ParCFD2024
35th International Conference on Parallel Computational Fluid Dynamics
Sep. 02-04, 2024, Bonn, Germany

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

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ARTICLE INFO[†]

Keywords:
Ammonia Combustion;
Direct Numerical Simulation;
Graph Convolution Neural Networks

ABSTRACT

The combustion of ammonia is accompanied by the release of NO_x, which refers to both NO and NO_2, i.e., the nitrogen oxides contributing to air pollution. A potential technology for complete combustion of ammonia and reduced NO_x emissions is combustion in porous media. Multiple test cases are defined using 2D burner configurations that are investigated computationally by means of Direct Numerical Simulations (DNS). The main objective of this work is to study the exhaust gas products for a wide range of burner configurations. However, simulating a large number of burner setups using DNS is time-consuming and costly. To reduce the number of DNS computations, a physics-informed deep-learning model based on Graph Convolution Neural Networks (GCNNs) is employed. In a first step, the effectiveness of data-driven GCNNs is validated for reactive flows in porous media and preliminary data is shown here. Subsequently, GCNNs augmented with constraints from combustion chemistry are implemented to train on sparse data and to predict the combustion characteristics of the porous media burner with high efficiency.

1. Introduction

Ammonia offers a promising possibility as a carbon-free energy carrier. Although it can easily be transported using the existing infrastructure and stored for future energy needs, combustion of ammonia poses considerable challenges. The three major challenges are its low burning velocity compared to hydrocarbons resulting in poor flame stability, its high levels of nitrogen oxide formation and its high toxicity even at trace levels. To tackle these challenges, combustion in porous media can be utilized. Porous media combustion (PMC) has long been investigated for conventional fuels [1, 2]. Conduction and radiation heat transfer between the porous medium and the reaction zone can help in stabilizing the flame for fuels with poor combustion characteristics [3, 4]. The porous medium is provided in the form of a ceramic structure, which forms a rigid matrix. Within the porous cavities of this rigid matrix the fuel and oxidizer flow, mix and react. Direct numerical simulations of combustion in porous media can aid in designing and optimizing porous media burners. Direct pore-level simulations (DPLS) require a coupling of such fully-resolved direct flow simulations with thermal simulations of the solid matrix. Such simulations are cost-intensive and performing DPLS for a wide range of burner configurations is computationally intractable. Data-driven graph neural networks have shown potential in predicting flow fields while training on data from numerical simulations [5, 6]. To study the effectiveness of such deep-learning based models in predicting NO_x emissions, the GCNN approach is employed to investigate porous media combustion. The performance of the proposed GCNN is evaluated against DNS results from the EBIdnsFoam solver [7] and results from a simplified 1D model.

2. Method

Two-dimensional burner configurations with porous solid structures are considered as shown in Fig. 1. The properties of the porous structure such as porosity and pore size as well as the initial/boundary conditions of velocity and temperature are varied for different burner configurations. Direct numerical simulations are performed for 10% of the total generated configurations. For the remainder of the configurations, training data for temperature is generated from 1D volume-averaged simulations (1D-VAS) of PMC [8]. Cantera is used to calculate the species reaction rates and material properties appearing in the governing equations. Thus, a combination of DNS and 1D-VAS results is used for the training of the GCNN model, which are considered via two data loss functions L_{data} from DNS and 1D-VAS. It should be noted that all GCNN outputs can be considered

[†]This paper is part of the ParCFD 2024 Proceedings. A recording of the presentation is available on YouTube. The DOI of this document is 10.34734/FZJ-2025-02463 and of the Proceedings 10.34734/FZJ-2025-02175.

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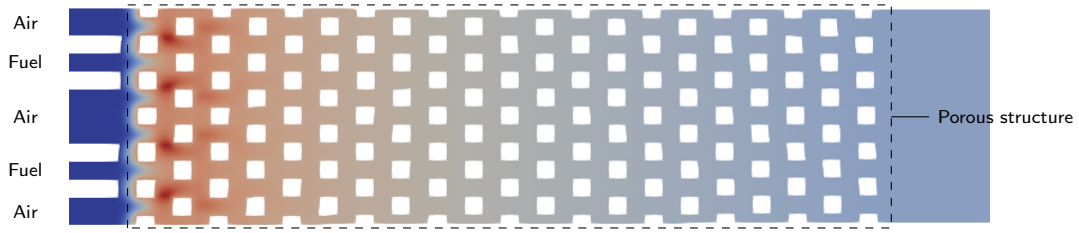
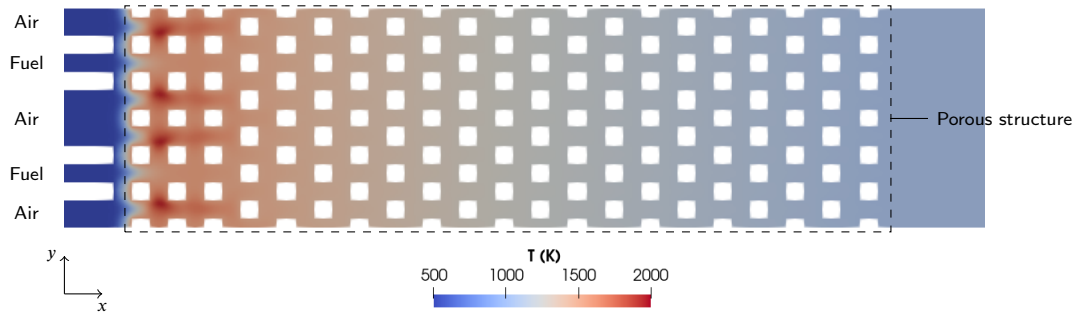


(a) Uniform porous medium.



(b) Regular porous medium with first three layers arranged in parallel.

Figure 1: Two-dimensional burner with solid structures representing the porous material.

in the L_{data} loss function when DNS data is available, while only temperature predictions are considered in L_{data} when using data from 1D-VAS. Physics-informed models can provide good accuracy in predicting solutions to boundary value problems. In addition to full DNS data, the inclusion of sparse temperature data from 1D-VAS can help to further improve the prediction quality. Due to the laminar flow in the porous media, steady state solutions for all configurations are obtained.

The proposed model architecture is shown in Fig. 2. A physics-informed GCNN is defined in which the governing equations for reacting flows are enforced as physical constraints. The input for the model is defined by the grid coordinates and the boundary conditions for velocity and temperature. The output of the model are the velocity, density, temperature, mixture fraction and NO_x mass fraction fields inside the burner. The NO_x emissions at the outlet of the burner are extracted from the predicted NO_x mass fraction fields. Assuming constant pressure, low velocity, equal species heat capacities, and no viscous heating, the physical constraints for the GCNN are defined using the simplified equations for continuity, momentum, energy, mixture fraction, and species (NO_x) mass conservation for steady laminar reactive flow [9]. The predicted value of the H_2O mass fraction serves as a progress variable and is used with Cantera to compute the source terms and material properties in the governing equations. The viscosity is obtained from Sutherland's law [10]. The physical constraints imposed by the governing equations are implemented as a loss function $L_{physical}$ for the GCNN

$$\begin{aligned} L_{physical} \quad = \quad & L_{continuity}(\rho, \vec{U}) + L_{momentum}(\rho, \vec{U}) + \\ & L_{energy}(\rho, \vec{U}, T) + L_{mix.fraction}(\rho, \vec{U}, f) + \\ & L_{NOx}(\vec{U}, Y_{NOx}), \end{aligned} \tag{1}$$

where ρ is the mixture density, $\vec{U}$ the velocity field, T the temperature, f the mixture fraction and Y_{NOx} is the NO_x mass fraction. Finally, the physical loss $L_{physical}$ is combined with the data loss L_{data} from both DNS and 1D-VAS, such that the total loss function for the model is defined as

$$L_{GCNN} = L_{physical} + L_{data}. \tag{2}$$

The automatic differentiation functionality of the `PyTorch` library is used for implementing the partial and ordinary differential equations (PDE/ODE) in the loss function. Thus, the proposed GCNN model uses the grid data from OpenFOAM as well as the boundary conditions as input and the species concentration of the NO_x species in the exhaust gas can be predicted from the output of the model. As the training progresses, the PDE/ODE residuals in the loss functions decrease, thus improving the predictive capability of the GCNN.

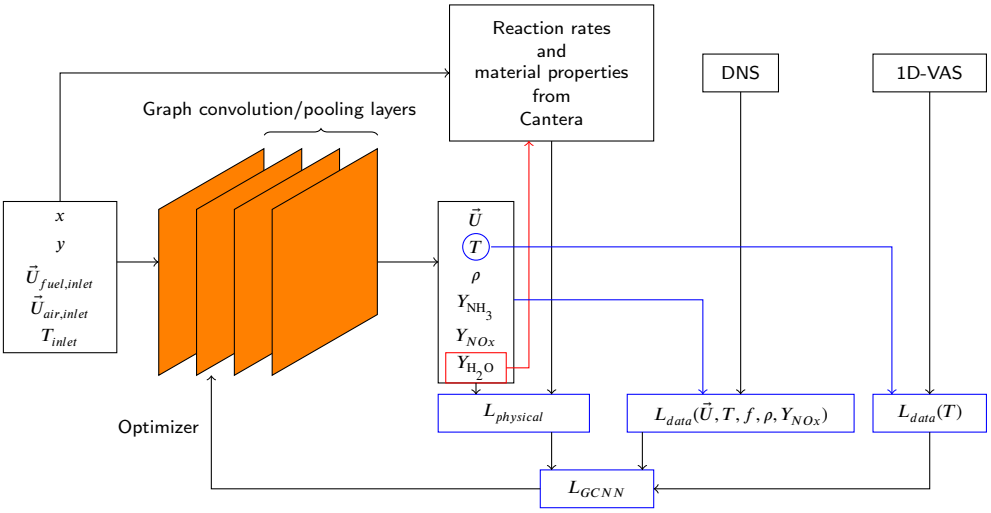


Figure 2: Schematic of the GCNN model.

ϕ	Fuel	Burner	$T_{max,PIM}$ (K)	Y_{NO_x} (DNS)	Y_{NO_x} (GCNN)	error (%)
0.9	NH_3	P1	1767	3.164×10^{-4}	2.307×10^{-4}	27.1
0.95	$0.9NH_3$+$0.1H_2$	P2	1591	2.207×10^{-5}	3.378×10^{-5}	67.8
0.95	NH_3	P1	1591	1.078×10^{-4}	5.393×10^{-5}	49.9

Table 1
Comparison of prediction results of data-driven GCNN with the interpolated DNS data. The burner configuration with uniform porous structures (Fig. 1a) is defined as P1 and the configuration with first three parallel layers of porous structures (Fig. 1b) is defined as P2. The fuel is defined using the mole fraction of fuel species.

3. Results

Here, we present preliminary results from the data-driven GCNN model which is trained with DNS data from 12 cases. The performance of the GCNN model is measured by the error in percent of the predicted values of the NO_x emissions from the exhaust of the burner. The DNS data is interpolated onto uniform grids and the adjacency list is generated for this uniform grid. Each uniform grid is set with an x-spacing of $0.5d$ and a y-spacing of $0.24d$, with d being the characteristic length of each solid strut in the porous medium. All variables except for the velocity are scaled to a range from zero to one. For the data-driven model, a 70:30 % split is used to distribute the data into training and testing datasets. The testing dataset is later also used for validation of the trained model. The hyperparameters for the model are tuned using the random search method and the model is trained on the the GPU partition of the JURECA-DC cluster [11] installed at the Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich. The model is comprised of six `GraphConv` convolution layers and two `EdgePooling` pooling layers coupled with two un-pooling layers. The intermediate dimensions in consecutive graph convolution layers are $(7, 256, 512, 1028, 1028, 512, 256, 7)$ and the hyperbolic tangent activation function is used. The ADAM optimizer is used with a learning rate of 0.0001 and the model is trained for 3,000 epochs.

As observed in Tab. 1, the deviation in prediction from the data-driven model from the DNS results is higher, as the NO_x mass fraction in the exhaust decreases. This deviation is likely attributed to the limited DNS data available for training. Further improvements are expected from the physics-informed model in future work.

4. Conclusion

A physics-informed graph convolution neural network is proposed to predict the NO_x emissions from the combustion of ammonia in porous media burners. Preliminary results from a data-driven GCNN are shown in the present work. The data-driven GCNN model is capable of predicting the order of magnitude of the NO_x emissions, with increasingly higher errors for lower absolute values of NO_x mass fraction. Based on the learning outcomes from the current configuration future work will enhance the data-driven part of the model and further develop the physics-informed model.

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