Reactive structures of Ammonia/Hydrogen Blends in MILD Combustion processes

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Abstract
The present work investigates the combustion behavior of ammonia and ammonia/hydrogen when they are used as fuels in MILD Combustion under diffusion-controlled conditions. Numerical simulations were performed through 1D counterflow flames in both steady and unsteady processes, under hot oxidant and diluted fuel conditions (HODF). Temperature and heat release patterns were analyzed to characterize the reactive region as a function of fuel dilution levels.
Main characteristics of the ammonia/hydrogen MILD Combustion were obtained to categorize the combustion regimes and to gain insights about the transition from conventional to MILD combustion regimes.

Introduction
MILD combustion is an innovative technology that effectively addresses the dual challenge of achieving high thermal efficiency and meeting stringent pollutant emission regulations [1-3] . This combustion method offers significant operational flexibility, adapting to varying conditions and fuel types without requiring major modifications to existing conventional plants. This makes it well-suited for handling the increasing complexity and diversity of the energy supply.
A key characteristic of MILD combustion is its use of high dilution and preheating levels that allow to operate in a distributed ignition regime, characterized by smooth gradients in scalar quantities. More recently, research has demonstrated the potential of MILD combustion for utilizing carbon-free fuels, such as ammonia and ammonia/hydrogen mixtures, with encouraging outcomes [2].
This work uniquely focuses on examining and defining the characteristics of the reactive structures that are obtained during the diffusion ignition process of ammonia and ammonia/hydrogen MILD Combustion. The study offers a classification of the various combustion behaviors that are obtained and peculiar features of diluted conditions.

Numerical Methodology

Ammonia-hydrogen/air igniting counterflow diffusion flamelets were generated with the 1D reactive flow solver CHEM1D [4]. A fixed strain rate of 50 s^{-1} was chosen for all cases. To replicate MILD conditions, a HODF (Hot Oxidizer Diluted

Fuel) configuration was employed. Inlet temperatures were set to 300 K and 1400 K for the fuel and oxidizer stream respectively. All simulations were performed at atmospheric pressure, with the fuel stream diluted by nitrogen at levels ranging from 0% to 93% N_2. Different fuel compositions were investigated including pure ammonia, pure hydrogen and blends of the two. A Bilger mixture fraction formulation is used for all fuel mixtures.

Results

MILD conditions are achieved for highly diluted mixtures, and distinctive features of the igni-diffusion process are observed, such as distributed reaction zone, lack of correlation between the heat release peak and the stoichiometric mixture fraction (Z_{st}). As illustrated in Figure 1, the temporal evolution of the maximum temperature increase relative to the frozen line reveals that highly diluted cases (90–93% N_2), classified as MILD, display a slower temperature rise compared to less diluted cases, with peak temperatures remaining below the autoignition threshold.

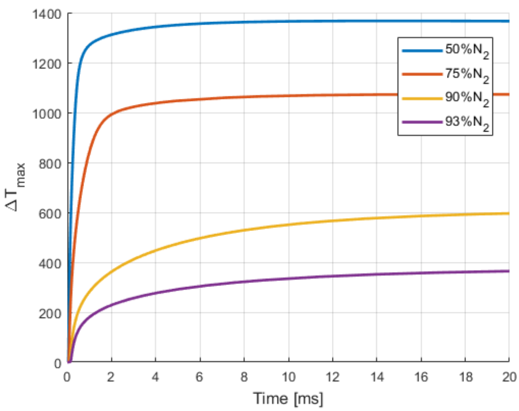

Figure 1. Evolution in time of the maximum temperature increase respect to the frozen line for different dilution levels.

Unsteady simulations highlight significant differences between MILD and conventional combustion regimes, as shown in Figure 2. In low-dilution, non-MILD conditions, higher transient heat release peaks and ignition events occurring in the rich zone are observed. In contrast, MILD cases consistently exhibit combustion confined to the lean region, with a gradual and monotonic increase in heat release over time. Additionally, achieving MILD conditions requires higher dilution levels when hydrogen is present in the fuel blend. Consequently, the NH_3/H_2 ratio strongly affects flame stability, the spatial distribution of heat release, and the dilution threshold necessary for entering the MILD regime.

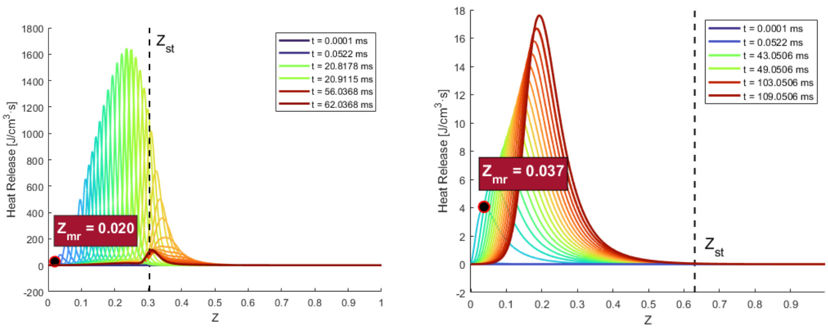

Figure 2. Evolution in time of heat release vs mixture fraction for 50% N_2 dilution (left) and 93% N_2 dilution (right).

Conclusions

The ignition behavior of ammonia-hydrogen/air counterflow diffusion flamelets under MILD and non-MILD conditions was investigated using unsteady 1D simulations. The results demonstrate that MILD combustion can be achieved at high nitrogen dilution levels (>70%), characterized by a distributed reaction zone, slower and smoother temperature rise, and the absence of correlation between the heat release peak and the stoichiometric mixture fraction. In contrast, low-dilution cases exhibit conventional combustion features, including sharp transient heat release and localized ignition in the rich zone. The transition between these regimes is gradual, with intermediate cases showing mixed ignition behavior. Furthermore, the NH_3/H_2 blending ratio plays a key role in determining the heat release dynamics, flame stability, and the dilution threshold required for MILD regime attainment. These findings highlight the potential of ammonia-hydrogen mixtures for flexible and low-emission combustion strategies under MILD conditions.

Acknowledgements

The authors gratefully acknowledge the partial financial support of the European Union, NextGenerationEU - in the framework of the National Sustainable Mobility Center - MOST, CN00000023, Italian Ministry of University and Research Decree n. 1033— 17/06/2022, Spoke 12, CUP B43C22000440001.

This research was partly funded by the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU – Project Title REACTANT – CUP B53D23026970001

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