Predicting NO_x Emissions From Porous Media Burners Using Physics-Informed Graph Neural Networks

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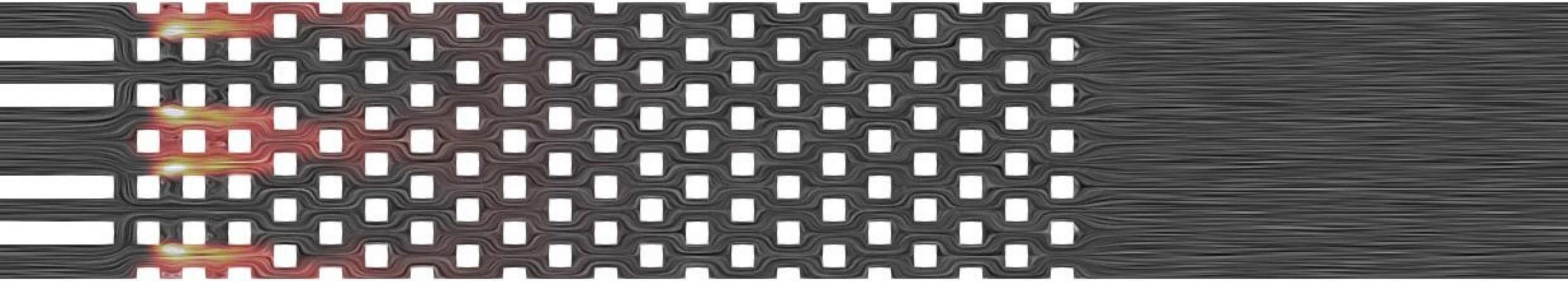


35th Parallel CFD International Conference 2024

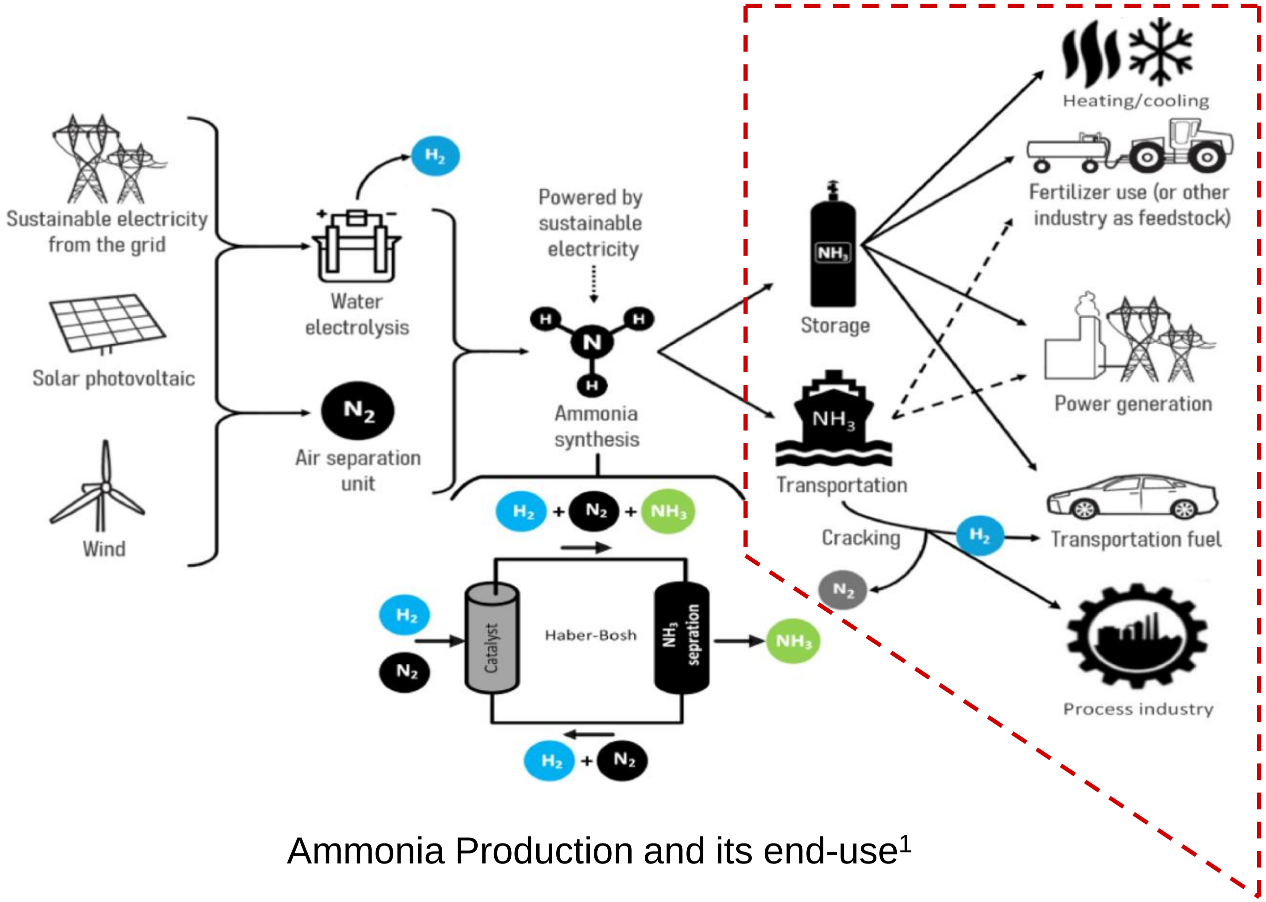
Agenda

- Why Ammonia?
- Challenges of Ammonia combustion
- Porous media burner
- CFD approach
- Machine learning approach
- NOx emissions

Motivation

Why ammonia?

- Carbon free fuel
- A suitable H_2 carrier
- Easy to transport in the liquified form using the existing infrastructure
- High energy density



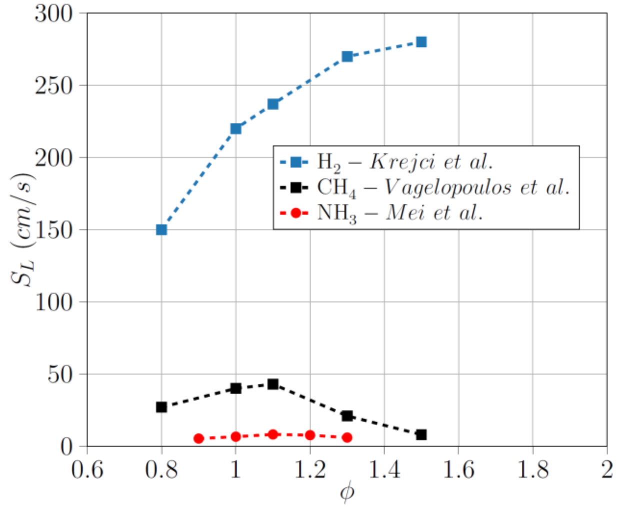
Ammonia Production and its end-use[1]

1. Service et al., Ammonia—a renewable fuel made from sun, air, and water—could power the globe without carbon, Science, 2018.

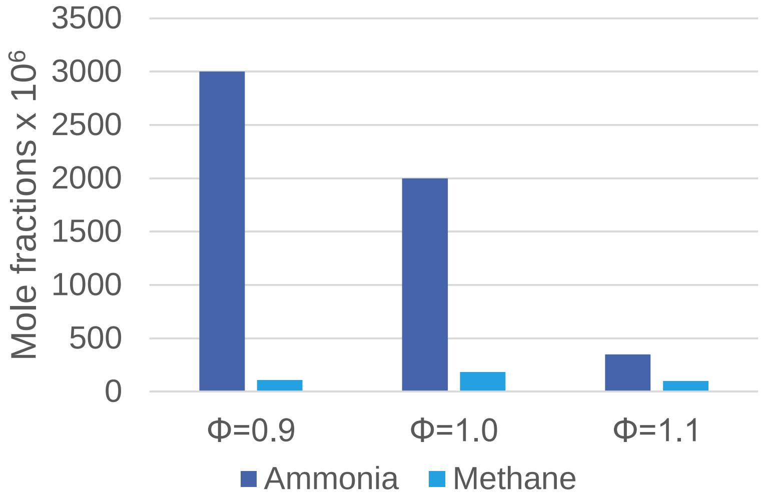
Motivation

Challenges of ammonia combustion

- Poor flame stability
- High NOx formation
- High toxicity at trace levels



Experimental measurements



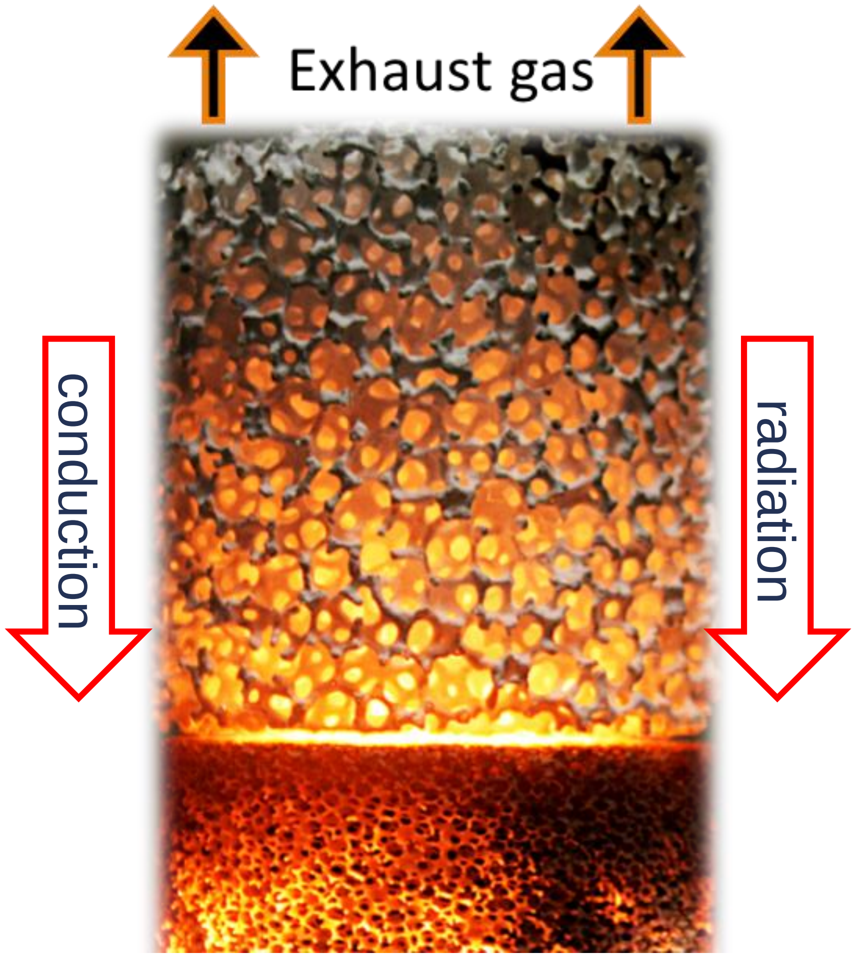
No_x emissions from 1D premixed free-flame simulations

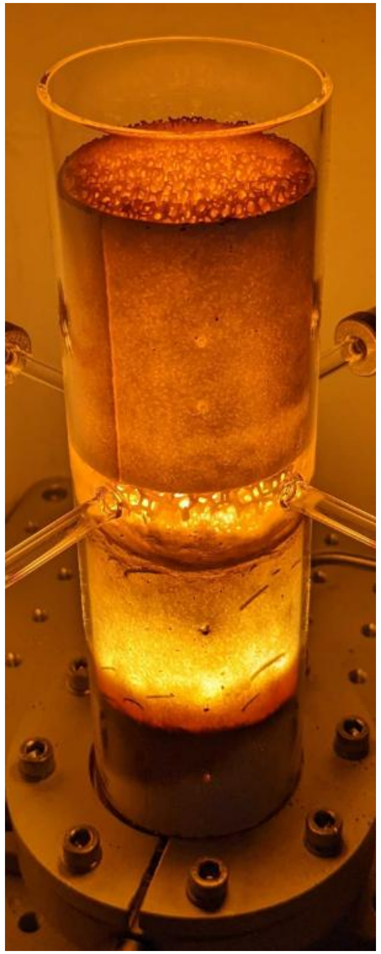
(Reproduced from Kobayashi et al.)

1. Krejci et al. https://doi.org/10.1115/1.4007737
2. Vagelopoulos et al. https://doi.org/10.1016/S0082-0784(98)80441-4
3. Mei et al. https://doi.org/10.1016/j.combustflame.2019.08.033
4. Kobayashi et al. https://doi.org/10.1016/j.proci.2018.09.029

Porous Inert Media (PIM) Burner

- Preliminary work on NH_3 and NH_3/H_2 combustion in porous inert media (PIM) at Stanford University[1]
- Result: Using the PIM combustion concept, ammonia can be stably burnt with low NOx formation.





1. T. Zirwes. et al. https://doi.org/10.1016/j.combustflame.2023.113020

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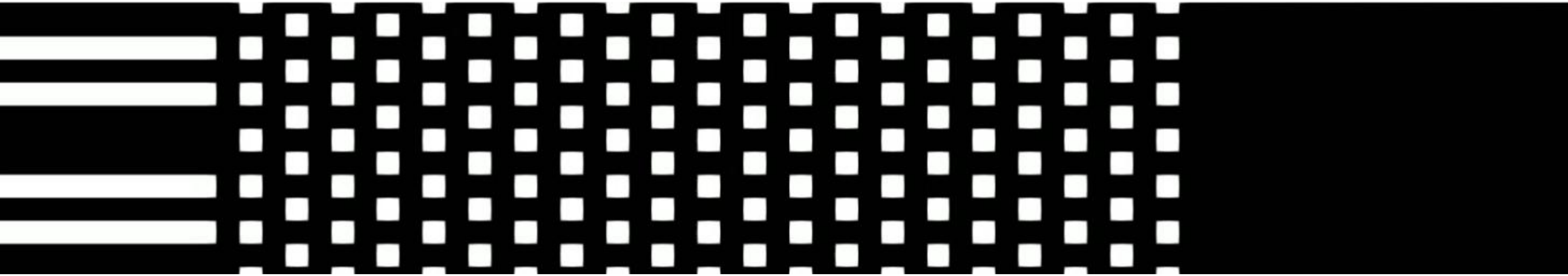
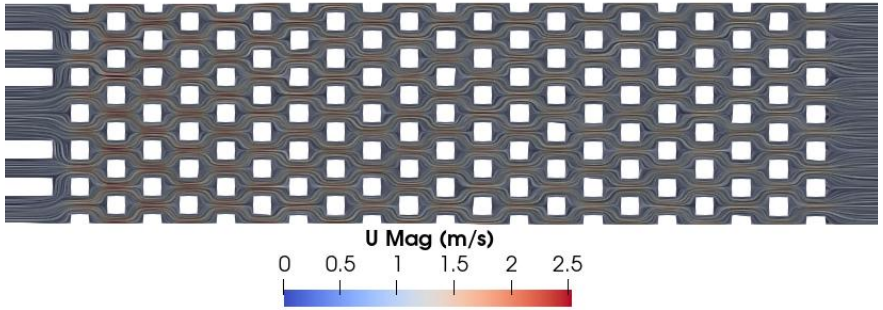
CFD approach

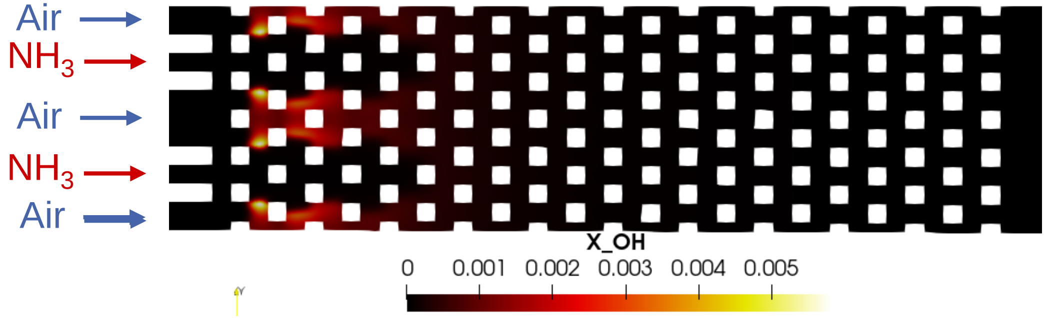


Simulation approach

- **In-house OpenFOAM extension with**
  - Detailed chemical reaction mechanisms (finite rate chemistry)
  - Coupled with open source chemical library "Cantera"
  - Detailed molecular diffusion for each species
  - Fully-resolved reaction zones
  - Fully-resolved flow field inside the porous structures
  - Excellent parallel scalability for use on modern supercomputers
  - Currently radiation and Conjugate Heat Transfer (CHT) not considered

- 2D combustion simulations in regular porous structures





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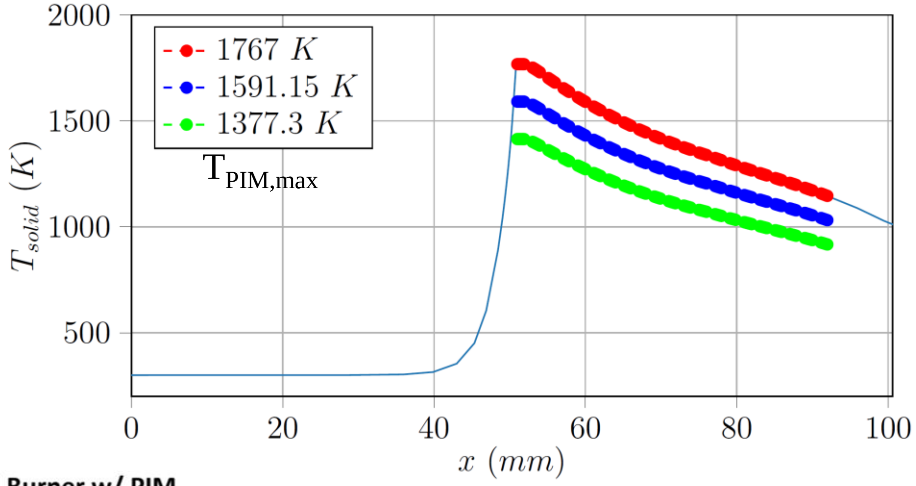
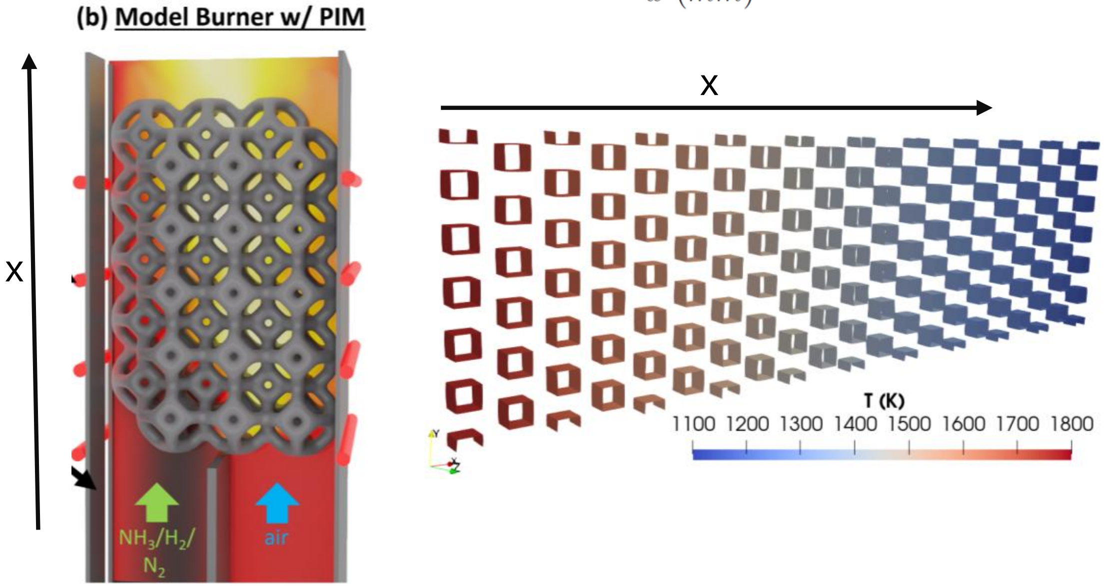
2D – Simulations with PIM

- PIM 1D temperature profile obtained from 1D-VAS and enforced as BC for 2D simulations
- Mechanism:
  - PoliMi (Stagni)[1] – 2020
- U_{fuel}: 0.3 m/s
- T_{inlet}: 500 K
- Ignition with initial hot gases
- Premixed burner: Initial species mole fractions taken from 1D free-flame
- Φ: 0.9, 0.95, 1.1

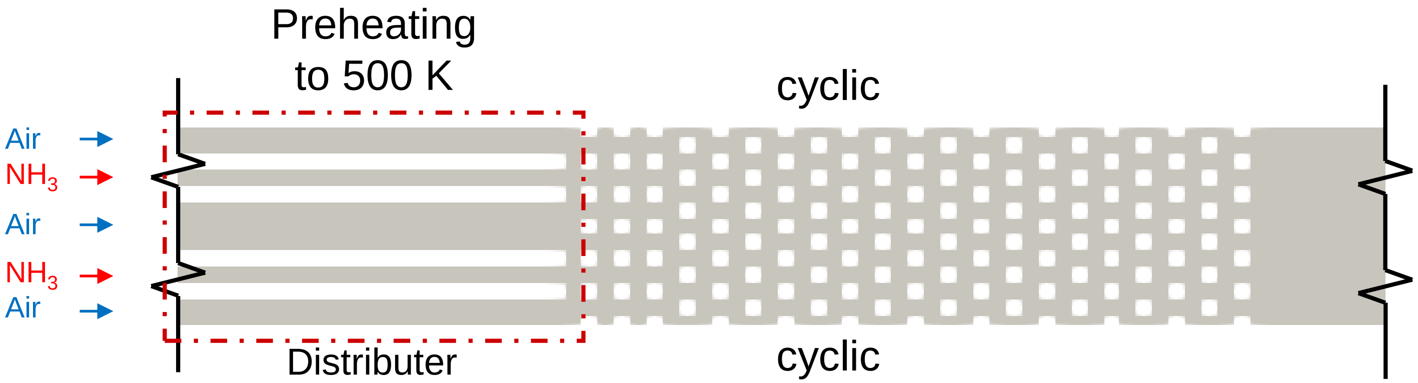




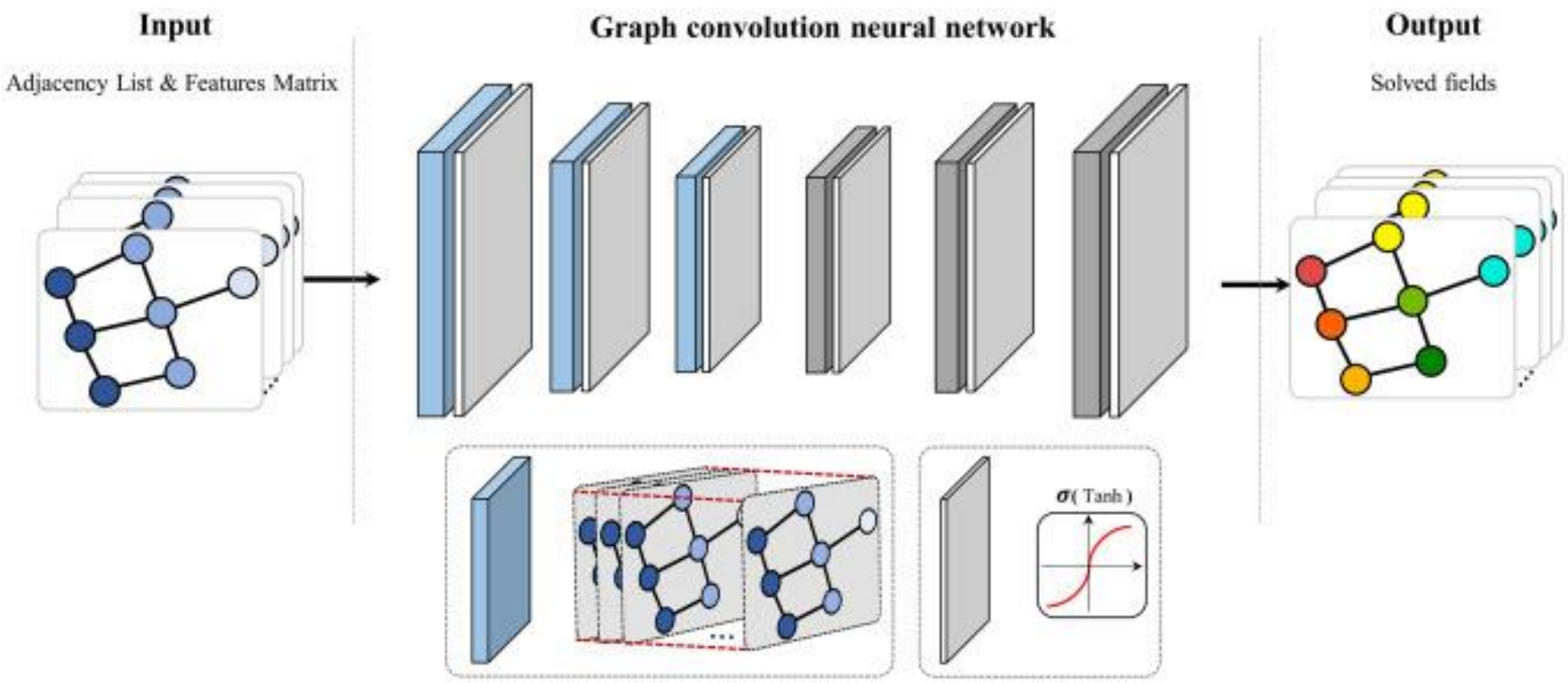
1. A. Stagni et al. doi:10.1039/c9re00429g

2D – Simulations with PIM

- Multi-channel geometry
- Strut size: 1x1 mm
- Pore size: 2x1 mm
- Solid structures defined by white squares
- Free flame thickness: 0.6 mm
  (Cantera, Φ=0.95, 0.7 NH_3 + 0.3 H_2)
- Smallest cell size:
  - Smaller than 10% of free flame thickness
  - Δx = 41 μm
  - Δy = 12.5 μm



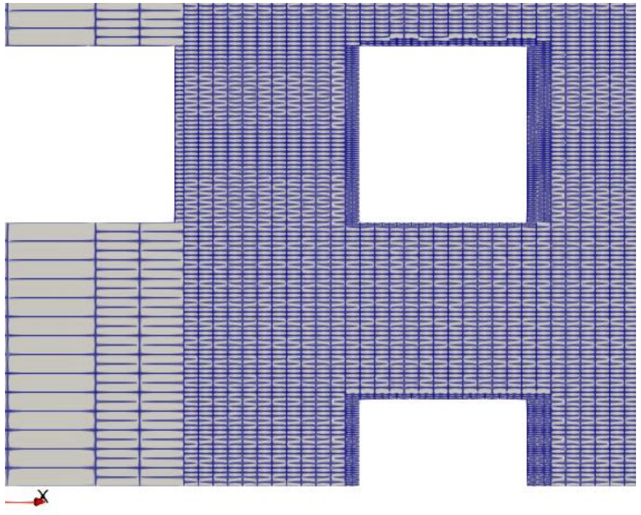
Machine learning approach



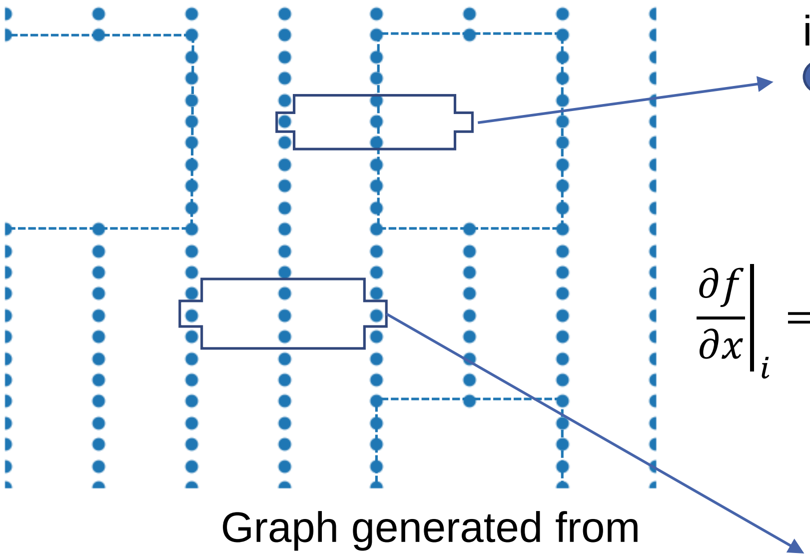
Peng et al. https://doi.org/10.1016/j.ijheatmasstransfer.2023.124593

Machine Learning approach

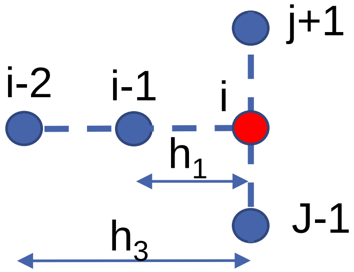
- Graph Convolutional Neural Networks (GCNN)



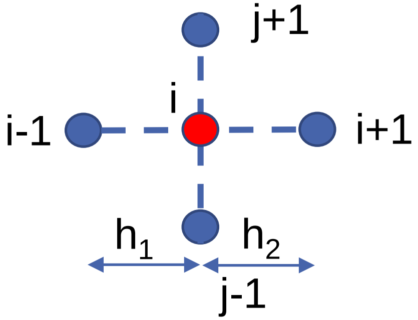
Sampling



Graph generated from computational mesh

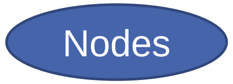


$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{h_1^2(f_{i-2} - f_i) + h_3^2(f_{i-1} - f_i)}{h_3 h_1 (h_3 - h_1)}$$



$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{h_1^2(f_{i+1} - f_i) + h_2^2(f_i - f_{i-1})}{h_1 h_2 (h_1 + h_2)}$$

$$\boxed{\vec{U}, T, \rho, Y_k}$$



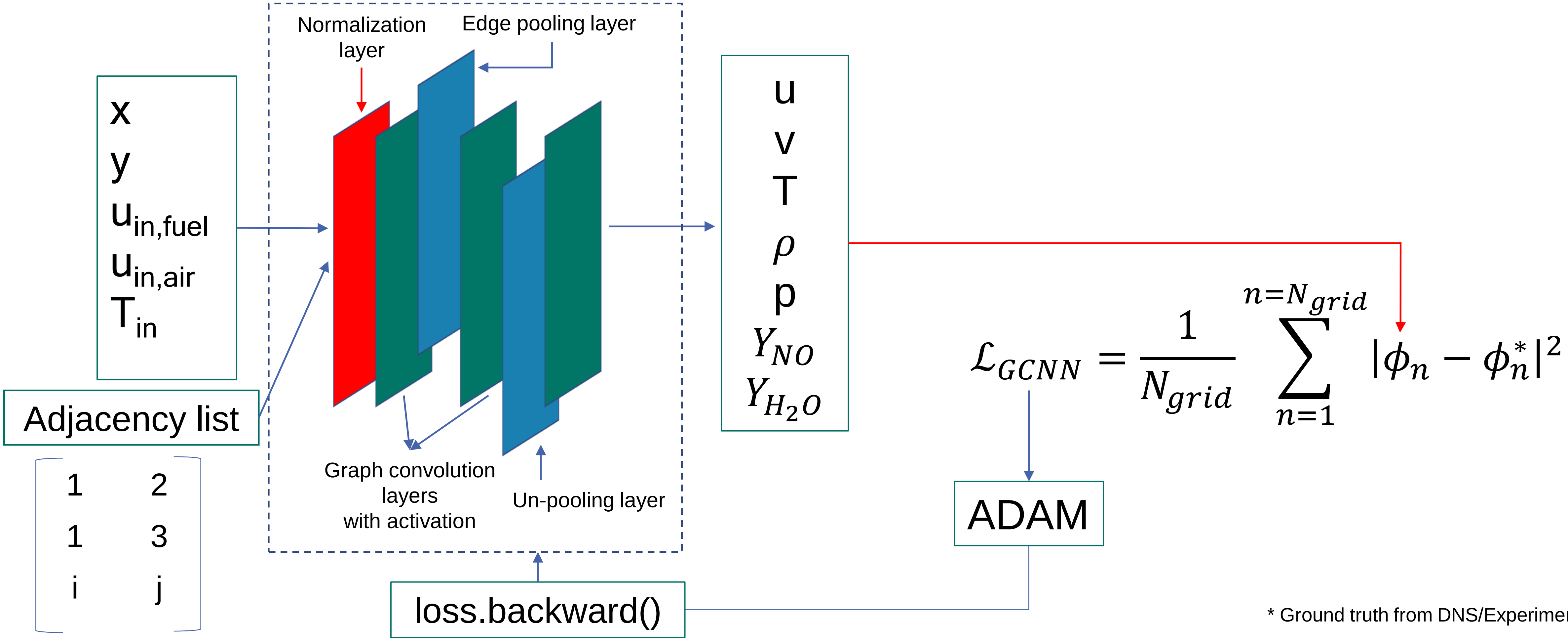
Coordinates, Dirichlet boundary conditions

Adjacency list, neighbors, edges (x_i-x_{i-1},y_i-y_{j-1})

Domain and PIM boundaries as indices

Machine Learning approach

- Data-driven GNN



$$\mathcal{L}_{GCNN} = \frac{1}{N_{grid}} \sum_{n=1}^{n=N_{grid}} |\phi_n - \phi_n^*|^2$$

* Ground truth from DNS/Experiment

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Machine Learning approach

- Simplified governing equations
- Mass conservation

$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial x}(\rho v) = 0$$

- Momentum conservation

$$\frac{\partial}{\partial x}(\rho uu) + \frac{\partial}{\partial y}(\rho vu) - \frac{\partial}{\partial x}(\tau_{xx}) - \frac{\partial}{\partial y}\left(\tau_{yx}\right) + \frac{\partial p}{\partial x} = 0, \qquad \frac{\partial}{\partial x}(\rho uv) + \frac{\partial}{\partial y}(\rho vv) - \frac{\partial}{\partial x}\left(\tau_{xy}\right) - \frac{\partial}{\partial y}\left(\tau_{yy}\right) + \frac{\partial p}{\partial y} = 0$$

- Energy conservation (Temperature based)

$$c_p \frac{\partial}{\partial x}(\rho uT) + c_p \frac{\partial}{\partial y}(\rho vT) - \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + \dot{Q} = 0$$

- Species mass conservation

$$\frac{\partial}{\partial x}(\rho uY_k) + \frac{\partial}{\partial y}(\rho vY_k) + \frac{\partial}{\partial x}\left(j_{k,x}\right) + \frac{\partial}{\partial y}\left(j_{k,y}\right) - \dot{\omega}_k = 0$$

- For unity Lewis number

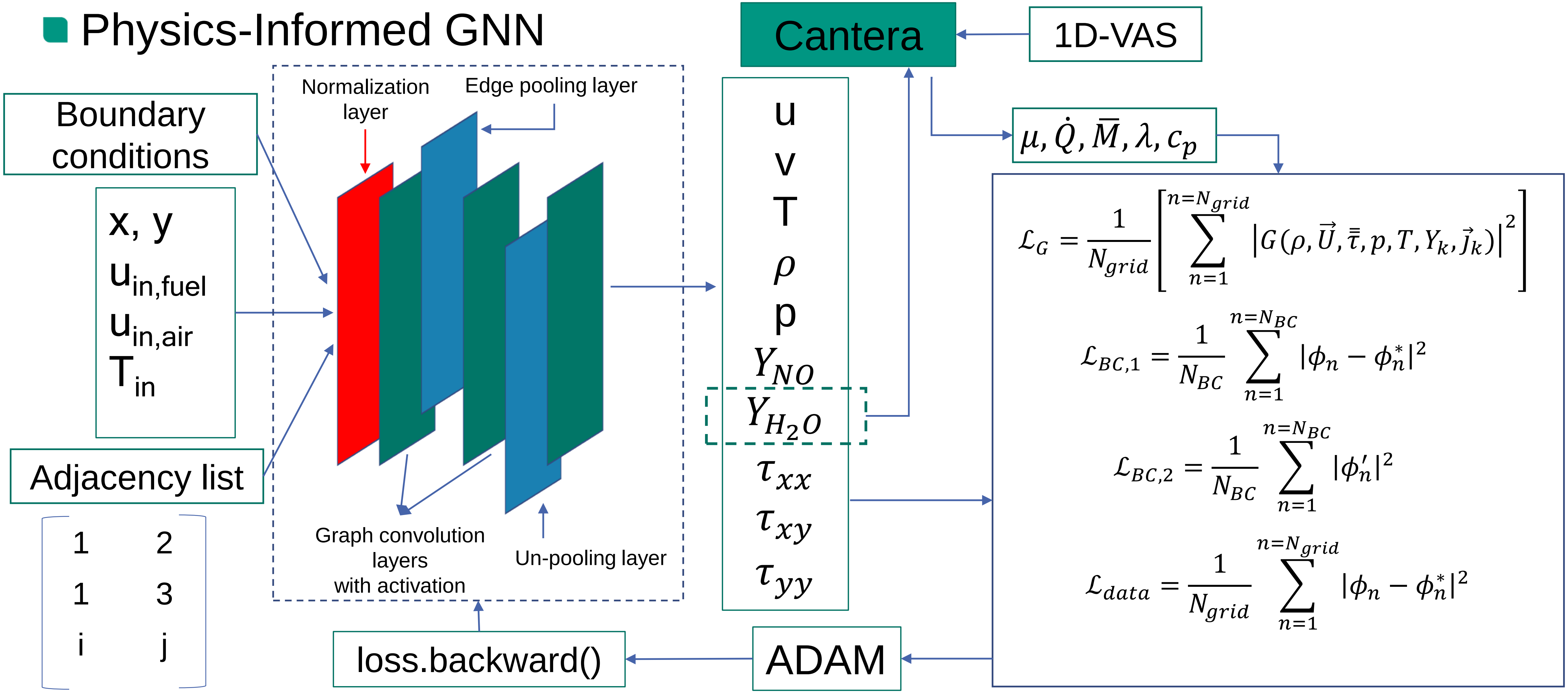
$$\overrightarrow{j_k} = -\frac{\lambda}{c_p}\nabla Y_k$$

- Equation of state

$$\rho = \frac{p\bar{M}}{\mathcal{R}T}$$

Machine Learning approach

- Physics-Informed GNN



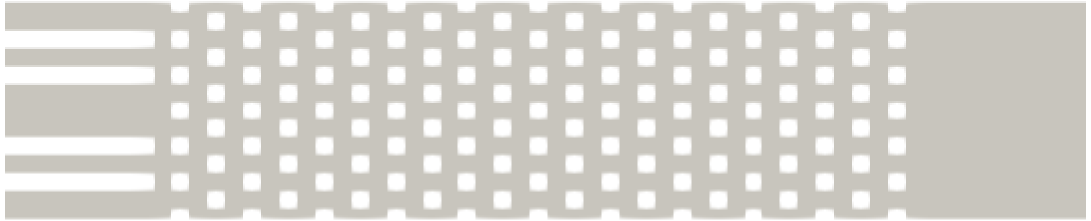
Machine Learning approach

- DNS data

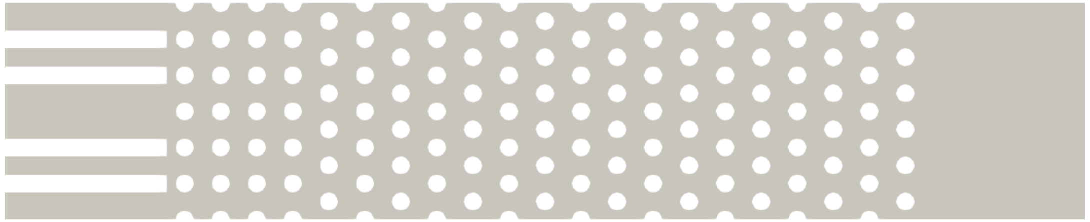
Variation in inlet conditions
and PIM temperature profiles

Case	Fuel composition at inlet (mole fraction)	Φ (global)	$T_{PIM,max}$ (K)
I	$0.9\ NH_3 + 0.1\ H_2$	1.1	1377.3
II	$0.7\ NH_3 + 0.3\ H_2$	1.1	1377.3
III	NH_3	1.1	1591.15
IV	NH_3	0.95	1591.15
V	$0.9\ NH_3 + 0.1\ H_2$	0.95	1591.15
VI	NH_3	0.9	1767

Variation in PIM structures



PIM A



PIM B

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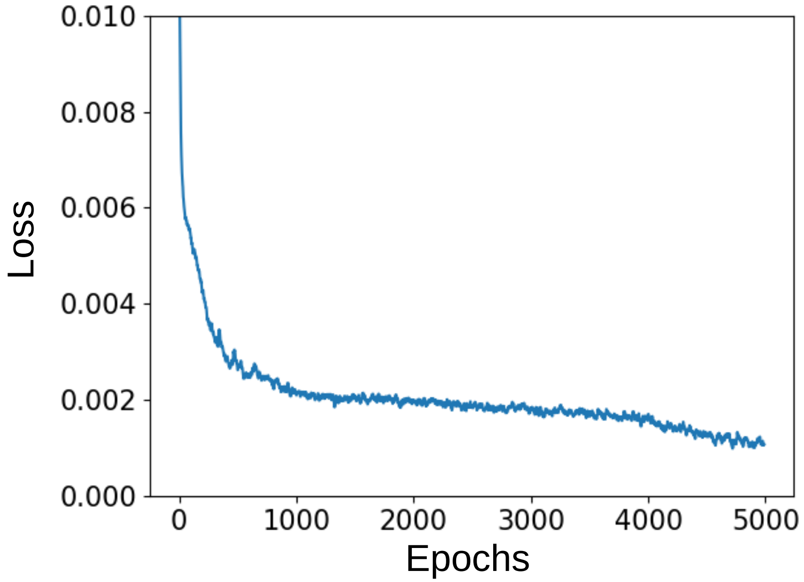
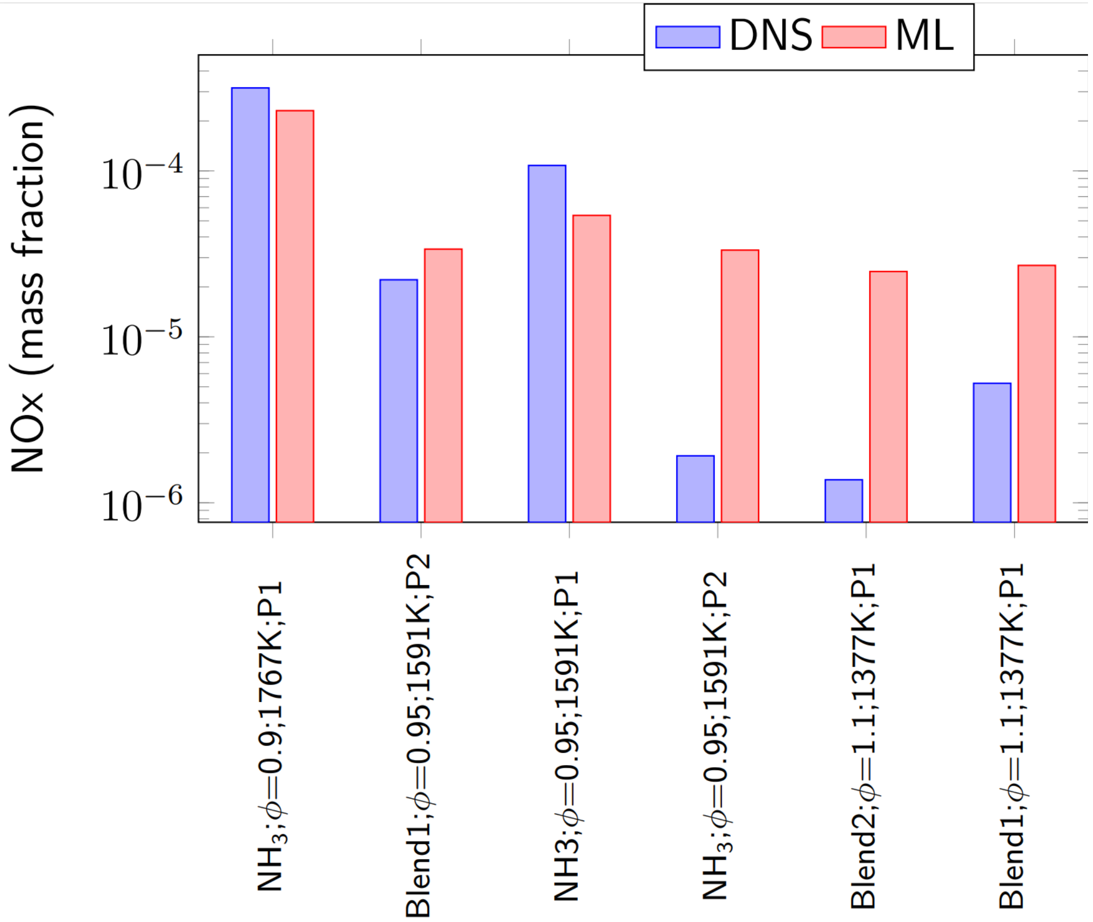
Initial results

- Data-driven model
  - Model architecture
    7 GraphConv layers with 3 EdgePooling and 3 un-pooling layers
  - Activation: Hyperbolic Tangent (Tanh)
  - Epochs: 5000





Blend1: $0.9NH_3 + 0.1\ H_2$,
Blend2: $0.7NH_3 + 0.3\ H_2$ by mol

Outlook and conclusions

- Challenges associated with combustion of ammonia
- Porous burners provide a potential solution to overcome the challenges
- High-fidelity reactive flow simulations in porous structures are computationally extensive
- Graph convolution neural networks (GCNN) provide a cost effective method to predict a solution
- Physics-Informed GCNN implemented for data-driven and data-free training
- Data-free PI-GCNN to be optimised for further PIM configurations

Thank you for your attention!