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Numerical Investigation on the Feasibility of the Micromix Combustion Principle for H_2/NH_3 Blends

[1,2]Pablo Barreiro, [1]Isabel Alava, [2]Jesus Maria Blanco
[1]Ikerlan Technology Research Center, Basque Research and Technology Alliance (BRTA), P°. J.M. Arizmendiarreta, 2, Arrasate-Mondragón, 20500, Spain
pbarreiro@ikerlan.es
[2]Energy Engineering Department, School of Engineering, Building I, University of the Basque Country, UPV/EHU, Plaza Ingeniero Torres Quevedo s/n, Bilbao, 48013, Spain

Abstract - This study aims to investigate numerically the feasibility of the micromix combustion principle (MCP) for hydrogen-ammonia blends in industrial combustion systems. The micromix combustion principle was originally designed for hydrogen burners in gas turbines, characterized by splitting the flame in a set of miniaturized turbulent diffusion flames. This principle reduces NOx emissions in an effective way and eliminates the risk of flashback, which are significant challenges when using pure hydrogen or hydrogen-enriched blends. A novel design micromix-type burner well adapted for 50-50% hydrogen-ammonia volume ratio was investigated through CFD (Computational Fluid Dynamics) modelling, considering an energy density of 10 MW/m^{2}bar and lean conditions ($\lambda = 2.5$). In addition, two other blends containing 40% and 60% ammonia respectively were also investigated. The numerical results showed that the micromix combustion principle could be perfectly adapted to ammonia and hydrogen blends by adjusting the design to the suitable crossflow penetration distance. Stable miniaturized flames and low concentrations of unburnt ammonia were obtained. Although ammonia combustion produces high NOx emissions, lean operating conditions promote relatively low emissions levels. This work thus establishes the groundwork for designing ammonia and hydrogen burners based on the micromix combustion principle.

***Keywords*:** Ammonia, Hydrogen, Micromix Combustion Principle (MCP), NOx, CFD modelling.

1. Introduction

To facilitate the decarbonization of the energy market, using ammonia as a fuel—either directly or blended with other fuels—offers several advantages. With its high volumetric energy density (compared to hydrogen) and a well-established production and transport infrastructure, ammonia is a sustainable fuel and an attractive energy carrier. However, using ammonia in combustion poses numerous significant challenges, such as low flame speed, narrow flammability limits, high NOx formation, etc. The use of ammonia-hydrogen blends in gas turbines and in industrial combustion systems has gained increasing attention, as hydrogen improves the combustion characteristics of ammonia. However, optimizing flame stability and reducing NOx emissions remain significant challenges. Two-stage combustion combustion processes have recently received increased attention for its NOx reduction capability and efficiency. This has been demonstrated over a wide range of operating conditions. Other strategies focused on emissions reduction continue to be studied, such as very lean combustion, flameless combustion and humidification [1, 2].

One promising combustion technology in the industrial sector that uses hydrogen as a fuel is the micromix combustion principle (MCP), which represents a novel approach that minimizes the drawbacks of hydrogen combustion [3]. The burner operates on the crossflow principle, using miniaturized nozzles to inject fuel perpendicularly into the air stream. Fuel jets and air guide panels (AGP) stabilize the flames by creating inner and outer vortices. This multi-flame method splits the reaction zone into diffusive turbulent flames, reducing high-temperature regions. In this context, computational fluid dynamics (CFD) will be demonstrated to be an effective tool for accelerating the industrial use of NH_3 and H_2 by investigating the combustion process itself. Thus, the main purpose of the present paper is to analyse the feasibility of adapting the MCP for different ammonia/hydrogen fuel blends, aiming to optimize it.

2. Numerical methodology

The burner design [4] and computational domain considered in the present study is shown in Fig. 1. Following the approach of previous CFD studies [5,6], the domain was simplified by considering symmetry flow conditions in both transverse and longitudinal directions instead of simulating the whole array of flames. The fluid domain was limited between the symmetry plane of the fuel inlet half and the symmetry plane of the free space between two consecutive flames. Previous numerical studies show that the adiabatic wall approximation leads to more than acceptable results. Therefore, due to the scope of the present work, all walls relative to the burner have been treated as adiabatic. In conclusion only one flame is modelled, considering the corresponding symmetry conditions.

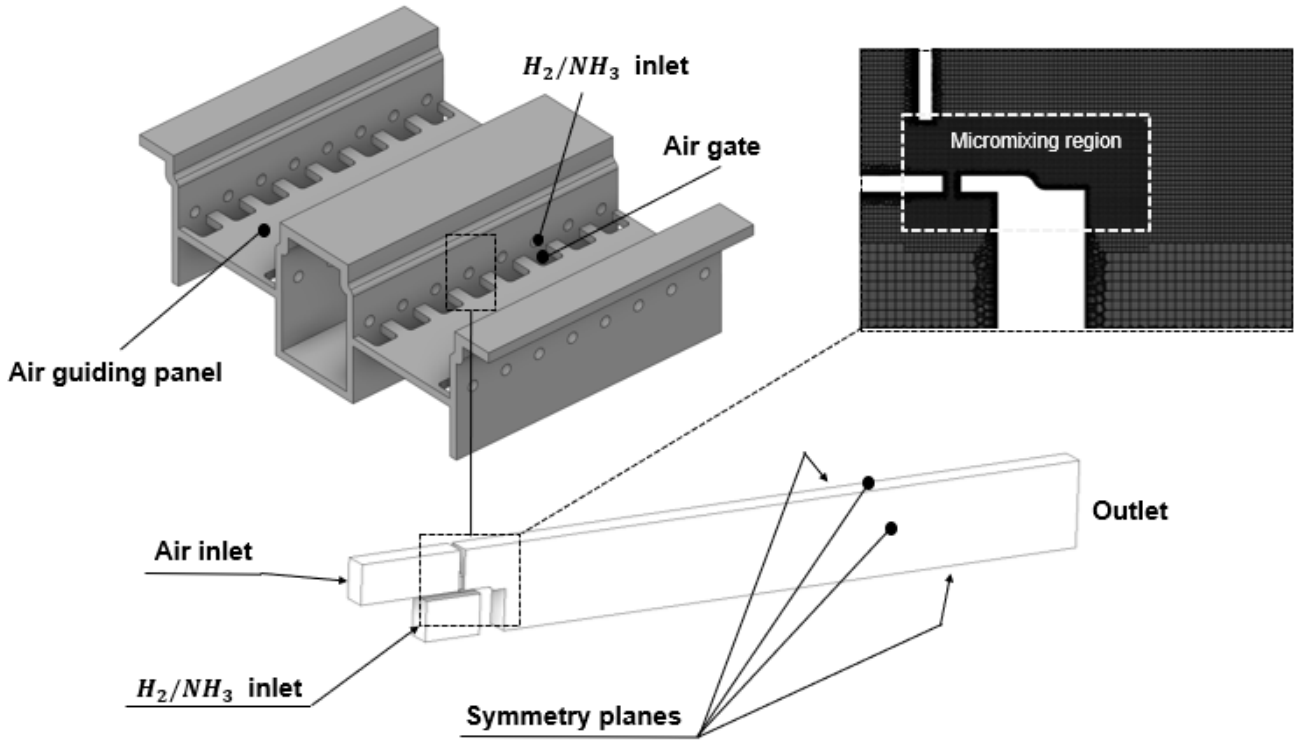

Fig. 1: The burner design, single fuel/air nozzle computational fluid domain and mesh.

The steady three-dimensional flow fields were obtained by solving the Reynolds-averaged Navier-Stokes (RANS) equations alongside transport equations for the scalars involved in the combustion model. The discretization of the convective terms was solved using a second-order upwind scheme, while gradients were computed through the Least Squares method. Pressure-velocity coupling was solved using the pressure-based coupled algorithm. The burner operating principle considers various turbulence scales based on the flow region; thus, k-omega turbulence models are used to capture the scale variability effects. Radiation effects have been also modelled through the discrete ordinate model. Regarding turbulent chemical interaction, the mechanism developed by Otomo et al. [7,8], optimized for hydrogen/ammonia blends was employed in combination with the FGM (flamelet generated manifolds) model. This mechanism allows modelling the NOx emissions from fuel and thermal source for combustion of hydrogen/ammonia mixtures. The complexity of the mechanism suggests that this combustion model is valuable for lowering computational costs, while representing the main features of MCP with same accuracy [6]. According to FGM theory the turbulent flame is approximated by an ensemble of laminar flames previously calculated. The main thermochemical variables (i.e. species mass fractions Y_i and temperature T) are defined by two variables: mixture fraction Z and the progress variable

c [9]. The transport equations for the mean mixing fraction, the reaction rate, and their variances were then solved. The thermochemical variable time-averaged values can be related to the instantaneous mixing fraction and progress variable through a probability density function (PDFs), according to Eq. 1,

$$\bar{\phi}_i = \int_0^1 \int_0^1 p(Z)p(c)\phi_i(Z,c,h)\, df\, dc \tag{1}$$

where $\bar{\phi}_i$ is a generic thermochemical variable (i.e. species mass fractions Y_i and temperature T) and h represent the enthalpy. For the mesh sensitivity analysis, a fine mesh of 1M cells, a medium mesh of 0.45M, and a coarse mesh of 0.2M were considered. The results shown in Tab. 1 indicated that the fine mesh with 1M cells was needed to guarantee a mesh-independent solution, showing negligible changes in the most representative variables.

Table 1: Grid sensitivity analysis results: the relative error to medium grid e_{f-m}, the extrapolated relative error e_f^{ext} and the Grid Convergence Index GCI.

$Quantity\ (\phi)$	ϕ_{Coarse}	$\phi_{Meidium}$	ϕ_{Fine}	e_{f-m} [%]	e_f^{ext}[%]	GCI_f [%]
$T_{max}\ (K)$	1850	1941	1942	0.05	0.07	0.09
$T_{Aver.}\ (K)$	1340	1360	1365	1.49	2.17	2.65
$NO_x(15\%\ O_2)\ (ppm)$	257	259	260	0.38	0.54	0.68

3. Results and discussion

This section exhibits the numerical results of ammonia-hydrogen blends combustion focusing on the effect of ammonia proportion. The MCP can be characterized by key design parameters related to the physical processes behind the jet in crossflow and combustion aerodynamics. This parameter is defined as the ratio between the fuel jet and the air crossflow momentum (Eq. 2), determining the injection depth of the hydrogen into the air crossflow:

$$r_m = \frac{\rho_{Fuel}U_{Fuel}^2}{\rho_{Air}U_{Air}^2} = \frac{\dfrac{\dot{m}_{Fuel}^2}{\rho_{Fuel}A_{Fuel}^2}}{\dfrac{\dot{m}_{Air}^2}{\rho_{Air}A_{Air}^2}} \tag{2}$$

where the velocity of fuel and air have been expressed in terms of the mas flow $\dot{m}$, jet area A_{Jet} and density ρ. The penetration depth is a critical parameter for optimal mixing. Better turbulent mixing between reactants in the jet crossflow region results in lower thermal NOx emissions. At shallow penetration depths, a high air flux adversely affects the mixing process between the fuel and the air, resulting in increased NOx emissions and ultimately impacting flame stability. Above a critical injection depth y_{crit}, the fuel jet penetrates into the shear layer and enters the inner recirculation vortex. The fuel–air mixture ignites in the inner vortex, leading to an opposing flame merging [3]. The fuel jet is well-mixed in the crossflow for optimal penetration depth and expands suddenly at the height of the hydrogen segments, resulting in anchored flames. Higher ammonia concentrations in the fuel increase its density and mass flow for a given energy density, increasing the momentum flux ratios and promoting the jet penetration into the inner vortex. Thus, as the concentration of ammonia in the fuel increases, the fuel jet area must also be increased to ensure proper mixing in the cross flow.

The burner design allows maintaining a penetration distance to ensure the micro mixing of the reactants for blends close to the 50% H_2 - 50 % NH_3 volume ratio. The operating conditions were close to gas turbine burners including an energy density (ED) of 10 MW/m^{2}bar, air excess $\lambda = 2.5$ and inlet air temperature of 560 K. The temperature contours for the three blends as well as the emissions and unburnt compounds are shown in Fig. 2. It follows from the numerical results that the lean conditions promoted a significant decrease of NOx emissions and demonstrated the potential of the burner to operate with hydrogen-ammonia blends. The adiabatic flame temperature decreased as the concentration of ammonia increased, which significantly reduced the thermal NOx emissions. However, the high concentration of nitrogen in the ammonia molecule appeared to react with the OH radicals, resulting in elevated fuel NOx emissions. The numerical results indicated a general trend of decreasing NOx levels as the amount of unburnt ammonia increased. For blends with an ammonia volumetric content greater than 60%, flame extinction occurred due to the reduction of the flame speed. Therefore, the lowest NO_X emissions were produced close to the flame extinction limit. In conclusion, operating in an ultra-lean regime with high air excess, which is very close to the extinction limit, provided distinct advantages by balancing NOx emissions and unburnt ammonia, as reported in previous studies [10, 11, 12].

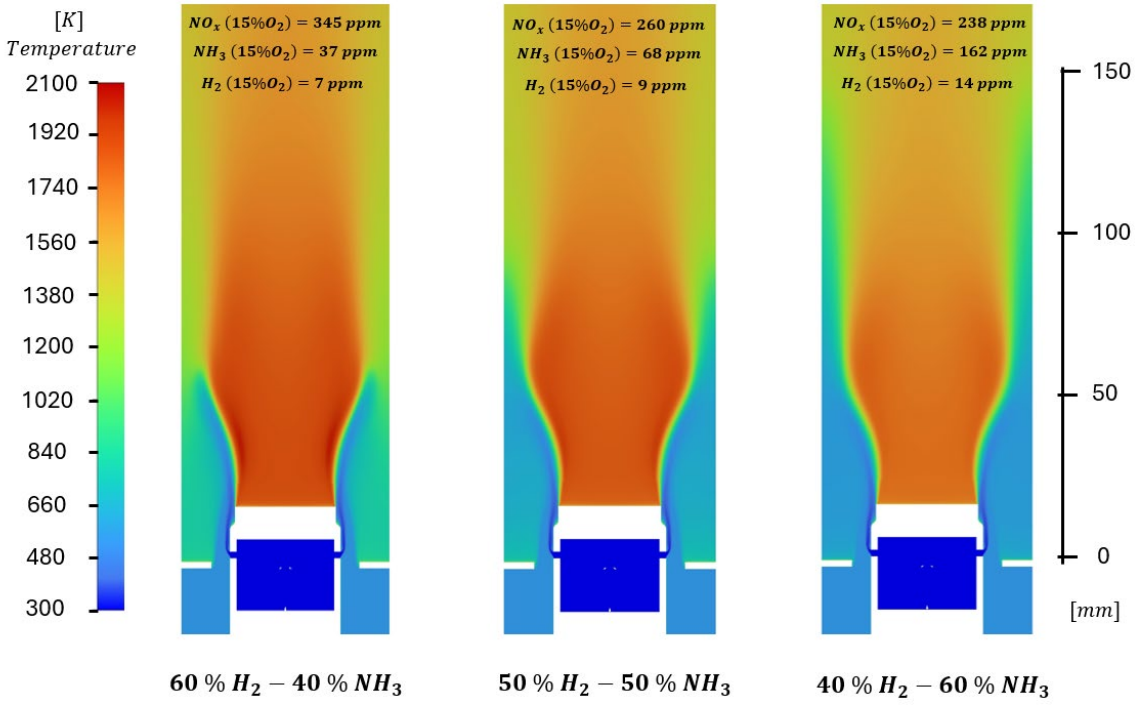

Fig. 2: Temperature contours, unburnt hydrogen/ammonia and emissions for different H_2/NH_3 blends.

4. Conclusion

The present study lays the groundwork for future research into using of H_2/NH_3 blends in micromix burners for industrial combustion systems. The burner operating condition was found to show stable flames and yield an acceptable trade-off between NOx and unburnt ammonia. Specifically, the design allows efficient combustion of a 50-50% volumetric blend of hydrogen and ammonia, resulting in NOx emissions below 400 ppm. In conclusion, the numerical results provide an initial baseline study, showing the potential of the micromix combustion principle to achieve greater fuel flexibility. Further research is necessary, especially experimental validation of the combustion model and reaction mechanisms, with a focus on accurately predicting NOx emissions.

Abbreviations

The following abbreviations are used in this manuscript:

MCP Micromix Combustion Principle
CFD Computational Fluid Dynamic
AGP Air Guiding Panel
FGM Flamelet Generated Manifolds
ED Energy Density

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