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# Implementation of a data-driven model for mesh-induced error corrections in CFD simulations of stirred tank reactors

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## Abstract

Using computational fluid dynamics (CFD) for reactor design is an established area in chemical engineering, and the emergence of machine learning (ML) approaches offers new possibilities for CFD. This work reports the integration of data-driven ML models with CFD to increase the efficiency of simulations for stirred tank reactors. By predicting and correcting mesh-induced errors in coarse-grid CFD simulations, it is demonstrated that ML models can significantly improve simulation results, reduce computational costs, and maintain high accuracy. This approach involves training ML models using data generated from CFD and applying them to predict and correct simulation inaccuracies. The study generated 43 datasets, ensuring turbulent flow, with each dataset containing 2,324 data points. An artificial neural network (ANN) model with three hidden layers was used for training. The results highlight the effectiveness of ML models for various scenarios, including interpolation and extrapolation error predictions. In interpolation cases, coarse-grid simulation errors were reduced by 58%–90%, while in extrapolation cases, simulation errors were reduced by over 30%, highlighting the potential of combining ML with traditional CFD methods in reactor design and optimization in chemical engineering. The study also explores the effect of selected physical features, providing valuable insight into how different flow and geometry variables influence the model performance. Feature importance was ranked using SHAP values, and correlations between features were analyzed to guide feature selection. This analysis offers a data-driven foundation for further model optimization and contributes to a better understanding of key drivers in complex flow systems.

**Keywords:** Stirred tank reactors, Machine Learning, Data-driven model, Computational fluid dynamics