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Modification of the Upstream Process Design in a Biorefinery by Modeling and combined Uncertainty and Sensitivity Analysis

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An integrated biorefinery is an essential concept for the sustainable production of food, chemicals and power generation, utilizing e.g. lignocellulosic waste from agricultural waste as feedstock [1]. The crux of this concept is a poor economic potential due to the multitude of costly process steps for the pretreatment of the feedstock and the downstream processing [2]. Therefore, the process design of a new biorefinery has to be performed systematically [3]. When opting for a specific co-product in the biorefinery, an essential decision already has to be taken for the upstream process, specifically for the biomass pretreatment and the following conversion reaction.

In the presented case, the considered process is the fermentative production of xylitol, a sugar substitute with manifold beneficial health properties and especially suitable for diabetics [4]. In lignocellulosic biomass, the hemicellulosic fraction consists mainly of xylose, which makes it an ideal feedstock for fermentation towards xylitol [5]. Hence, requirements for the pretreatment technology to be employed can be postulated: (1) an optimal fractionation between hemicellulose and the cellulosic and lignin fraction; (2) a high yield of xylose monomers; and, (3) a low amount of inhibiting substances. The first requirement directly results from the biorefinery concept, since the highest value is achieved when all the feedstock is processed to value-adding products. Secondly, a higher yield of xylose monomers implies an increased volumetric productivity for the following fermentation. Accordingly, lower amounts of inhibitors results in better growth conditions for the microorganisms during the fermentation.

For the investigation of this interplay between pretreatment and fermentation, first-principle models are built. The pretreatment model incorporates mechanisms for Liquid Hot Water (LHW) and Dilute Acid (DAc) pretreatment. The fermentation model is designed based upon data acquired from experiments with a yeast under aerobic conditions. The following key analysis step is a combined Uncertainty and Sensitivity analysis of both models, with the focus on Sobol indices for the global sensitivity analysis and Monte-Carlo techniques for the uncertainty analysis.

The output of this combined analysis is twofold: Apart from an extended insight into the robustness of the models, their functioning and their interactions, it yields valuable output for a following process design based on superstructure optimization. Based on the results, conclusions for the process and its design can be drawn, e.g. whether additional unit operations must be taken into consideration. High uncertainty in the output of the pretreatment model regarding the concentration of certain inhibiting compounds, could indicate a necessary integration of an intermediate unit operation in order to remove the compound for better yields in the fermentation step. Different possible conclusions from the output of the Uncertainty and Sensitivity Analysis influencing the composition of the process design superstructure are discussed.

With this cornerstone, following optimization steps for the superstructure and operations optimization of the biorefinery and an extended supply chain analysis based on robust optimization can be performed soundly. Finally, this contributes to the development of a consolidated, economically viable biorefinery process.

References

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