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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 agriculture as feedstock [1]. The crux of this concept is a poor economic potential due to the multitude of process steps for the pretreatment of the feedstock and the downstream processing (DSP) [2]. In terms of the latter, the separation and purification of a desired substance from fermentation broth is a complex and versatile procedure [3]. Hence, classic heuristic approaches in process design for biorefineries will succumb to a methodic approach. Superstructure optimization is a well-proven approach to tackle this exact challenge [4]. In order to utilize it, models for every considerable unit operation have to be developed. Apart from the issue of which unit operations to employ, the predominant question targets the robustness of the implemented models, which exceedingly affect the results of the superstructure optimization.

The considered case is the DSP of xylitol produced by fermentation. Xylitol is a sugar substitute with manifold beneficial health properties and especially suitable for diabetics [5]. Xylitol is highly soluble in water, which is the bulk substance in fermentation broth. Moreover, it contains salts, byproducts and – in the case of lignocellulosic feedstock – inhibitory compounds. Hence, the downstream process has to segregate xylitol from water and the other named compounds. To this end, the unit operations, which are represented in the superstructure by first-order models, are an evaporation unit, a liquid-liquid extraction unit and a crystallization unit. All three are incorporated as unit operation in the separation section of the DSP, where the latter one is also considered as the unit operation for the purification step.

In order to address the arisen question regarding the robustness, a Sensitivity and Uncertainty analysis with the three unit operation models is performed. The Sensitivity analysis is conducted globally and comprises Sobol indices, the Uncertainty analysis is performed by utilizing Monte-Carlo techniques. This key analysis step now provides various insights into the functionality of each of the models and allows for conclusions regarding the following interactions of the model by performing the superstructure optimization. Firstly, the sensitivity analysis serves as design space exploration, yielding information about whether similar parameters in the models are more sensitive. This allows conclusions towards which of them should be included in the objective function of the following superstructure optimization, which is a valuable contribution in order to improve its efficiency. Secondly, the principal question about the robustness is answered by the combined Uncertainty and Sensitivity analysis: with the knowledge about sensitive model parameters and the error-propagating properties of the model valuable insights about the reliability of the interconnection of several of these models are provided. In case the

downstream process should involve several repetitive separation and purification steps in order to match the presumed purifications, the overall resilience of the suggested design can be assessed.

With this cornerstone, the 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 will contribute to the development of a consolidated, economically viable biorefinery process.

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