Indian Institute of Technology Delhi

Summer Undergraduate Research Award (SURA)

# Analysing Multiphase Flows through Catalytic Converters using Graph Neural Networks


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# 1 Introduction

Catalytic converters are integral components of modern vehicles, serving as critical emissions control devices. These ingenious devices play a pivotal role in reducing harmful pollutants emitted from internal combustion engines into the atmosphere, thereby mitigating environmental pollution and safeguarding public health. Understanding their chemical, mechanical, and flow properties is essential to grasp their significance in environmental protection
A multiphase reactor is a type of chemical reactor in which more than one phase (solid, liquid, or gas) is present during the reaction process. These reactors are used in various industries for e.g:- energy for different purposes due to their ability to handle complex reactions involving multiple phases simultaneously.
Machine Leraning is a valuable toolkit that complements incomplete domain-specific knowledge in conventional experimental and computational methods. Machine Learning can provide flexible techniques to facilitate the conceptual development of new robust predictive models like:-GNNs for multiphase flows and reactors by finding hidden pattern/information/mechanism in a data set. We thereby comprehensively analyze multiphase flow systems using such predictive models.

# 2 Objectives

The Primary objective of the research is the analysis of small and large-scale simulated flow behavior in catalytic converters and industrial multiphase reactors by training a Graph Neural Network Model on small scale multiphase flows through catalytic converters and using the trained model to find patterns/information in large scale multiphase flows.

# 3 Concepts

We briefly describe the main components of multiphase flows thourgh catalytic converters.

1. **Catalytic Converters**
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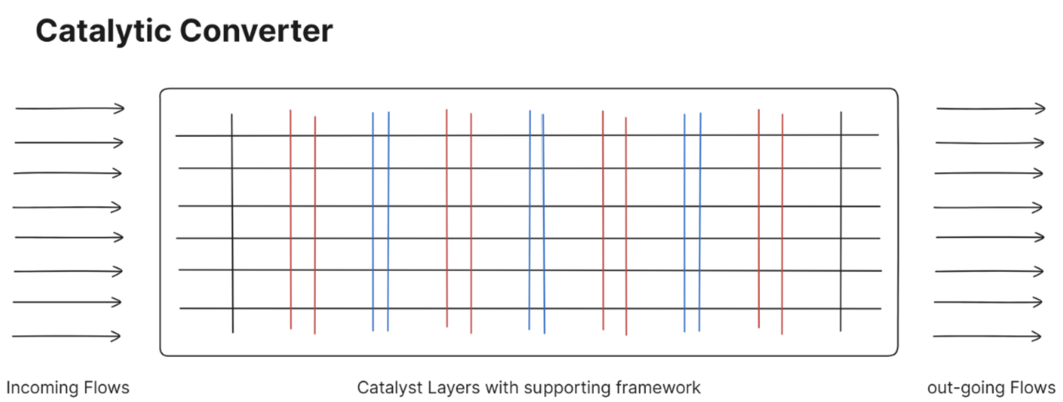


Figure 1: Flows thorugh Catalytic Converters

2. **Chemical Processes**
   At the heart of catalytic converters lie intricate chemical reactions facilitated by catalysts, typically composed of precious metals like platinum, palladium, and rhodium. These metals serve as active sites where pollutants undergo transformation. When exhaust gases containing unburned hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NOx) pass over the catalyst surface, a series of chemical reactions occur

3. **Mechanical Processes**
   Beyond the chemical reactions, catalytic converters exhibit crucial mechanical properties to ensure optimal performance. The physical structure of the converter is designed to maximize the contact between exhaust gases and the catalyst surface. Honeycomb-like structures made of ceramic or metallic substrates provide a large surface area for catalytic reactions to take place.

4. **Graph Neural Networks**
   Graph Neural Networks (GNNs) have gained significant importance in various fields of science and engineering, including multiphase flow analysis. Multiphase flow refers to the movement of multiple phases of matter, such as gas, liquid, and solid, within a system.Here's why Graph Neural Networks are particularly important for multiphase flow analysis:

   (a) **Complexity of Multiphase Flows**
   Multiphase flow systems are inherently complex, with interactions occurring between different phases and various spatial and temporal scales. Traditional computational fluid dynamics (CFD) methods often struggle to capture these complexities accurately due to their reliance on structured grids or meshes. GNNs offer a promising alternative by allowing for the representation of complex multiphase flow systems as graphs, where nodes represent entities such as particles or cells, and edges represent interactions between them.

   (b) **Learning Complex Dynamics**
   GNNs are capable of learning complex dynamics and patterns directly from data. In multiphase flow analysis, this means that GNNs can learn the behavior of different phases, interfaces, and interactions without relying heavily on handcrafted features or domain-specific knowledge. This data-driven approach allows for more accurate modeling and prediction of multiphase flow phenomena.

   (c) **Scalability and Efficiency**
   Traditional CFD methods often face scalability issues when dealing with large-scale multiphase flow systems or complex geometries. GNNs offer scalability and efficiency advantages, as they can process graph-structured data in a parallel and distributed manner, making them suitable for handling large-scale multiphase flow simulations.

   (d) **Integration with Simulated and Experiment data**
   GNNs can be integrated seamlessly with simulation data generated from CFD simulations or experimental data obtained from laboratory measurements. By combining GNN-based approaches with traditional simulation techniques, we can leverage the strengths of both methods to enhance the accuracy and efficiency of multiphase flow analysis.

   These points also serve as the **MOTIVATION** behind this project.

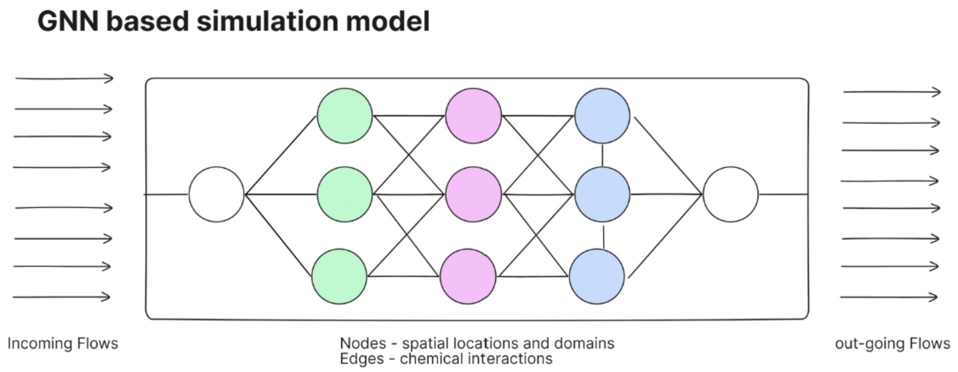


Figure 2: GNN based Simulation Model

# 4 Approach

(a) **Simulation of Multiphase Flows through Catalytic Converters**
The first phase of study will gravitate towards simulating the multiphase flows through Catalytic converters that we wish to study. These converters rely on intricate flows of different phases through densely packed catalyst particles to achieve optimal conversion rates.

(b) **Representation of the Simulated Data as Graphs for training a Graph Neural Network Model**
Multiphase flow domains can be represented as graphs, where nodes correspond to discrete spatial locations or computational cells, and edges denote interactions between neighboring nodes.GNN architectures are designed to learn and infer the behavior from the graph-structured representation of the simulated multiphase flow data. Through iterative training, GNNs adaptively learn the underlying relationships and dependencies within the flow system.The performance of GNN-based models is assessed through validation procedures, including comparison against experimental data, traditional computational methods, or analytical solutions

(c) **Optimization of the GNN Model**
The third phase will be focused on the study of different optimizations techniques to improve both the precision and the accuracy of the GNN model which will be trained on our simulated data.This model will also serve as the basis for construction and analysis of different architectures of catalytic converters to improve their operational efficiency

(d) **Extrapolation to Large Scale Flows in Industrial Reactors**
Later we would like to extend the study to multiphase flows on large scale reactors. It's speculative that extrapolation of the small scale simulated flow data would lead to compromise in accuracy and precision or spike in computational power requirement making it impractical for design and study purpose, therefore the third phase of this project will be about counterbalancing the loss of accuracy and computational intensity of this GNN model for achieving results for large scale multiphase flows through industrial reactors.

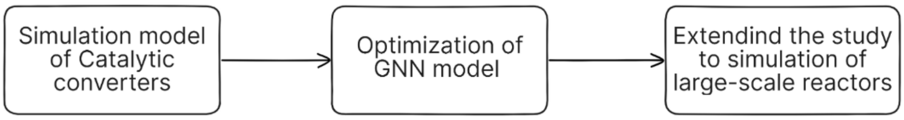


Figure 3: Approach to our research project

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## 5 Budget, Duration and Facilities

The duration of the project will roughly be of 2 months but, We would continue to work beyond this point if required to bring the project to a meaningful conclusion.

We may require access to the following resources for the project:

(a) GPUs for training the models

(b) We will need approximately ₹10,000 to get high priority access to HPC resources.

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