

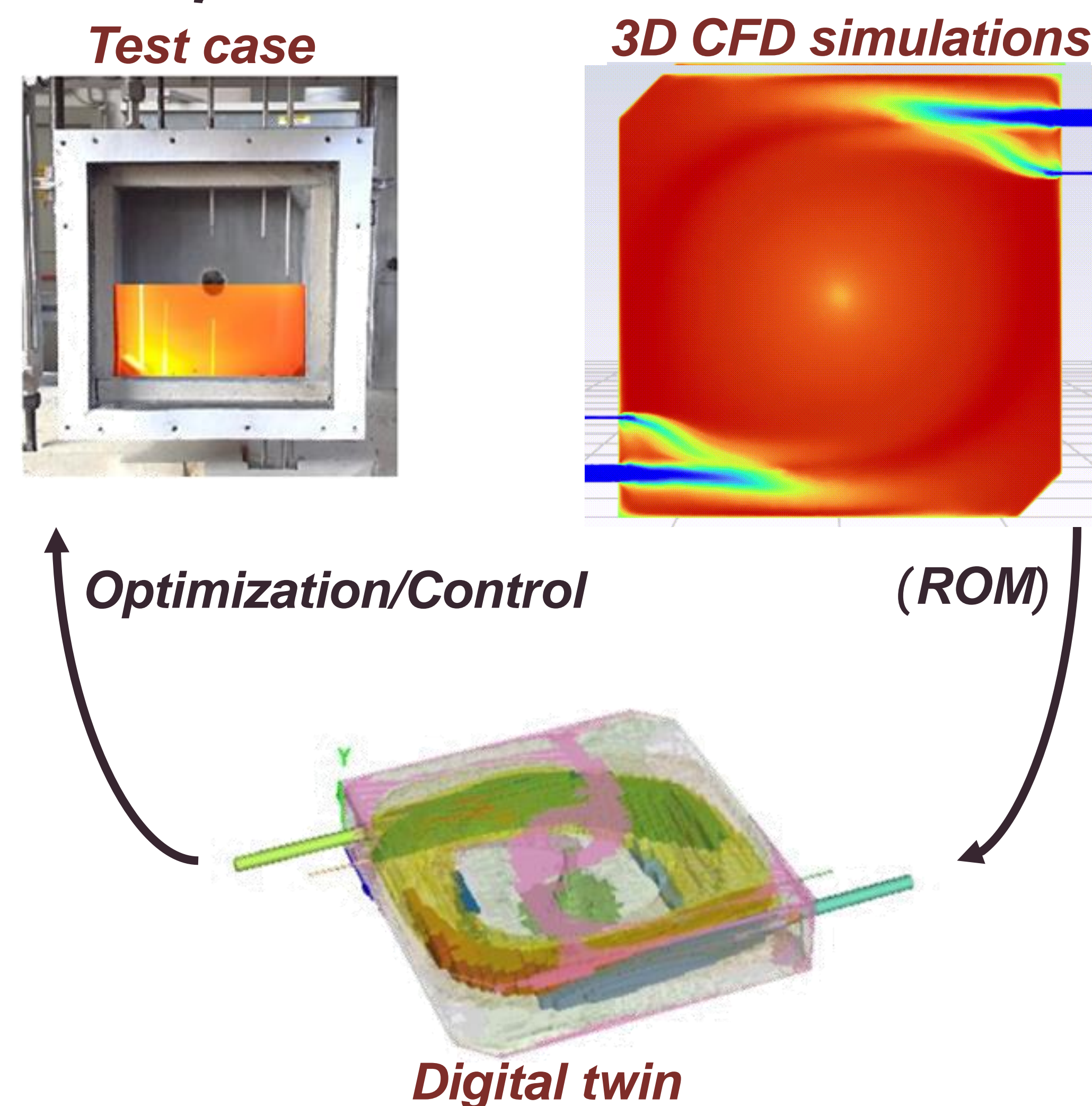
Introduction

The present work investigates the thermo-chemical conversion of Hydrogen blends with ammonia in an innovative combustion system, such as the **Laboratory Unit CYclonic (LUCY) burner**. This reactor can operate in **Moderate or Intense Low-oxygen Dilution (MILD)** combustion conditions due to a strong internal recirculation of burned gases.

Such combustion process needs adequate numerical models for the characterization of its fluid-dynamical and thermo-chemical behaviors.

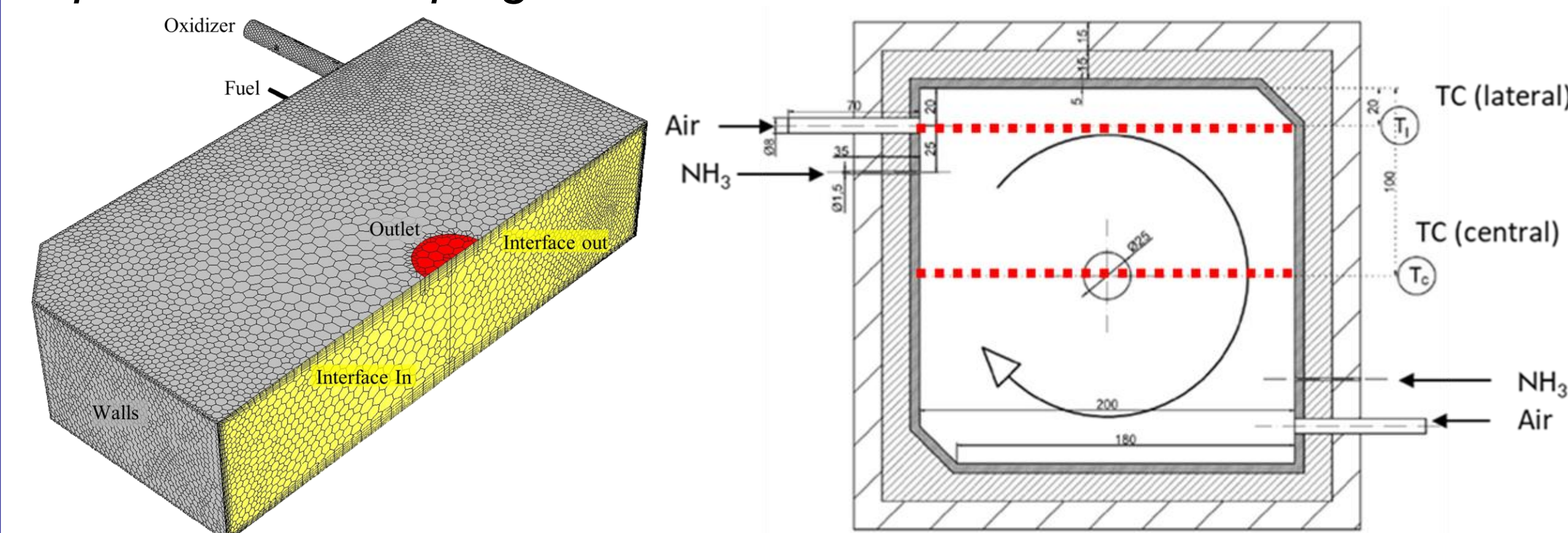
Computational Fluid Dynamics (CFD) methods are applied to predict Ammonia/Hydrogen combustion in MILD regime to create a reliable models that can be used for generating a **Digital Twin** via **Reduced Order Methods (ROM)**.

Model development and validation



Methodology

A **polyhedral mesh with periodic condition** with 300k cells was thus generated, validated on data collected from numerous experimental campaigns.



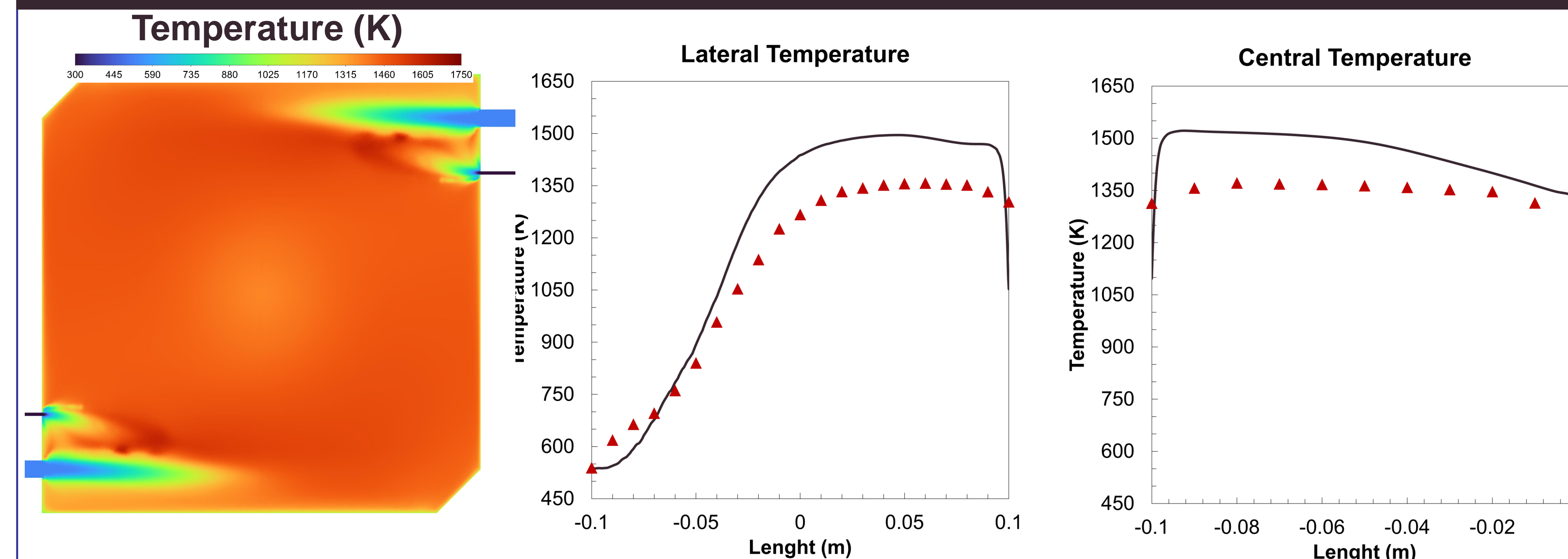
Numerical simulations were performed using **Fluent** software from the **ANSYS 2022 R2** package, specifically the following table shows the boundary conditions entered for the case under consideration.

BOUNDARY CONDITIONS	
Thermal Power	7 kW
Equivalence Ratio	1.0
Oxid	Air
Oxid Temperature	515 K
Oxid Velocity	31.33 m/s
Fuel	50% H ₂ - 50% NH ₃
Fuel Temperature	298 K
Fuel Velocity	173.35 m/s
Bulk Temperature	500 K
Heat Transfer Coefficient	50 W/(m ² K)

As a result of a thorough sensitivity analysis, the following models were chosen:

- **Reynolds Stress Model (RSM)** for turbulence with Enhanced Wall Treatment setting for near wall Treatment;
- **Flamelet Generated Manifold (FGM)** model to describe the Turbulence-Chemistry;
- **Discrete Ordinate** for modeling the internal radiation the reactor and the spectral properties of the gas were evaluated with the **Weighted-Sum of Gray Gases (WSGG)** model.

Results



OUTLET SPECIES

	Molar Fraction NO _x	Molar Fraction H ₂	Molar Fraction O ₂	Molar Fraction NH ₃
Experimental value	0.000621	0.002068	0.008174	0.000192
Simulation	0.004482	0.002359	0.033569	0

Summary

- Simulations obtain temperatures comparable to those recorded by thermocouples with a maximum deviation of 100 Kelvin degrees in the recirculation zone.
- Remarkable performance in terms of Stabilization of the oxidation process and Low Pollutants has been verified in a wide range of operating conditions.
- Preheating the oxidizer inlet flow allows to reach very low NO_x emissions for stoichiometric and rich mixtures, while for lean mixtures lower emissions have been obtained without preheating.
- For higher Thermal Power, the minimum NO_x shifts toward higher equivalence ratios, according to the lower maximum working temperatures.

Open Issues

- LES simulations based on the optimized model.
- Model and grid validation for different ammonia-hydrogen mixtures and feeding conditions.
- Creation of a digital twin model based on the simulations performed.