

Theoretical Bachelor/Master Thesis or Scientific Internship

Theoretical study of plug flow reactors for enzymatic cascades

Description

In the Laboratory of Chemical Process Engineering the model-based optimization of reactors for enzymatic cascades is carried out using Python and the Python-based, open-source optimization modeling language Pyomo. Plug flow reactors containing immobilized enzymes are expected to play an important role in developing sustainable reaction processes. Some fundamental theoretical questions about carrying out enzymatic cascade reactions in plug flow reactors remain open. In particular, the optimal selection of a combination of a spatial immobilization strategy inside the particle pores and a distribution for particles inside the plug flow reactor is of interest. The main tasks of the project are to study and compare three designs for a plug flow reactor that carries out a two-step enzymatic cascade reaction. A mechanistic model of the process will be developed based on previous work completed in our laboratory and used for the comparison. Python and Pyomo will be used for modeling and model-based optimization. The results will be used to extract general guidelines for the design of such processes and where appropriate they will be generalized to cases that are more complex.

Requirements

An interest in reaction engineering is required.

To start

Immediately

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