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Coaches	**Supervisors**	**Funding**
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CFD Simulation of CO_2 Capture Based on Artificial Neural Network

Aim

To develop an artificial neural network as a tool to predict the liquid side reaction in CO_2 capture using the training date of Lagrangian PDF method

Justification

Many practical applications, such as the liquid side reaction in CO_2 capture process, involve turbulent reactive flow. Turbulent reactive flow is an interdisciplinary and broad topic. To simulate a turbulent flow, probability density function (PDF) transport methods are increasingly used in many cases. One of the main advantages of the PDF transport method is that the crucial turbulence-chemistry interaction (TCI) is accurately accounted for. By implementing this method, the actual reaction rate depends on not only the intrinsic dynamics, but also the turbulent characteristics in each computational grid. Therefore, using PDF transport methods is an ideal way to turbulent reactive flow but with an extremely high computational cost. However, a novel way needs to be developed to reduce the computational cost while maintaining model accuracy.

With the development of deep learning artificial neural networks (DL ANNs), the possibility of coupling the ANN with TCI in CFD simulations shows its promising prospect to both reduce the computational cost and improve the model accuracy. In order to build this framework, on the one hand, the reaction rates for each computational grid will be obtained by using Lagrangian PDF methods in FLUENT, which will generate matrixes as the training data. On the other hand, considering the ANN algorithms, Keras is an open-source neural network library written in Python, which will be used in this project. This is a high-level application programming interface (API) to build and train models that includes first-class support for TensorFlow-specific functionality, such as eager execution, pipelines, and Estimators. It makes TensorFlow easier to use without sacrificing flexibility and performance. The basic flow information, turbulent characteristics and concentration will be considered as the input data for the neural network. This project aims to predict the TCI-based reaction rate in each computational grid. Combining the ANN with Lagrangian PDF method in CFD simulation, this project will show a novel way for turbulent reactive flow simulations.

Program

1. To develop a CFD simulation of CO_2 capture based on the Lagrangian PDF method in FLUENT to provide the training data, which will be mainly finished by the coach.
2. To develop an ANN for a 2D reactive flow using Keras and TensorFlow framework and the training data from Lagrangian PDF method.
3. Validation and prediction of ANN-based turbulent reactive flow simulation.