DNS STUDY OF THE IMPACT OF THERMODIFFUSIVE EFFECTS ON THE TURBULENT FLAME SPEED IN PARTIALLY CRACKED AMMONIA FLAMES

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Abstract
In this work, Direct Numerical Simulations (DNS) of turbulent premixed partially cracked ammonia/air flames in a three-dimensional box shaped numerical domain at atmospheric conditions are performed to investigate the impact of flame-turbulence interaction and thermodiffusive effects on the turbulent flame speed.
To this scope, three levels of ammonia cracking (5%, 20% and 40%), one level of turbulent intensity (1.13 m/s), and one value of equivalence ratio (0.8) are selected to investigate specific flame-turbulence interaction regimes.

Introduction
Ammonia (NH_3) combustion is considered a promising solution to reduce anthropogenic carbon emissions. Nevertheless, it presents several modeling and scientific challenges, since NH_3 flames are characterized by low reactivity [1]. To solve these issues, two strategies are commonly used: (1) doping ammonia with other more reactive fuels and (2) partial cracking of ammonia molecules (PCA). This second solution is particularly interesting, due to its easier implementation in practical industrial-scale combustion systems.
Given the complexity of the phenomenon, high-fidelity numerical simulations are required to complement experiments and gain an understanding. Therefore, this work aims to improve the knowledge in ammonia combustion for both low and high Karlovitz number (Ka) combustion regimes, focusing on flame-turbulence interaction, thermodiffusive (TD) effects and their impact on turbulent flame properties. Specific attention is given to turbulent flame speed to gain an understanding of the mechanism behind its peculiar “bending effect” found in [2].

Numerical Methodology and Configuration
To achieve these objectives, this work proposes a set of DNS of planar ammonia-air flames stabilized in a three-dimensional (3D) box-shaped numerical domain submitted to Homogeneous Isotropic Turbulence (HIT) (Fig.1). The numerical simulations are performed in the massively-parallel compressible Navier-Stokes

solver AVBP (https://cerfacs.fr/avbp7x). The HIT field is forced within the computational domain following the linear forcing model provided by Bassenne et al. [3]. To properly solve the flame and capture velocity gradients of the highly corrugated flame front, a sufficiently refined grid is required, with at least 10 points in the flame front, whose thickness is estimated by 1D unstretched premixed flame calculations. The Pope criterion is adopted to ensure turbulent flow resolution. A previously validated Analytically Reduced Chemistry (ARC) mechanism [4] is adopted to solve the ammonia-hydrogen-air chemical reactions.
Based on the experimental work by Zitouni et al. [2], simulations are performed considering three levels of ammonia cracking γ=5%, 20% and 40%, one level of turbulent intensity u'=1.13 m/s, and one value of equivalence ratio φ =0.8. These operating conditions are chosen to investigate multiple flame-turbulence interaction regimes.

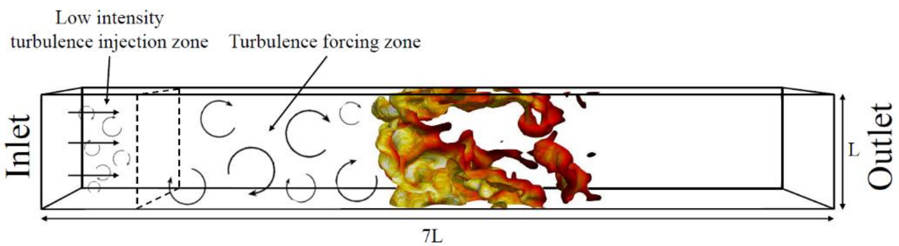

Figure 1. Computational domain and methodology scheme.

Results
Preliminary results show that the interaction between flame and turbulence varies with mixture composition. It is worth noting that mixtures with the highest amount of NH_3 have the highest Karlovitz numbers, due to their laminar properties [2].
The effects of turbulence-flame interaction and flame dynamics impact the turbulent flame speed S_C. In fact, as illustrated in Fig. 2A, it is evident that for γ=5% the S_C increases predominantly because of turbulence, which tends to augment the flame surface area A_T rather than the TD effects which varies the local flame structure (e.g., local reactivity) [5]. These are represented by the stretch factor I_0, which remains close to unity in this case. In contrast, for γ=20% (Fig. 2B), I_0 is greater than this

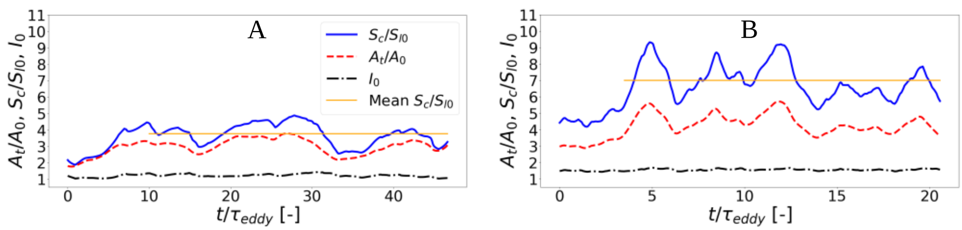

Figure 2. Temporal evaluation of the stretch factor I_0, normalized turbulent flame speed S_C/S_{l0} and flame surface area A_T/A_0 for γ=5% (A) and γ=20% (B) ($\tau_{eddy} = 2.3 \cdot 10^{-3} s$).

value. Thus, the combined effect of enhanced H_2 and low Ka is such that TD instabilities are more pronounced than in the high Ka case, resulting in a more wrinkled flame surface, as can be seen in Fig. 3. Consequently, in the latter case, turbulence and TD effects both impact S_C. These phenomena are even more evident in $\boldsymbol{\gamma}$=40% case.

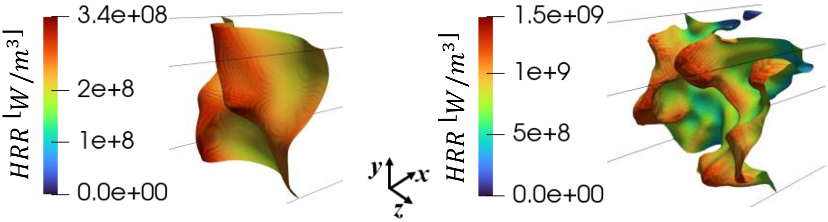

Figure 3. Instantaneous isosurfaces of progress variable c for γ=5% (left, c=0.93) and for γ=20% (right, c=0.87) cases. Isosurfaces are coloured by Heat Release Rate.

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References

[1] Valera-Medina, A., Amer-Hatem, F., Azad, A.K., Dedoussi, I.C., De Joannon, M., Fernandes, R.X., Glarborg, P., Hashemi, H., He, X., Mashruk, S. and McGowan, J., "Review on ammonia as a potential fuel: from synthesis to economics", *Energy & Fuels*, *35*(9): 6964-7029 (2021).

[2] Zitouni, S., Brequigny, P. and Mounaïm-Rousselle, C., "Turbulent partially cracked ammonia/air premixed spherical flames" *Fuel Communications*, 20: 100126 (2024).

[3] Bassenne, M., Urzay, J., Park, G.I. and Moin, P., "Constant-energetics physical-space forcing methods for improved convergence to homogeneous-isotropic turbulence with application to particle-laden flows", *Physics of Fluids*, *28*(3) (2016).

[4] Ruiz, H.V., Laera, D., Lartigue, G., Mashruk, S., Valera-Medina, A. and Gicquel, L., "Extension of the dynamic Thickened Flame model for partially-premixed multi-fuel multi-injection combustion and application to an ammonia–hydrogen swirled flame" *Combustion and Flame*, 274: 113992 (2025).

[5] Tingas, E.A. (Ed.), "Hydrogen for Future Thermal Engines", *Springer Nature*, 93-265 (2023).