Professur für Chemische und Thermische Verfahrenstechnik
Campus Straubing für Biotechnologie und Nachhaltigkeit
Technische Universität München

Theoretical Bachelor thesis, Master thesis, Research internship

Developing a Surrogate Model of Thermodynamic Equilibrium Processes for Direct Air Capture

Description
At the Professorship of Chemical Process Engineering, processes for capturing carbon dioxide directly from ambient air are investigated. Such Direct Air Capture (DAC) processes can involve complex thermodynamic interactions, including gas-liquid equilibria, chemical reactions in electrolyte solutions, and solid formation. Thermodynamic models can be used to describe these phenomena and provide the basis for process simulation. However, evaluating such models can be computationally demanding.

The aim of this project is to investigate and develop Machine Learning-based surrogate modeling for thermodynamic calculations relevant to Direct Air Capture with significantly reduced computational effort. The work involves generating and preprocessing data, implementing and training Machine Learning models, and evaluating and improving their predictive performance. Various modeling approaches and strategies to improve model performance may be investigated.

Requirements
Basic knowledge of thermodynamics and Python is required. Prior knowledge in Machine Learning is encouraged.

Start date
Flexible

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