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Systematic analysis of tabulated chemistry methods for lean hydrogen flames

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Thermodiffusive instabilities in lean hydrogen flames strongly influence local consumption speeds and reaction rate distributions, posing significant challenges for the development of reduced-order modeling (ROM) approaches [1]. One possible ROM approach is the tabulated chemistry method, which relies on defining one or more control variables and requires a precomputed chemistry database. This database is typically generated by solving one-dimensional flamelets with detailed chemistry and transport, thereby accounting for the flame structure. The selection of relevant control variables and the approach used to build the chemistry database are, however, of critical importance for the model's accuracy.

While previous studies have adopted a progress variable defined as either H_2 or H_2O mass fraction, along with the mixture fraction to account for local equivalence ratios variations [2, 3], the appropriate selection of control variables remains a crucial modeling aspect to be addressed. Preliminary *a priori* investigations demonstrated that a H_2O-based progress variable consistently led to an overprediction of the chemical source term, particularly in high curvature regions, resulting in artificially increased flame speeds. This unphysical behavior might stem from using unstretched flames to build the chemistry database, which fails to correctly capture superadiabatic regions. In contrast, although accurate predictions of the chemical source term can be obtained using an H_2-based progress variable, the inability to represent superadiabatic regions remains a critical limitation for capturing thermodiffusive instabilities. These findings suggest that the definition of the progress variable may be adjusted according to the modeling framework employed, and the approach used to build the chemistry database may significantly affect the ability to map all chemical states.

To address these issues, the performance of tabulated chemistry methods, specifically tailored for thermodiffusive instabilities, is evaluated through both *a priori* and *a posteriori* analyses of canonical hydrogen flame configurations. Key global metrics, including flame consumption speed, wrinkling factor, and stretch factor, are examined, along with local quantities such as joint probability distributions. These findings aim to contribute to a deeper understanding of the modeling of thermodiffusive instabilities and to further support the development of more accurate tabulated chemistry methods for realistic configurations.

References

[1] Berger, L., Attili, A., Gauding, M., and Pitsch, H., "LES combustion model for premixed turbulent hydrogen flames with thermodiffusive instabilities: a priori and a posteriori analysis," *Journal of Fluid Mechanics*, Vol. 1003, 2025, pp. A33.

[2] Regele, J. D., Knudsen, E., Pitsch, H., and Blanquart, G., "A two-equation model for non-unity Lewis number differential diffusion in lean premixed laminar flames," *Combustion and flame*, Vol. 160, No. 2, 2013, pp. 240–250.

[3] Schlup, J. and Blanquart, G., "Reproducing curvature effects due to differential diffusion in tabulated chemistry for premixed flames," *Proceedings of the Combustion Institute*, Vol. 37, No. 2, 2019, pp. 2511–2518.