

VGPS

Direct Numerical Simulation of Flame-Wall Interaction for Low-Carbon Gas Turbine Combustion





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Context

- Green hydrogen (H₂) and ammonia (NH₃) are emerging as carbon free alternatives to hydrocarbon fuels [1, 2].
- · In gas turbines, flames interact with the combustor liner (wall), which affects the pollutant emissions, the burning efficiency, and the thermal load on the liner. We lack understanding of this important flame-wall interaction (FWI) for alternative fuels
- FWI occurs at the scale of the flame thickness, and such scales are only resolved by direct numerical simulation.
- Here, we resolve the FWI for NH₃ and H₂ flames. Preliminary results of two distinct projects are presented.

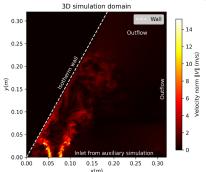
Configurations

2D laminar case: anchored "V" NH₃/H₂ flame

- · Chemical kinetics model with 21 species and 64 reactions [3]
- Effective resolution: 14 µm (maximum refinement level)
- Computational cost: 3-5k cpuh/case

3D turbulent case: lab-scale swirling CH₄/H₂ flame (70% H₂ by vol.) 0.00 0.25 0.50 0.75 1.00

- Bulk Reynolds number: ~ 20,000.
- Reduced Aramco chemical kinetics model for lean CH combustion (24 species and 105 reactions) [4].
- Effective resolution: 4096x4096x4096 (80 μm)
- Only 1024x1024x1024 (300 µm) shown
- Computational cost: ~ 10M cpuh (500k cpuh so far)



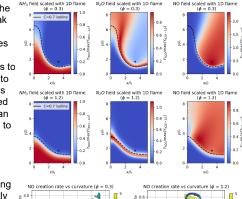
- Solver: PeleLMeX [5], a low-Mach number, reactive flow solver with embedded boundaries, adaptive mesh refinement and finite rate chemistry.
- **Definitions:** Equivalence ratio (ϕ) fuel to air ratio, normalized by stoichiometric value; l_f – flame thickness; C - progress variable; Y - mass fraction

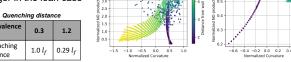
Role of quenching on pollutants

NH₃/H₂ laminar flames

- Flame quenching at the wall allows NH3 to leak and increases N₀O emissions, but reduces NO emissions.
- Partly due to heat loss to the wall, which leads to reduced reaction rates
- Phenomenon amplified (attenuated) in the lean (rich) case. Attributed to positive (negative) correlation between reaction rates and curvature.
- Consistently, quenching distance is significantly larger in the lean case

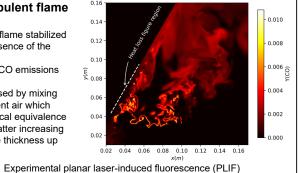




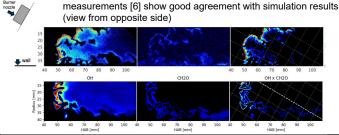


CH₄/H₂ turbulent flame

- Ultra-lean flame stabilized by the presence of the wall
- Important CO emissions identified
- Likely caused by mixing with ambient air which reduces local equivalence ratio, the latter increasing local flame thickness up to O(1) m

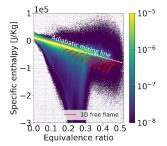


CO mass fraction field

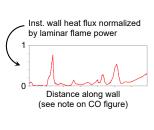


Heat loss (turbulent case)

Significant wall heat loss identified locally



· Leads to non-adiabatic thermochemical space



Conclusions

- · Quenching and pollutant emissions strongly affected by fuel/air ratio
- An inclined wall can stabilize very lean turbulent CH₄/H₂ flames, but prone to large CO emissions
- Wall heat loss affects flame response to curvature (shown in 2D case) and leads to non-adiabatic thermochemical space (shown in 3D case). These effects imply modeling challenges for LES or RANS of turbulent flame-wall interaction in advanced gas turbine engines

References

[1] Ministère des ressources naturelles Québec, "Hydrogène vert," 2022.

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[3] Y. Jiang, A. Gruber, K. Seshadri, and F. Williams, "An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications," Int J Energy Res, vol. 44, no. 2, pp. 795–810, Feb. 2020. [4] W. K. Metcalfe, S. M. Burke, S. S. Ahmed, and H. J. Curran, "A Hierarchical and Comparative Kinetic Modeling Study of C1 - C2 Hydrocarbon and Oxygenated Fuels," International Journal of Chemical Kinetics, vol. 45, no. 10, pp. 638-675, 2013.

[5] M. Day et al., "Pele: An Exascale-Ready Suite of Combustion Codes," National Renewable Energy Lab. (NREL), Golden, CO (United States), NREL/PR-2C00-82880, Jun. 2022. Accessed: Mar. 13, 2023. [Online]. Available: https://www.osti.gov/biblio/1873112

[6] L. Fan et al., "Simultaneous stereo-PIV and OH×CH2O PLIF measurements in turbulent ultra lean CH4/H2 swirling wall-impinging flames," Proceedings of the Combustion Institute, Nov. 2022.

Acknowledgements



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