Chair of Bioseparation Engineering
TUM School of Engineering and Design
Technical University of Munich

In cooperation with WACKER

BioSE

Master's Thesis
"Simulation of Silica-Based Affinity Chromatography with a Mechanistic CADET Model"

Keywords: chromatography, process design, protein purification, protein A, CADET, mechanistic model, Python, programming

Project Description

Due to its high mechanical strength and easy manufacturing, silica is often used as a stationary phase in chromatographic processes. To achieve high-purity protein purification, silica resins can be combined with silica-binding amino acid tags. A novel octapeptide $(RH)_4$ tag, the PosH-Tag, has been developed in our group. Purifying PosH-tagged proteins with low-cost silica resins enables an economical and efficient affinity chromatography process. The next step is to purify industry-relevant proteins (e.g., Protein A variants), which are currently produced through complex and expensive purification schemes.

Developing mechanistic models for silica-based affinity chromatography allows a deeper understanding of binding phenomena and provides predictive capabilities for process optimization. Using the CADET framework, adsorption and mass-transfer mechanisms can be described mathematically and validated with experimental data. The focus of this project lies on developing, extending, and refining the existing CADET-based mechanistic model to accurately describe protein binding on silica. These models will serve as a foundation for transferring the process from batch to continuous multi-column chromatography.

The student will be responsible for implementing and parameterizing the models in CADET, analyzing simulation data, and integrating experimental results for model validation. **This project is of high industrial relevance**, as the shift from empirical experimentation to mechanistic, model-driven process development is one of the key goals in modern bioprocess engineering.

Research objectives

- Refine the existing CADET model by integrating protein adsorption data.
- Optimize binding and elution conditions for PosH-tagged proteins on silica.
- Validate the refined model using experimental chromatography results.

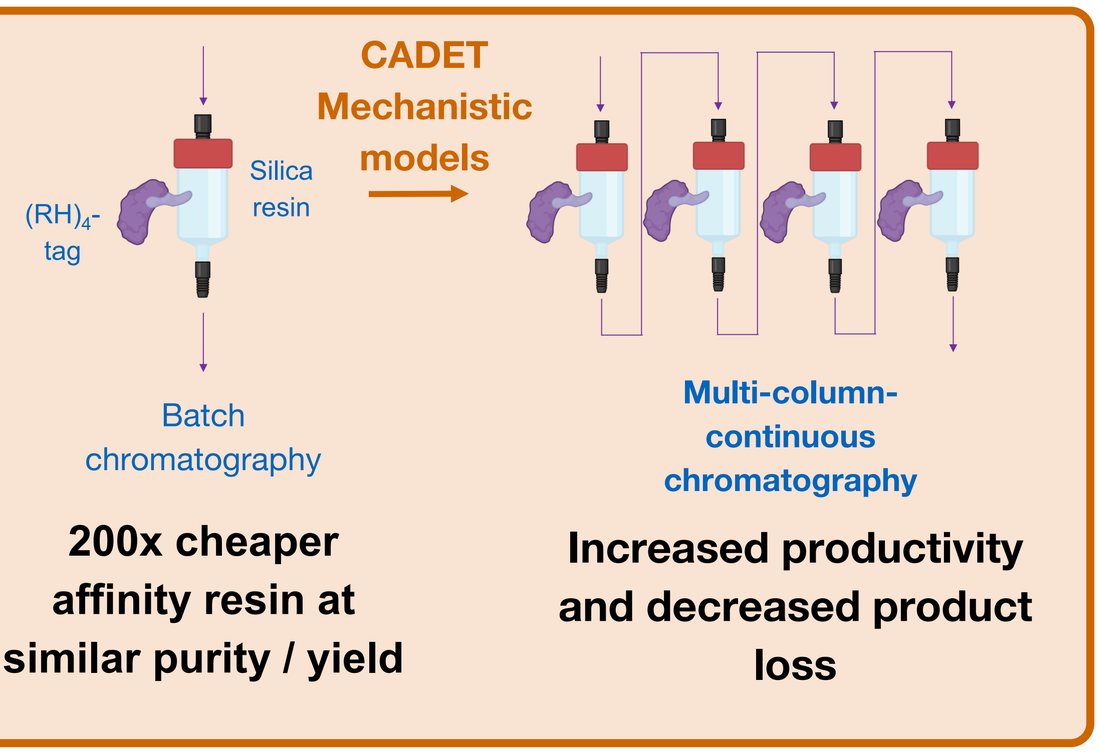
Profile

- Background in IBT, Bioprocess-, Chemical-, Mechanical, Data Engineering, computational science or similar.
- Solid Python skills, experience with scientific libraries and interest in chromatographic process modeling.

Start information

- Start date: As soon as possible / flexible.
- Location: Garching.
- Spoken languages: English, German, Spanish.

„Imagination is more important than knowledge." - Albert Einstein



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