A Physics-Informed Graph Neural Network Framework for Reduced-Order Modeling of Synthetic Fuel Combustion

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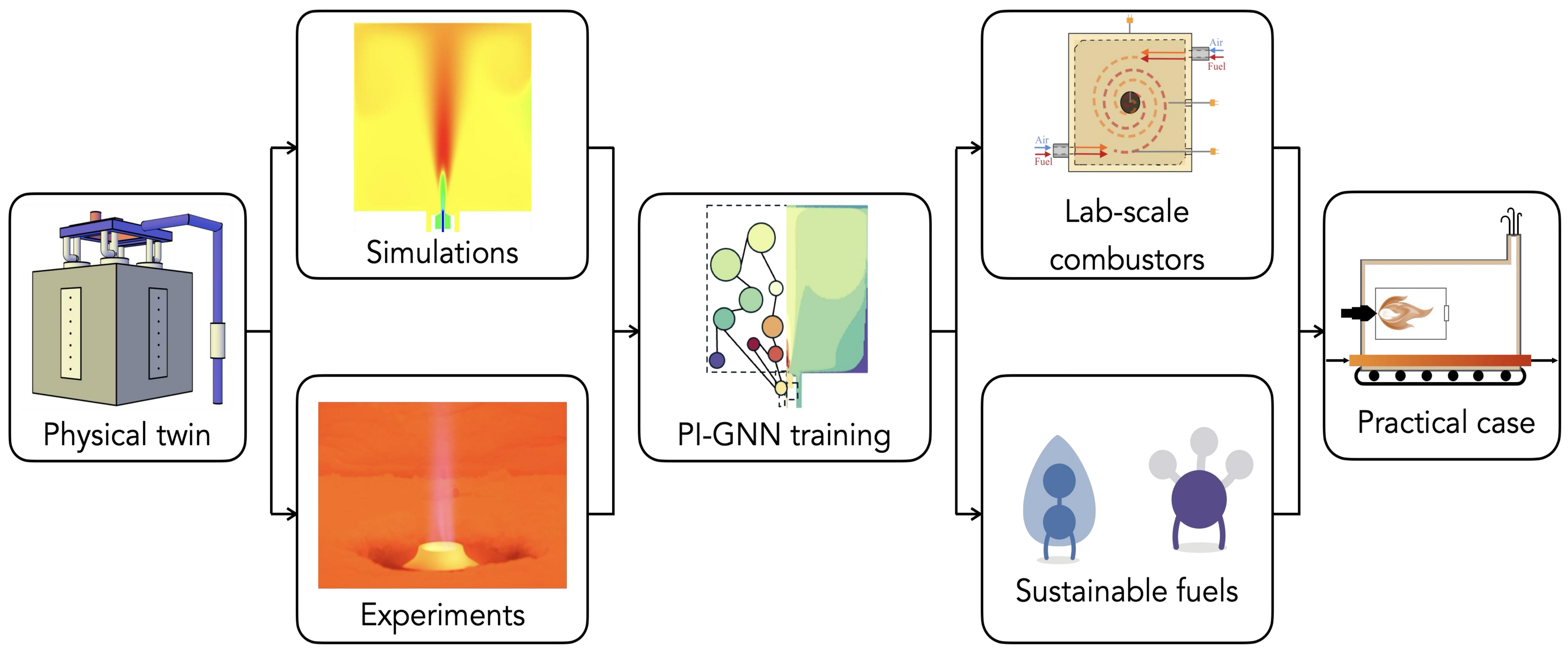
A hybrid methodology involving **Chemical Reactor Networks** (CRNs) and **Computational Fluid Dynamics** (CFD) is employed to build **Graphical Neural Networks** (GNNs) to assess the impact of retrofitting industrial furnaces with **sustainable fuels**.

Context:

Energy transition has introduced new renewable fuel candidates such as **ammonia** and **hydrogen**. Retrofitting of the current plants will be needed, but first, the impact of switching from conventional fuels to **carbon-free fuels** (H_2, NH_3). To do so, experiments and simulations are first conducted at a smaller scale. Still, the repetition of experiments can be challenging, and the computational cost of **CFD** can increase drastically when resorting to detailed chemistry.

Hence, this work approach aims to develop a **Graph Neural Network (GNNs)** for investigating the feasibility of burning sustainable fuels in industrial-scale furnaces. The model is first developed on a large CFD dataset before the addition of **physical information** in the model, with a lab-scale test case.

The final objective will extend this capability to direct CFD field **prediction**, enabling rapid evaluation of **alternative fuel combustion** without the need for full CFD calculations.



Test case: Modified SPRF of ULB

Originally built for CH_4 combustion.

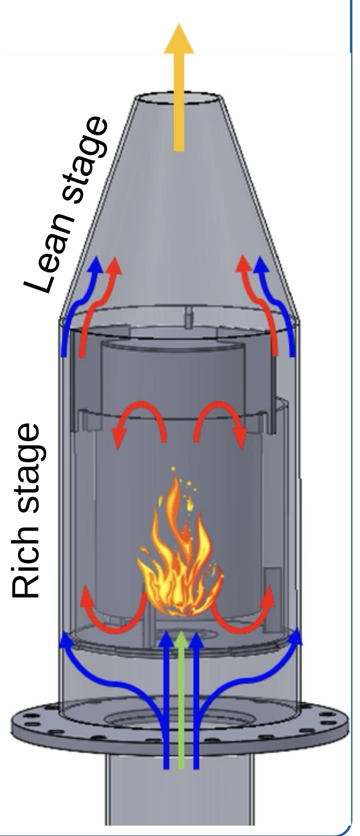
Adapted for NH_3 combustion in [1].

Investigated for NH_3/H_2 blends in [2].

Eq. ratio rich stage: $\phi_1 \in$ [1-1.6].

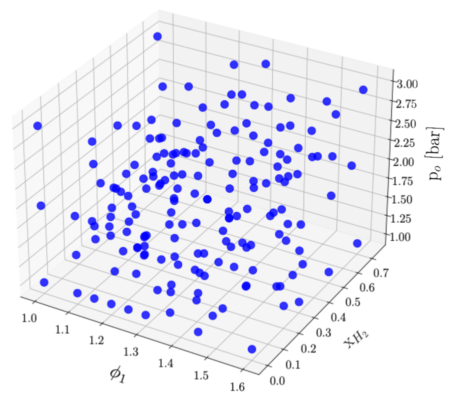
Hydrogen content: $x_{H_2} \in [0 - 0.75]$.

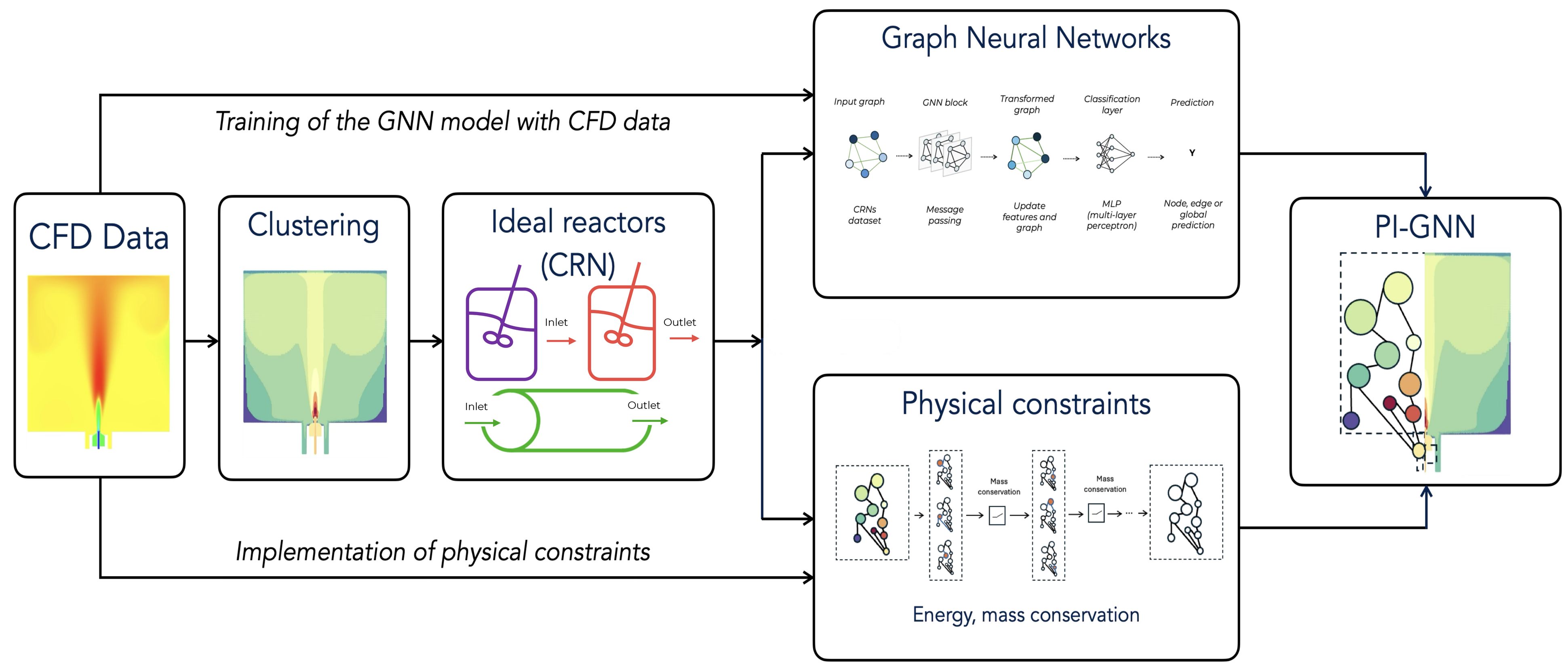
Operating pressure: $p_o \in$ [1-3] bars.



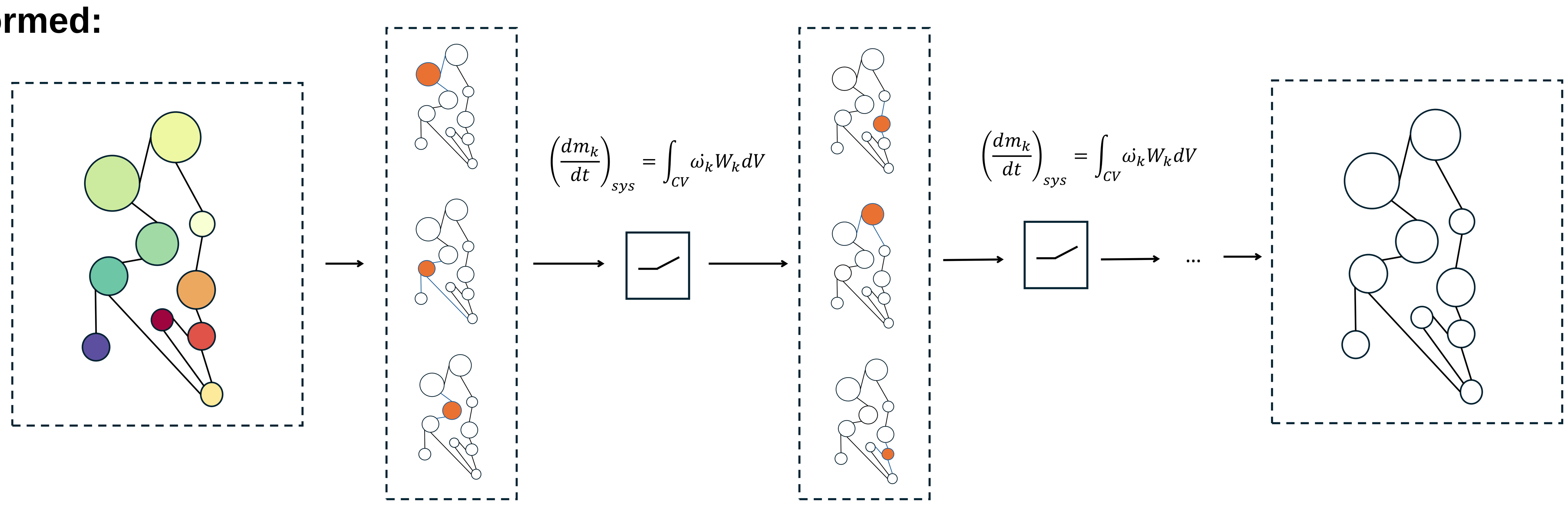
Methodology:

- 175 CFD simulations
- GNN tuning
- Detailed kinetics



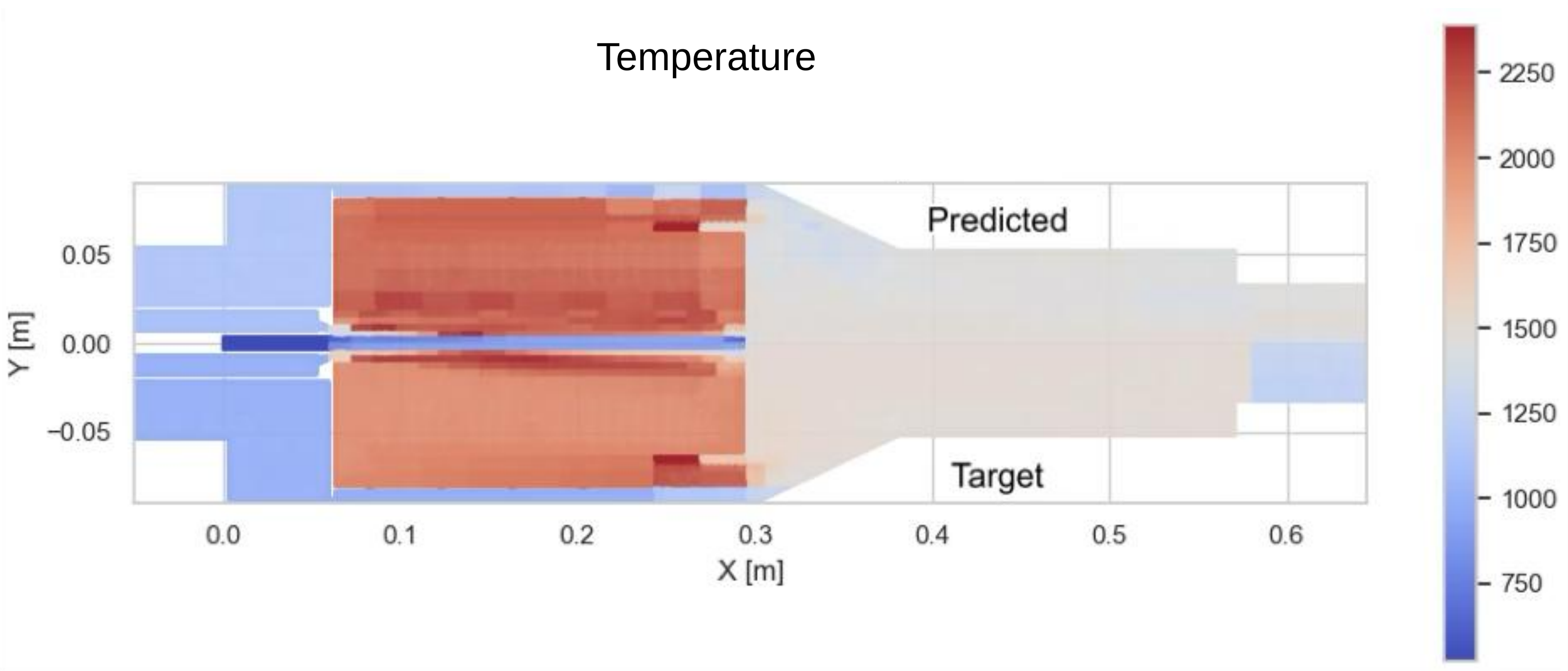


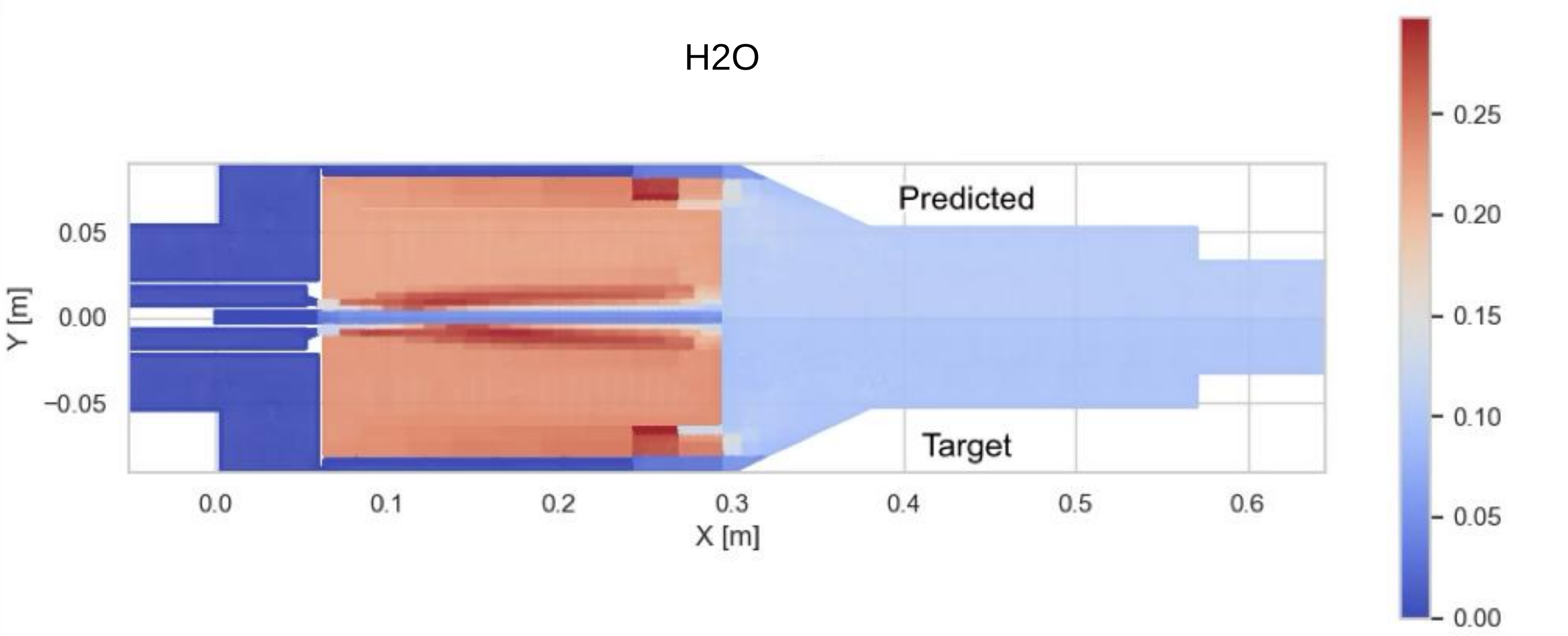
Physically informed:



- Mass conservation at each node and across the entire CRN,
- Energy conservation,
- Enthalpy balance.

Results:





Conclusions:

Training the GNN enables us to predict various operating conditions, which will be valuable for designing burners and assessing alternative fuel combustion.

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References :

[1] L. Giuntini, *et al.* Continuously-staged NH3 oxidation in a stagnation-point reverse-flow combustor for low NOx emissions, Proceedings of the Combustion Institute, 40, 1–4, 2024, 105674, https://doi.org/10.1016/j.proci.2024.105674.

[2] A. Piscopo, *et al.* Burning ammonia–hydrogen mixtures in a staged combustor with high efficiency and low pollutant emissions, International Journal of Hydrogen Energy, 118, 2025, 343-355, https://doi.org/10.1016/j.ijhydene.2025.03.099.