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New experimental data on laminar flame speed to improve ammonia kinetic mechanisms

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Topic: Combustion Fundamental

Introduction

As one of the best hydrogen carriers and a zero-carbon fuel, ammonia (NH₃) will play a main role for future energy production, marine transport, and industrial processes. To help to design or retrofit systems able to accept ammonia as a fuel, numerical simulations are useful. To perform simulations accurate kinetic mechanisms of ammonia oxidation and pollutant formation are needed. To validate and improve them, different experimental data are still needed for a wide range of conditions (equivalence ratio, pressure, and temperature) and with different combustion improvers as for example hydrogen (generated by cracking ammonia itself) [1]. The objective of this study is to provide new experimental data for laminar flame speed (S_L) and to compare them with the last kinetic mechanisms and literature data to further improve existing kinetic mechanisms.

Materials and Methods

Laminar flame speed is obtained with the spherical combustion chamber and a Schlieren optical diagnostic setup fully described in [2]. The study parameters of the experimental set-up are summarized in Table 1. For this study laminar flame speed measurements were performed under normal pressure and temperature conditions and for equivalent ratios from 0.8 to 1.2 with a 0.1 step. Ammonia/hydrogen blend from 0 to 15% vol. of H₂ were studied and compared to a selected panel of mechanisms [3-10] and experimental data from the literature [2,11].

Main Study Parameters	Values	Optical Parameters	Values
Internal Volume [NL]	4.2	Camera Resolution [pxl]	1280x800
Viewport Diameter [mm]	70	Camera Frame rate [fps]	3000-5000
Temperature Range [��C]	25	Open Shutter time [��s]	20
Pressure Range [bar]	1	Magnification [mm/pxl]	0.095

Table 1. Experimental setup parameters

Results and Discussions

The experimental results are gathered on Figure 1. As well known, the addition of H₂ enhances S_L but the effect is noticeable when 10% vol of H₂ is used in NH₃/air mixture. The effect of H₂ addition is more important to the rich sides due to the laminar flame speed evolution of H₂ itself as a function of the equivalence ratio. But for these 4 cases, the maximum of S_L is kept around 1.1 of equivalence ratio. The comparison with numerical simulations, Figure 2., gives spread results. For pure ammonia none of the simulated mechanisms fits with experimental data. At higher H₂ content mechanisms tends to have a better fit for lean mixture but there are still inaccuracies between simulated and experimental data for rich mixtures. Furthermore, the maximum of S_L is reached at different equivalence ratio, depending on the mechanisms, mainly between 1.0 and 1.15.

NH₃/H₂/Air, 298K, 1bar

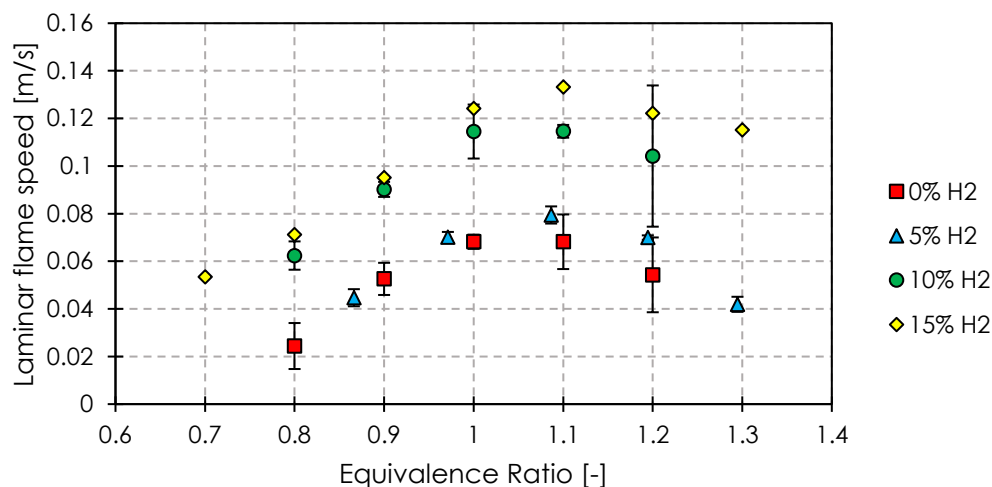


Figure 2. Experimental data

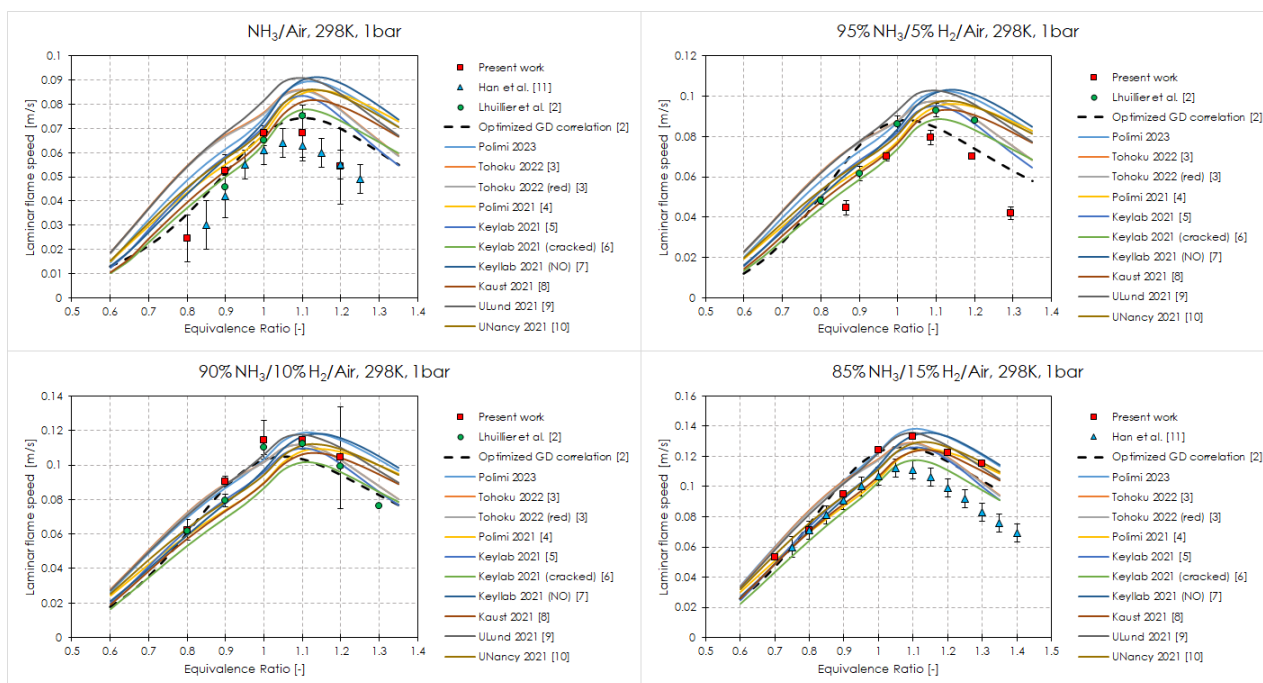


Figure 1. Comparison with numerical and literature data

Conclusions

Most of the mechanisms recently available (from 2021 to 2023), provide a global good prediction of SL as a function of equivalence ratio in comparison to the experimental data. However, for rich and lean mixtures, with less than 10% vol. H₂, more discrepancies can be noticed for the ambient pressure and temperature conditions. No studied mechanisms provide a perfect fit on laminar flame speed as a function of H₂ content and equivalence ratio.

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References

- [1] Nakamura O. 2nd Workshop on Ammonia Combustion, May 2023, Taiwan
- [2] Lhuillier, C., Brequigny, P., Lamoureux, N., Contino, F., Mounaïm-Rousselle, C., 2020. Experimental investigation on laminar burning velocities of ammonia/hydrogen/air mixtures at elevated temperatures. *Fuel* 263, 116653. <https://doi.org/10.1016/j.fuel.2019.116653>
- [3] Gotama, G.J., Hayakawa, A., Okafor, E.C., Kanoshima, R., Hayashi, M., Kudo, T., Kobayashi, H., 2022. Measurement of the laminar burning velocity and kinetics study of the importance of the hydrogen recovery mechanism of ammonia/hydrogen/air premixed flames. *Combustion and Flame* 236, 111753. <https://doi.org/10.1016/j.combustflame.2021.111753>
- [4] Bertolino, A., Fürst, M., Stagni, A., Frassoldati, A., Pelucchi, M., Cavallotti, C., Faravelli, T., Parente, A., 2021. An evolutionary, data-driven approach for mechanism optimization: theory and application to ammonia combustion. *Combustion and Flame* 229, 111366. <https://doi.org/10.1016/j.combustflame.2021.02.012>
- [5] Wang, Z., Han, X., He, Y., Zhu, R., Zhu, Y., Zhou, Z., Cen, K., 2021. Experimental and kinetic study on the laminar burning velocities of NH₃ mixing with CH₃OH and C₂H₅OH in premixed flames. *Combustion and Flame* 229, 111392. <https://doi.org/10.1016/j.combustflame.2021.02.038>
- [6] Mei, B., Zhang, J., Shi, X., Xi, Z., Li, Y., 2021b. Enhancement of ammonia combustion with partial fuel cracking strategy: Laminar flame propagation and kinetic modeling investigation of NH₃/H₂/N₂/air mixtures up to 10 atm. *Combustion and Flame* 231, 111472. <https://doi.org/10.1016/j.combustflame.2021.111472>
- [7] Mei, B., Ma, S., Zhang, X., Li, Y., 2021a. Characterizing ammonia and nitric oxide interaction with outwardly propagating spherical flame method. *Proceedings of the Combustion Institute* 38, 2477–2485. <https://doi.org/10.1016/j.proci.2020.07.133>
- [8] Zhang, X., Moosakutty, S.P., Rajan, R.P., Younes, M., Sarathy, S.M., 2021. Combustion chemistry of ammonia/hydrogen mixtures: Jet-stirred reactor measurements and comprehensive kinetic modeling. *Combustion and Flame* 234, 111653. <https://doi.org/10.1016/j.combustflame.2021.111653>
- [9] Han, X., Lubrano Lavadera, M., Konnov, A.A., 2021. An experimental and kinetic modeling study on the laminar burning velocity of NH₃+N₂O+air flames. *Combustion and Flame* 228, 13–28. <https://doi.org/10.1016/j.combustflame.2021.01.027>
- [10] Arunthanayothin, S., Stagni, A., Song, Y., Herbinet, O., Faravelli, T., Battin-Leclerc, F., 2021. Ammonia–methane interaction in jet-stirred and flow reactors: An experimental and kinetic modeling study. *Proceedings of the Combustion Institute* 38, 345–353. <https://doi.org/10.1016/j.proci.2020.07.061>
- [11] Han, X., Wang, Z., Costa, M., Sun, Z., He, Y., Cen, K., 2019. Experimental and kinetic modeling study of laminar burning velocities of NH₃/air, NH₃/H₂/air, NH₃/CO/air and NH₃/CH₄/air premixed flames. *Combustion and Flame* 206, 214–226. <https://doi.org/10.1016/j.combustflame.2019.05.003>
- [12] Kawka, L., Juhász, G., Papp, M., Nagy, T., Zsély, I.Gy., Turányi, T., 2020. Comparison of detailed reaction mechanisms for homogeneous ammonia combustion. *Zeitschrift für Physikalische Chemie* 234, 1329–1357. <https://doi.org/10.1515/zpch-2020-1649>