



Development, Validation and Comprehensive Sensitivity Analysis of a Fermentation Model Expediting the Process Design of a Biorefinery

Vollmer, Nikolaus I.; Gernaey, Krist V.; Mussatto, Solange I.; Sin, Gürkan

Publication date:
2019

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

Vollmer, N. I., Gernaey, K. V., Mussatto, S. I., & Sin, G. (2019). *Development, Validation and Comprehensive Sensitivity Analysis of a Fermentation Model Expediting the Process Design of a Biorefinery*. Abstract from 5th European Congress of Applied Biotechnology, Florence, Italy.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.



Development, Validation and Comprehensive Sensitivity Analysis of a Fermentation Model Expediting the Process Design of a Biorefinery

Nikolaus I. Vollmer¹, Krist V. Gernaey¹, Solange I. Mussatto², Gürkan Sin¹ *

¹ PROSYS, Department of Chemical and Biochemical Engineering, Technical University of Denmark;

² Biomass Conversion and Bioprocess Technology Group, Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark.

*Corresponding author: gsi@kt.dtu.dk

Highlights

- Systematic Fermentation Model Development for Biorefinery Process Design.
- Production of Xylitol from Lignocellulosic Biomass.
- Validation and Comprehensive Sensitivity Analysis consolidating the Development Strategy and showing potential for Extended Applications.

1. Introduction

The Sustainable Development Goals of the United Nations (UN-SDG) demand inter alia a transition towards sustainable and responsible economic production patterns [1]. A key approach in achieving these goals is the concept of a biorefinery, in which the processing of lignocellulosic biomass (LB) serves to provide multiple value-adding products [2]. A major drawback though still remains its economic profitability. Therefore, extensive research and development efforts are required to design, analyze and holistically optimize biorefinery concepts in order to enhance their economic feasibility [3]. For these purposes, tools from Process Systems Engineering (PSE) can be employed to give adequate responses to questions from unit level up to the plant-in-market level. The focus of this contribution lies on the production of xylitol by fermentation in a biorefinery. Xylitol can be a highly value-adding product due to its increasing demand in e.g. the health industry [4]. Therefore, a first-principles fermentation model is developed to describe mechanistically the yield of xylitol and the process dynamics. A multi-stage approach is used to develop a customized model which is able to support the process synthesis and design for the biorefinery including performance prediction, sizing and costing analysis. To this end the model accounts for various process phenomena from different scale levels such as biological (e.g. the specific metabolism), chemical (e.g. acid-base equilibria) and physical (e.g. gas-liquid mass transfer) in a fermentation reactor.

2. Methods

The model development incorporates seven subsequent steps, which allow for a gradual implementation: *step (1)* - Simple Substrate-Product-Biomass correlations, *step (2)* - Oxygen Uptake, *step (3)* - CO₂ production, *step (4)* - Nitrogen Consumption + weak acid-base equilibrium, *step (5)* – Gas-Liquid Mass transfer and Energy Balance, *step (6)* - Internal metabolism reactions and *step (7)* - Additional Products and Substrates. A model framework based upon the matrix formulation of Sin et al [5] is chosen, since it facilitates the desired stepwise implementation.



Exemplary, during *step (1)* an overall mass balance and component mass balances for the substrates, the cell biomass and the products are derived. Conversion rates for all the components are calculated with a stoichiometric matrix of all the components and a process rate vector with all the occurring reactions in the fermentation, which are biomass formation, maintenance and the production of the products [5]. All the further steps aim to add further components and processes to the matrices/vectors and introduce new component or overall mass balances and energy balances. The steps are consecutively validated with data for a specific microorganism employed for xylitol production. Finally, a comprehensive local and global sensitivity analysis is conducted.

3. Results and discussion

The purpose of this approach is to guarantee a sufficient model complexity, while taking into account all necessary mentioned factors avoiding excessive complexity. Hence, *step (1)* is supposed to serve as fundamental model base. Since most microorganisms grow under aerobic conditions, oxygen is integrated into the model in *step (2)* to yield information about the oxygen demand. Since CO₂ is an important end product in the aerobic metabolism, a quantification is important, since it can be sold as by-product. The inclusion of nitrogen in *step (4)* contributes furtherly to the accurate prediction of the biomass growth since the microorganisms require nitrogen to grow. The weak-acid base model is introduced in the same step, because nitrogen sources serve as proton donors and influence the pH value of the liquid directly, which itself influences the concentration of CO₂ in liquid. The consideration of mass transfer refines these phenomena and yield a quantitative response for oxygen and CO₂ concentrations in gas and liquid phase. Considering the evaporation of H₂O is important, since it quantifies its loss and hence equally a necessary compensation to maintain a constant reaction volume. Other contributing factors here a potential heating of the system due to thermophilic conditions or increasing viscosity which influences the mixing effort. The assessment after *step (5)* considers the sufficiency of the prediction qualities of the model. Both *step (6)* and *(7)* denote a trade-off between the model complexity and its final purpose of prediction. Due to the flexibility of the framework this assessment can always be revised, depending on the further needs of the desired application. The validation with data in the chosen case shows a sufficient result in terms of yield prediction for xylitol and the process dynamics after the fifth step, implying to cease the implementation here. The sensitivity analyses show expected results.

4. Conclusions

The presented model structure and in particular its sequential implementation with increasing complexity proves to be a perfectly suitable approach in order to provide a model for this purpose. It ascertains a flexible and easy implementation for all seven steps in case of adaption of the model framework for various microorganisms, products or substrates. Hence, it yields simple yet adequate models for the process design of a biorefinery and thus can support the transition towards more sustainable processes as demanded by the UN-SDG.

References [Calibri 10]

- [1] United Nations, Transforming our world: The 2030 agenda for sustainable development, 2015.
- [2] F. Cherubini, Energy Conversion and Management 51 (2010) 1412-1421.
- [3] S.S. Mansouri et al, in M. Tabatabaei, M. Aghbashlo (Eds.), Biodiesel, Springer, Cham, 2018, pp. 127-148.
- [4] S.I. Mussatto, in: S. da Silva, A. Chandel (Eds.), D-Xylitol. Springer, Berlin, Heidelberg, 2012, pp. 309-323.
- [5] G. Sin et al, Biotechnology and Bioengineering 101 (2008) 153-171.