution - NonCommercial - NoDerivatives 4.0 International License

THE JOURNAL OF Ammonia Energy

Cardiff University Press | Gwasg Prifysgol Caerdydd

1st Symposium on Ammonia Energy

EXPERIMENTAL AND NUMERICAL STUDY OF LAMINAR FLAME SPEED OF AMMONIA/METHANOL AND AMMONIA AT HIGH PRESSURE AND TEMPERATURE

Pelé R[a*], Dayma G[b], Rousselle C[a], Brequigny P[a], Halter F[b]

[a]*Univ. Orléans, INSA-CVL, EA 4229 – PRISME, F-45072 Orléans, France*

[b]*Univ. Orléans, CNRS-ICARE, Orléans, France*

Introduction

Ammonia, mainly produced from the Haber-Bosh process [1], is considered one potential carbon-free fuel for internal combustion engines, gas turbines, or industrial burners. Ammonia has a high auto-ignition temperature and research octane number, narrow flammability range, and low laminar flame speed [2] which are unfavorable combustion properties. However, these properties can be improved by mixing with a more reactive fuel to improve ignition/combustion properties, as reviewed in Mounaïm-Rousselle and Brequigny [3] and Dimitriou and Javaid [4]. Hayakawa et al. [5] performed measurements for different initial pressures (0.1, 0.3, and 0.5 MPa) and $0.7 \leq \Phi \leq 1.3$, at an initial temperature of 298 K using a constant pressure combustion chamber. Lhuillier et al. [6] measured NH3/air laminar flame speeds for temperatures ranging from 298 to 473 K, at 1 atm. All results confirmed the extremely low values, around 8 cm.s-1 at 298 K and 1 bar [14, 15]. Therefore, blending ammonia with another fuel is one solution to boost its laminar flame speed. Lhuillier et al. [2] confirmed that ammonia/hydrogen is a suitable fuel for current spark-ignition engines with no design modifications. Other blends with methane [7,8], syngas [9], or DMM [10] were also explored. Mixtures of ammonia and methanol have received less attention [1], while the maximum laminar flame speed of methanol is 42 cm.s-1 in identical conditions. Moreover, methanol is promised to be one of the most important synthetic fuels shortly produced by H_2 electrolysis and CO_2 captured or by biomass in gasification processes [11].

The present work aims to provide laminar flame speed data for NH_3/methanol blend at different levels of temperature and pressures as usual in an internal combustion engine. A kinetic analysis is done to investigate the performances of a kinetic mechanism available compared to experimental data.

Materials and Methods

The constant volume spherical flame method is employed in this study to determine the laminar flame speed of blends of ammonia and methanol. This method allows the measurement of the laminar flame speed of expanding spherical flames by using both pressure and flame radius growth. This method relies on the hypothesis of an isentropic compression of the unburned gases following the ignition: thus, resulting in a simultaneous increase of both pressure and temperature within the vessel. Therefore, each flame propagation is submitted to pressure, and temperature simultaneous increase thus giving flame speed values as a function of the couple (P, T). A pressure transducer records the change in pressure, whereas the temperature change is calculated for each pressure using Laplace's law. Flame chemiluminescence visualization was adopted to obtain the radius evolution by means of a CMOS camera (PHANTOM V1611). Images were captured at an adapted rate of 5 000 fps for ammonia only and up to 15 000 fps for methanol only due to the laminar flame speed difference. Then, the laminar flame speed is calculated using the radius and pressure evolution by Equation (1).

$$S_u = \frac{dR_f}{dt} - \frac{\left({R_0}^3 - {R_f}^3\right)}{3\gamma_u {R_f}^2 P}\frac{dP}{dt} \qquad (1)$$

Where Rf and Ro are the radius of the flame and the spherical chamber respectively, P, the pressure, and γu, the heat capacity ratio of the unburnt gases at the corresponding radius Rf.

The initial pressure P_0 is set at 1 and 2 bar and the initial temperature T_0 is fixed at 423.15 K for each blend, enabling to process data up to 650 K and 10 bar (for P_0=2bar). The fuel/air ratio is set at the stoichiometric ratio with the equation of combustion:

$$X_{NH_3}NH_3 + \left(1 - X_{NH_3}\right)C_2H_5OH + \frac{3\left(1 - 0.75X_{NH_3}\right)}{0.21}\left(0.21O_2 + 0.79N_2\right) = Products \qquad (1)$$

* Corresponding author.
E-mail address: ronan.pele@etu.univ-orleans.fr

With :

$$X_{NH_3} = \frac{n_{NH_3}}{n_{C_2H_5OH} + n_{NH_3}}$$

Results and Discussions

Figure 1 illustrates the isentropic evolution of the laminar flame speed as a function of (P,T) simultaneously from an initial unburned condition (T_0, P_0). The laminar flame speed, y-axis, is plotted for the couples (P,T) with a split x-axis, on the left: the temperature trace and, on the right: the pressure trace. The simultaneous increase of both pressure and temperature within the vessel due to the isentropic compression increase the laminar flame speed. A horizontal line on the y-axis determines (P,T) conditions of the measurement of the laminar flame speed. The thick traces represent the laminar flame speed including the experimental uncertainty of 5%. The increase of methanol content in the blend increases proportionally the laminar flame speed. The experimental values of coefficient of temperature and pressure dependences were also determined. The coefficient of temperature dependence is equal to 1.9 for ammonia and increases to 2.6 for methanol with a polynomial form. On the contrary, the coefficient of the pressure dependence decreases from -0.13 for pure ammonia to -0.32 for pure methanol.

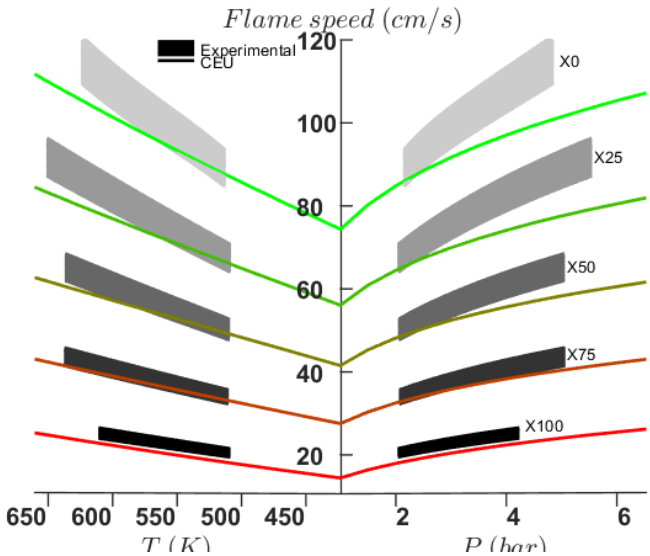

Figure 1. Comparison of predicted laminar flame speed with one kinetic mechanism with experimental values for ammonia/methanol blends; experimental values: Thickened line colored with greyscale and the continuous line correspond to the laminar flame speed simulated with the mechanism (green for methanol and red for ammonia) for P_0=1 and T_0=423.15 K.

The mechanism available for NH_3/methanol, CEU-mechanism from Wang et al. [1] is optimized for a blend of ammonia with hydrogen, methane, methanol, and ethanol and validated with data obtained with the heat flux method for an initial temperature between 298-448 K at 1 atm. The PREMIX module from the ANSYS CHEMKIN-PRO package [12] was used for numerical simulations with a 10 cm grid, curvature and gradient criteria of 0.1 and 0.05 respectively, multicomponent transport, and Soret effect. The kinetic reproduces correctly the pure ammonia condition and the X75 condition but fails for blends with high content of methanol.

Conclusions

This work proposes new laminar flame speed data for ammonia/methanol blends using the isochoric methodology. The results indicate a linearity dependency of the laminar flame speed with ammonia mole fraction. The coefficient of temperature and pressure were measured and follows a polynomial dependence on the ammonia ratio in the blend. The laminar flame speed sensitivity to the temperature and the pressure is higher for the methanol than pure ammonia. A correlation based on this behavior is developed and a good agreement is found with the isochoric data. A kinetics mechanism was compared to the experimental data. CEU mechanism catches well for a low ratio of methanol (X100 and X75). In future work, improvement of the kinetic mechanism is still required to better capture the laminar flame speed for blends with high content of methanol.

* Corresponding author.
E-mail address: ronan.pele@etu.univ-orleans.fr

THE JOURNAL OF Ammonia Energy

Cardiff University Press | Gwasg Prifysgol Caerdydd

References

[1] Z. Wang, X. Han, Y. He, R. Zhu, Y. Zhu, Z. Zhou, K. Cen, Combust. Flame 229 (2021) 111392.
[2] C. Lhuillier, P. Brequigny, F. Contino, C. Mounaïm-Rousselle, Fuel 269 (2020) 117448.
[3] C. Mounaim-Rousselle, P. Brequigny, Front. Mech. Eng. (2020).
[4] P. Dimitriou, R. Javaid, Int. J. Hydrogen Energy 45 (2020) 7098–7118.
[5] A. Hayakawa, T. Goto, R. Mimoto, Y. Arakawa, T. Kudo, H. Kobayashi, Fuel 159 (2015) 98–106.
[6] C. Lhuillier, P. Brequigny, N. Lamoureux, F. Contino, C. Mounaïm-Rousselle, Fuel 263 (2020) 116653.
[7] E.C. Okafor, Y. Naito, S. Colson, A. Ichikawa, T. Kudo, A. Hayakawa, H. Kobayashi, Combust. Flame 204 (2019) 162–175.
[8] H. Xiao, A. Valera-Medina, P.J. Bowen, Energy 140 (2017) 125–135.
[9] S. Wang, Z. Wang, A.M. Elbaz, X. Han, Y. He, M. Costa, A.A. Konnov, W.L. Roberts, Combust. Flame 221 (2020) 270–287.
[10] A.M. Elbaz, B.R. Giri, G. Issayev, K.P. Shrestha, F. Mauss, A. Farooq, W.L. Roberts, Energy and Fuels 34 (2020) 14726–14740.
[11] S.M. Sarathy, P. Oßwald, N. Hansen, K. Kohse-Höinghaus, Prog. Energy Combust. Sci. 44 (2014) 40–102.
[12] R.J. Kee, F.M. Rupley, J.A. Miller, J. Chem. Inf. Model. 53 (1989) 1689–1699.

* Corresponding author.
E-mail address: ronan.pele@etu.univ-orleans.fr