Global sensitivity analysis on cost evaluation via the development of process flow diagram using detailed kinetic model: application to γ-valerolactone production

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Highlights

- Kinetic modeling for the hydrogenation of butyl levulinate
- Simulation of a process flow diagram using detailed kinetic models
- Effect of inlet parameters on cost evaluation

1. Introduction

The valorization of biomass with various methods are highly investigated nowadays and many breakthroughs were achieved for the industrialization of such complex systems. Flowsheeting simulators also play a crucial role in investigating and developing processes for industry. Although a significant amount of research has been done in process simulation for the development of biomass valorizing processes, the literature is sparse on implementing detailed and or intrinsic kinetic models.

In most cases process flowsheet diagrams are developed based on experimental data, but without implementing existing kinetic models, only using conversion-based methods. Kinetic data for such complex systems is challenging to develop and often requires more complex kinetic models, that are not suitable to implement directly to process simulators. However, there are methods available targeting this specific issue [1]. Kinetics containing simulation models have the advantage of providing a wider spectrum of sensitivity analyses and process investigation, based on the range of experimental data used for developing the kinetic model. Conversion methods could only be used for modeling a single scenario, based on ratios in the specific experimental dataset. Performing analysis and modifying initial conditions in this case, like temperature, pressure, and initial concentration ratios is not possible.

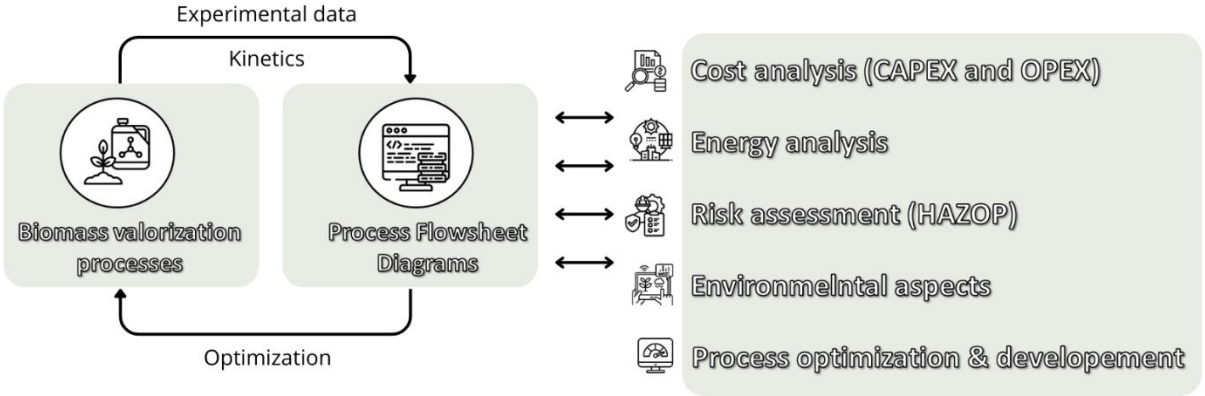

Figure 1. Examples of analysis with Process Flowsheet Diagrams developed on an experimental basis.

This work aims to develop a process flow diagram for the catalytic conversion of lignocellulosic biomass monomer glucose, to obtain γ-valerolactone as a product. The main goal is to utilize kinetic models in an expression directly usable in process simulator Aspen Plus to develop a robust PFD for accurate process optimization and cost evaluation purposes.

2. Methods

Experimental datasets were available with different initial and operating conditions, kinetic parameter identification and validation of the results were both possible for these datasets [2,3]. The identification framework was written in MATLAB, where genetic algorithm was used. For the flowsheet simulator we had chosen Aspen Plus V12, performing steady state simulation.

3. Results and discussion

The process flow diagram consists of three main reactors: the glucose-fructose isomerization reactor, the fructose to butyl levulinate reactor and the butyl levulinate to γ-valerolactone producing reactor [4]. All three of them operates in kinetic mode, where the main challenge during the simulation development was to find a form of the kinetic models that are suitable to implement in Aspen Plus.

The chosen kinetic models were modified Arrhenius type for the glucose isomerization and the fructose dehydration reactions and, LHHW type for the hydrogenation of butyl-levulinate [5]. First, identification to multiple experimental datasets was performed with an objective function of quadratic error minimization in MATLAB environment. The results were validated to the remaining datasets. Then the process flowsheet was built in Aspen Plus stationary simulator with the use of the identified kinetic constants.

The results with the developed kinetic models and the identified kinetic constants resembled the experimental concentration profiles well. The process flow diagram could utilize these models and provided a reliable simulator for a scaled-up process of biomass derived product valorization.

4. Conclusions

Process simulators play an important role in development and implementing kinetic models to widen the spectrum of possible analysis and obtain reliable results with the use of them. The main disadvantage is however to develop kinetic models that could be directly used inside these simulators, which is severely limiting the complexity of the models, therefore their performance replicating the real reaction rates. In our case study we successfully modified and identified kinetic models for various biomass processing reactions and created a robust process model inside Aspen Plus environment for further analysis.

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Keywords

biomass valorization; process simulation; kinetic modelling; Aspen Plus