Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Efficient Integration of Physically Enhanced Neural Networks in Particle-Resolved CFD Simulations of Industrial Packed-Bed Reactors



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Project Term
2022 - 2025

Clusters
Lichtenberg II Cluster Darmstadt

Software
OpenFOAM

Additional Software
catalyticFOAM

Institute
Reaction Engineering of Catalytic Processes

University
Technische Universität Darmstadt

Introduction

The investigation of novel or optimizing established processes is of paramount importance in chemical engineering in the pursuit of mitigating the effects of climate change and environmental pollution. Heterogeneous catalysis is utilized in a multitude of industrial chemical plants on a vast scale. A fundamental objective in heterogeneous catalysis is to comprehend the interactions between the catalytic mechanism and transport phenomena in geometries of interest. In this context, the use of reactive CFD simulations has become increasingly prevalent. Nevertheless, solving micro-kinetics schemes represents a substantial computational challenge, necessitating the consumption of a considerable amount of computational resources. The goal of this study is to resolve the aforementioned computational bottleneck. In collaboration with the research group of Prof. Dr. M. Maestri of the Politecnico di Milano, physically enhanced neural networks have been incorporated into a specialized catalytic CFD. The proposed methodology is evaluated using three-dimensional packed-bed reactor models of industrial scale under methane steam reforming conditions.

Methods

The objective of this work is to accelerate particle-resolved, catalytic CFD simulations of packed-bed reactors of industrial

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scale, while maintaining the highest level of mechanistic details. However, heterogeneous reactions on the catalyst side occur on atomistic length scales and fast time scales (< *1* □□□□. The time and length scales of transport phenomena observed in industrial reactors are several orders order of magnitude larger. Coupling the two is therefore a multi-scale problem and requires specialized CFD software The progression of chemical species in catalytic processes is typically described using micro-kinetic models, which are sets of stiff ordinary differential equations. In catalytic CFD, such a scheme must be solved in each computational cell - often exceeding one million - of the model and in every iteration of the solver. This introduces a significant computational bottleneck, limiting the scales of a reactor model that can be modelled. To mitigate this, surrogate models are trained on a set of pre-solved solutions of the scheme. In a simulation, the surrogate model can predict the solution of the scheme, thereby retaining the mechanistic details while achieving a significant increase in simulation speed. The use of physically enhanced neural networks represents the current state of the art for the task at hand. Neural networks have the potential to approximate any multi-variate function with arbitrary accuracy, depending on the number of parameters. They are primarily based on matrix operations, which are well optimized and scale well on large amounts of data. The incorporation of physical and/or chemical information into the network architecture has the effect of reducing the amount of required training data while simultaneously increasing the accuracy and extrapolation behavior. In this study, the OpenFOAM-based catalyticFOAM steady-state solver has been modified for the utilization of neural network surrogates. The Global Reaction Neural Network architecture has been selected for the prediction of chemical source terms of the methane steam-reforming process.

Results

In the second and early stages of the third phase of this project, the CFD solver catalyticFOAM has been successfully modified to efficiently enable flexible incorporation of neural network-based surrogate models for catalytic rate predictions. As previously stated, the Global Reaction Neural Network architecture has been selected and trained to describe the occurring steady-state chemical source terms in the methane steam-reforming process. The methodology has been examined with packed-bed reactor models. A campaign of simulations with varying operating conditions has been carried out. The simulations with the employed learning-based surrogate model demonstrated high accuracy with deviations of less than 1 % to reference simulations with full evaluation of the micro-kinetic scheme. This resulted in a steady 20-fold and 100-fold total-simulation speed-up and chemistry speed-up, respectively.

Discussion

In the initial phase of the project, the objective was to simulate ammonia oxidation in the Ostwald process, which is one of the largest in the chemical industry. The substantial computational

necessitated a reconsideration of the employed reactive CFD solver, with the aim of enhancing its efficiency. In the second and the early stages of the third phase, this optimization has been successfully accomplished. The newly developed methodology is now capable of efficiently describing heterogeneous systems in the geometries of interest. at least to some extent. In the following time period, the focus will switch back to ammonia oxidation and in particular of high-pressure plants. The plan is to investigate the coupling of micro-kinetics with transport phenomena in non-ideal reactor models.

Publications

Biermann, F.: "Coupling ANNs with reactive CFD in microkinetic simulation of packed-bed reactors: from the catalytic site to the catalytic reactor via artificial intelligence", International Symposium on Chemical Reaction Engineering 2024 / ISCRE, Turku, Finland, June 16-19, 2024

Biermann, F.: A"I accelerated micro-kinetic modelling in heterogeneous catalysis: an application of physically enhanced ANNs to CFD simulations of industrial packed-bed reactors", Annual Meeting on Reaction Engineering 2024 / DECHEMA, Würzburg, Germany, May 6-8, 2024

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