



Master Thesis

Programming

Surrogate-Based Batch-to-Batch Optimization of Consolidated Bioprocessing

Keywords: consolidated bioprocessing; surrogate modeling; batch-to-batch optimization; machine learning; bioethanol; process optimization

Conditions:

Duration: 6 months
Requirements: MATLAB or Python knowledge (demonstrated):
Diagnosis and Prognosis course (Passed)
Language: English
Target group: Master students

Contents:

Consolidated bioprocessing (CBP) is a promising approach for bioethanol and biochemical production, integrating enzyme production, lignocellulosic hydrolysis, and fermentation into a single process step. However, optimizing CBP is difficult due to the time-consuming nature of experiments, nonlinear process responses, and strong interactions among operating variables such as temperature, pH, substrate loading, and pretreatment. Machine learning-based surrogate models can assist in process development by learning the relationships between operating conditions and measurable process outputs, such as ethanol concentration, substrate conversion, and time-related performance.

In this thesis, surrogate-based batch-to-batch optimization strategies are implemented and compared for improving the CBP process. Surrogate models such as random forests, Extra Trees, Gaussian process models, gradient boosting, or neural networks will be trained on simulation data and/or secondary literature. The trained models will then be used to propose improved operating conditions that meet selected process objectives, e.g., maximizing ethanol formation while accounting for substrate conversion or process duration. The comparison will be based on prediction accuracy, optimization performance, robustness to noise, and appropriateness for future experimental planning.

The goals of this work are:

- Identification of relevant CBP operating variables, measurable outputs, and optimization objectives
- Implementation and comparison of selected surrogate models for CBP response prediction
- Development and testing of batch-to-batch optimization strategies using simulation
- Complete and detailed documentation/presentation of the research results