Systematic Multivariate Analysis (sMVA) Strategy for Improved Process Understanding of Industrial Biorefinery Processes with Applications in Fatty Acid Production

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The pronounced variability in biomass composition and quality is one of the key bottlenecks in the development of biorefineries.[1] Mechanistic and statistical modelling are used in petroleum refineries to tackle this challenge of feedstock diversity and adapt process conditions for the compositional variability of the incoming crude oil.[2] Applying these techniques to biorefinery processes would aid in utilizing biomass more efficiently. However, due to the complexity of biomass, mechanistic modelling is highly challenging. Alternatively, statistical process modelling can be used to support identification of effects of feedstock and process variability on product quality and to gain insight in how control strategies can aid in managing this variability. Thereby, statistical modelling could serve as an important basis to steer further research and modelling efforts for the optimization, monitoring and control of biorefinery processes. However, a lack of systematic practices and methods is often seen as one of the main disadvantages of this statistical modelling.[3] This motivates the development of general strategies for applying statistical modelling in industrial biorefinery processes.

In this work, a systematic multivariate analysis (sMVA) strategy for improved process understanding of industrial biorefinery processes is proposed to support identification of effects of feedstock and process variability on product quality.[4] The sMVA strategy comprises nine steps categorized in dataset organization, exploratory analysis and regression. Different multivariate analysis techniques are used, such as principal component analysis (PCA) and sequential multi-block Partial Least Squares Regression (SMB-PLS).[5] As a case study, two main operations in fatty acid production, both operated by Oleon NV in Belgium, are investigated: oil hydrolysis and fatty acid distillation.

The case study showed that applying our proposed sMVA strategy improves the understanding of a biorefinery process by identifying critical sources of process and feedstock variability, which allows more targeted decisions for optimization and control. It was found that single and multi-block PCA analysis of product properties, feedstock properties and process parameters allow identification of grouping, outliers and background effects. The optimal PLS regression methodology, which results in the easiest to interpret results, can be chosen based on the observed correlation between feedstock properties and process parameters. For fatty acid production, the type of fat or oil used, such as canola or palm oil, largely influences product quality due to the large difference in composition between the oil types. However, if a single oil type is used, the variability in product quality does not always critically depend on the variability in feedstock properties. For both operations, flow rate variations, mainly caused by planning issues, were identified as a main cause. In oil hydrolysis, the feed flow rate influences the residence time and thereby directly influences the hydrolysis and side reactions. In fatty acid distillation, a better control is required of the middle reflux ratio in relation to this changing flow rate. Based on these findings, control improvements were proposed, such as a higher and fixed middle reflux ratio instead of a fixed valve% controlling the reflux rate in fatty acid distillation. The findings of these case studies can be used to develop or improve mechanistic or hybrid models of both processes to further steer the optimization and control of both operations.

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