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Unraveling Turbulent NH_3/H_2 Flames Using High Performance GPU Computing: A Series of Spectral Element Method-Based High-Fidelity DNS

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ABSTRACT

Ammonia-hydrogen blends are crucial for future carbon-free combustion systems, with staged-combustion technologies like rich-quench-lean being proposed to minimize emissions. However, the combustion behavior of turbulent rich ammonia-hydrogen mixtures is not well understood, particularly regarding phenomena like partial cracking, hydrogen slip, and post-flame stratification. Recent HPC advancements, particularly in GPU-based systems, enable combustion DNS beyond academic configurations. Utilizing nekCRF, a new GPU-based spectral element solver based on nekRS, we perform finite-rate chemistry DNS of a rich, turbulent premixed jet flame. The analysis focuses on NH_3/H_2 interaction, revealing residual H_2, minimized NH_3 slip, and enhanced heat release through turbulent mixing. By leveraging GPU acceleration and employing a novel spectral element solver, this research not only advances our understanding of ammonia combustion but also showcases a paradigm shift in computational efficiency, offering a promising avenue for developing sustainable energy solutions.

1. Introduction

To address the pressing issue of climate change, society confronts the formidable task of transitioning away from fossil fuels in our energy system. Gas turbines for power generation and aviation are at the heart of our energy infrastructure. Renowned for their high thermal efficiencies and unmatched power densities, these machines have traditionally used hydrocarbon-containing fuels. Efforts are underway to develop gas turbines that efficiently use zero-carbon fuels, leading to a sustainable energy future. Although gas turbines are theoretically fuel-flexible, they can face significant operational challenges related to flame stability and emissions due to the vastly different combustion properties of H_2 and NH_3 fuels compared to conventional hydrocarbon fossil fuels [1].

For example, hydrogen's high diffusivity and reactivity drive its strong turbulent burning rate, influenced by turbulent fluctuations and intense thermo-diffusive instabilities from differential diffusion [2, 3]. Conversely, ammonia, a promising hydrogen carrier, requires precise NOx emission control during partial decomposition. Recent experimental and numerical evidence indicates that an RQL (Rich-Quench-Lean) operational strategy ensures both flame stabilization and low emissions in ammonia-fired combustors [4, 5, 6]. This study aims to fill the knowledge gap on pressure effects on these fuels, focusing on H_2/NH_3 flames with controlled flame propagation. By leveraging advanced high-performance computing tools, we seek to unlock the potential of fuel-flexible, high-power density combustion systems for zero-carbon gas turbines.

To fully exploit the potential of current and future HPC centers, a highly scalable reactive flow simulation code (nekCRF) [7] based on nekRS as part of the Center of Excellence in Combustion (CoEC) project during the last three years was developed, enabling high-fidelity direct numerical simulations (DNS) of configurations at technically relevant operating conditions. Here, nekCRF will be leveraged to study ammonia-hydrogen jet flames. The novel benchmark data will enable the assessment and further development of

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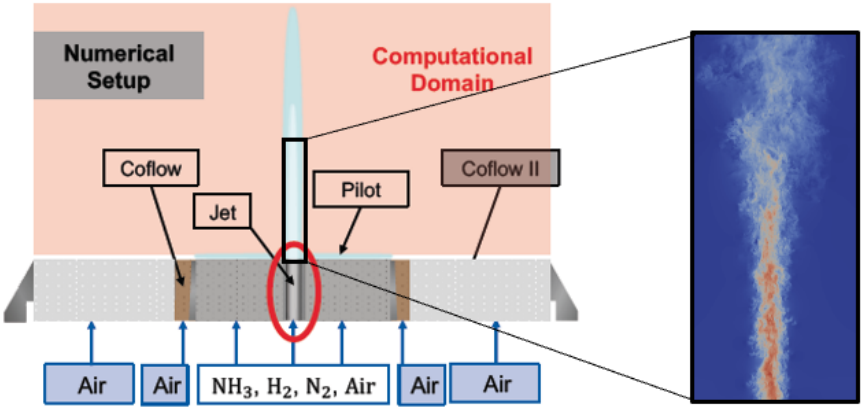

Figure 1: Schematic depiction of the McKenna burner configuration. Zoom shows the jet-flow field.

combustion models urgently needed for designing ammonia-hydrogen-fueled gas turbines.

2. Computational methodology

As simulation framework, nekRS [8] is used in combination with the chemistry plugin nekCRF developed as part of CoEC. It employs high-order spectral elements in which the solution, data, and test functions are represented as locally structured Nth-order tensor product polynomials on a set of E globally unstructured conforming hexahedral brick elements. Time integration in nekRS employs a semi-implicit splitting scheme, utilizing kth-order (k up to three) backward differences (BDFk) to approximate the time derivative, resulting in an implicit treatment of the viscous and pressure terms, and kth-order extrapolation (EXTk) for the advection and forcing terms. The discretization leads to a sequence of symmetric positive definite linear systems for pressure, velocity and temperature. Its scalability to millions of MPI ranks is based on the gsLib communication library, which handles all near-neighbor and other stencil type communications [8].

The thermochemistry (energy and species equations) is treated with the highly optimized chemistry plugin nekCRF that generates optimized kernels for the source term, thermodynamic and transport properties evaluation for GPUs. It also provides consistent advection and diffusion transport operators acting efficiently on multiple scalars. The resulting large system is integrated without further splitting of the convection, diffusion and reaction term using CVODE [9].

3. Configuration

The setup involves a turbulent premixed $NH_3/H_2/N_2$ jet flame operating under slightly rich conditions with an equivalence ratio of $\Phi = 1.2$. This configuration, illustrated in Fig. 1, is adapted from a McKenna burner studied experimentally at TU Darmstadt. This offers the advantage of benchmarking the base operating condition with 45 vol-% H_2 against available experimental data, enabling the exploration of uncertainties in the chemical mechanism. For the experimental conditions, the central jet velocity is set to 50 m/s, resulting in a REYNOLDS number of 15,000. The coflow, which stabilizes the flame, operates with a fuel-lean hydrogen mixture at an equivalence ratio of $\Phi = 0.7$. The flame is stabilized directly above the burner exit, and the exhaust gas velocity of the flame is used as an inlet condition for the DNS domain. The overall objective is to unravel the fundamental combustion physics of propagating hydrogen and ammonia flames under diverse operating conditions, spanning from atmospheric to high pressure (unlike the experiments). A critical free parameter in NH_3/H_2 combustion is the precracking ratio of ammonia. Determining

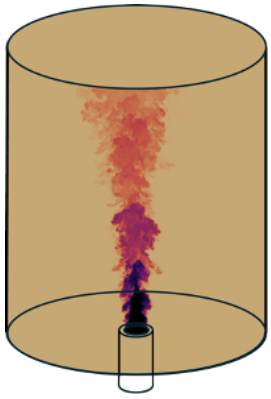

Figure 2: Instantaneous temperature of field of the McKenna burner.

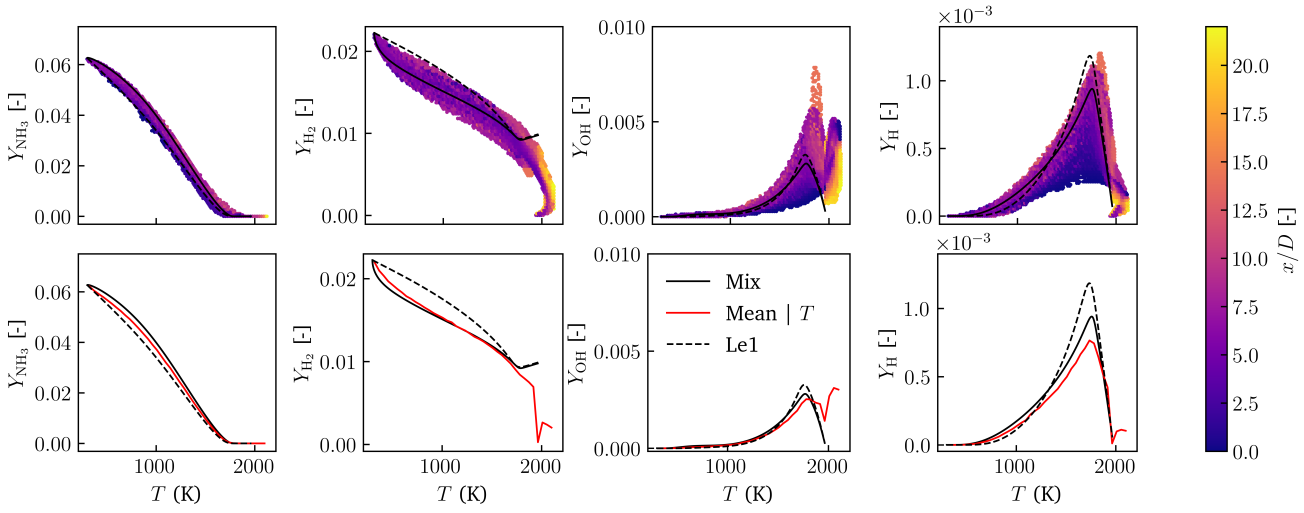

Figure 3: Top row: Instantaneous scatter plots of the thermochemical state together with unity LEWIS numbers and mixture-averaged flamelets. Bottom row: Conditional averaged of DNS data.

an optimum balance between flame stability (with high H_2 content), low emissions, and energy efficiency (with high NH_3 content) is crucial. Given the fully premixed state, this configuration is predestined for the analysis of turbulence-chemistry interactions. Of particular interest are processes of thermal ammonia decomposition, the impact of equivalence ratio variations on NOx formation.

4. Results

The flame depicted in Fig. 2 exhibits significant influence from turbulent flow, leading to intricate interactions between chemical reactions and mixing processes. In the instantaneous temperature field, sharp gradients and fluctuating regions of high and low temperatures are observed. These variations highlight the intense mixing and reaction zones within the flame, where hot combustion products and cooler reactants interact continuously, creating a highly dynamic and ever-changing thermal structure. Capturing these dynamics remains a challenge for state-of-the-art combustion models.

Figure 3 showcases the high-fidelity data from these DNS studies, illustrating flame structures as a function of temperature for the main fuel species (NH_3, H_2), and the OH and H radicals. Additionally, one-dimensional freely propagating flames with unity LEWIS number and mixture fractions are displayed, which are used to build manifold-based combustion models [3]. The scatter in the DNS data demonstrates reasonable agreement with both models. To establish a better comparison, temperature conditional averaging of the DNS data is performed, shown in the bottom row of Fig. 3. This comparison shows a favorable match of the conditional average with the mixture-averaged flamelets for both fuel species, with high-temperature differences attributed to unmodeled mixing with the surrounding co-flow of burnt gases, and low-temperature deviations due to turbulent mixing with ammonia pre-cracking. These effects are not included in current combustion models, which require extensions. Notably, the radicals OH and H also align well with the mixture-averaged flamelet. As these species are markers for curvature and strain impacts on turbulent flame structures, it can be concluded that NH_3/H_2 flames are less sensitive to curvature and strain than hydrogen flames, as reported in previous studies [3]. The scatter data used for conditional averaging are derived from the entire domain. Given that the co-flow is fuel-lean (providing sufficient oxygen for the flame) and the jet is fuel-rich, a mixing process occurs. This process involves the mixing of flue gases from the jet flame with the surrounding co-flow, resulting in the tails observed in the conditionally averaged DNS data. Additionally, the excess hydrogen burns in a weak secondary flame, which is suggested by the temperature increase after the main flame.

5. Conclusions and outlook

In this study, a series of SEM DNS simulations of NH_3/H_2 flames is conducted to explore the complexity of this novel fuel blend. Utilizing the advanced GPU flow solver NekRS with the chemistry plugin NekCRF, we vary parameters such as pressure and pre-cracking ratio. These high-fidelity results enable a thorough evaluation of state-of-the-art combustion models, including the manifold-based

models demonstrated here. At the conference, this assessment will be expanded to cover the entire parameter space and include a performance evaluation of the reactive flow solver.

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