Modelling-based Catalytic Bio-refining Reaction Engineering

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Highlights

- High-performance computing, machine learning and artificial intelligence are crucial for the development of innovative bio-based processes.
- Exemplary approaches for the use of lignocellulose, lipids, and marine sources.
- Multiscale modeling proves to be crucial for development of bio-based chemicals.

1. Introduction

Biomass as an abundant and sustainable resource plays a pivotal role in reducing the carbon emissions and replacing fossil-based resources with renewable alternatives.

To overcome the challenges of biomass valorization a model-based process design using mechanistic models has proven to be a crucial approach for predicting the chemical behavior in various biomass valorization processes relevant to biorefineries. Such methodology enables a better understanding and process optimization to achieve desired products. This presentation will discuss and evaluate studies in which novel in-silico strategies are combined with the experimental methods and applied to various aspects of biorefining, highlighting the challenges encountered when using conventional modeling approaches.

The critical evaluation of such kinetic models leads to recommendations for improving their applicability and predictability in future of bio-based chemical production. As computational power advances, such complex mathematical models are expected to become integral technologies in the emerging bioeconomy and contribute to innovative biorefinery concepts.

2. Biomass relevance

Currently, biomass plays a crucial role in the production of liquid bio-fuels and bio-based platform chemicals. The cascade utilization of lignocellulosic biomass, through thermochemical or biochemical fractionation allows later valorization of cellulose, hemicellulose and lignin, which enables a sustainable production of valuable raw material for various applications. Isolated lignin fractions can be based on their specific properties incorporated in various bio-polymers and -resins, while also offering multiple valorization routes including depolymerization towards bio-aromatics. Furthermore, (hemi-)cellulose can be depolymerized into sugars, leading to the production of C5 and C6 building blocks and chemicals that are crucial for the polymer industry. The modification of pulp and cellulosic fibers by (de)functionalization enables the adjustment of surface and mechanical properties providing an alternative to synthetic fibers with functionalized natural fibers.

3. Examples and key findings

Efforts to fractionate lignocellulosic biomass are directed towards unlocking the potential of cellulose, hemicelluloses, and lignin for the targeted production of high value-added chemicals. The authors are working intensively on optimizing organosolv fractionation to preserve the molecular structures and improve the quality of the resulting biopolymers. The aim is to go beyond the traditional methods of biomass fractionation used in the pulp and paper industry to achieve a more sustainable and economical process.

The catalytic hydrotreatment of lignin is a solution for the conversion of lignin, a by-product of various industries, into bio-monoaromatics. This approach not only addresses the challenge of underutilized lignin, but also contributes to sustainable chemical production. At the same time, valorization of (hemi)-cellulose derived monomers offers a sustainable production of targeted bio-chemicals. Therefore, the authors are focused on glucose conversion by initial oxidation towards glucaric acids and its subsequent conversion into adipic acid, which is essential to produce nylon 66 [1,2].

Correspondingly, (hemi)-cellulose valorization route entails the saccharide hydrolysis and dehydration towards furanics known as bio-based platform chemicals [3]. Therefore, an ongoing research entails the production of 5-(hydroxymethyl)furfural (HMF) and furfural and its further conversion via hydrogenation and hydrodeoxygenation. By employing different process conditions and innovative catalysts, 5-HMF particularly, revealed its immense potential to obtain valuable bio-based poly/dios such as 1,2,6-hexanetriol and bis(hydroxymethyl)tetrahydrofuran [4].

Overall the methodology applied includes a high-throughput screening of catalysts and reaction conditions, to obtain the time dependent concentration profiles, which is often guided by computational methods, Figure 1a. On the other hand, computational modelling is often combined with experimental kinetic studies with an aim to elucidate various mechanisms of selective conversion of model compounds to value added products to value added products such as glucose oxidation to glucaric acid in base free aqueous solution, Figure 1b. Importantly, the obtained data and kinetic parameters can be later used to predict the optimal reaction time and temperature to achieve the highest yield of desired [2].

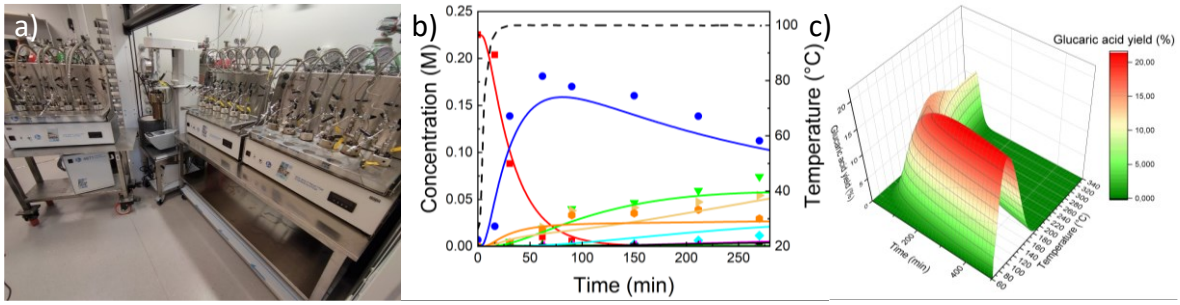

Figure 1 a) Reactor system used for high throughput screening, b) descriptive modelling by simultaneous regression analysis of multiple experiments, c) process parameters optimization by the predictive modelling [3].

4. Conclusions and Outlook

Next to CO_2, biomass is our most important sustainable carbon resource. Nevertheless, the inherent challenges of its utilization due to its high complexity so far limits the scale of conversion, especially when it comes to applications beyond powerful methods such as pyrolysis, combustion, or gasification, with a focus on bio-based chemicals. Therefore, the combination of high-throughput screening and high-performance computing, including machine learning and artificial intelligence, can be a valuable tool for catalyst and process optimization, particularly within the field of biorefining.

In this context, we describe and present a roadmap for several exemplary cases dealing with lignocellulose biomass. The integration of multi-scale modeling simulations proves helpful to either support or entirely solve key challenges. While the uniqueness of these approaches remains remarkable today, this dynamic field is poised for future developments. As technological tools continue to advance, there is optimism of overcoming existing limitations and fully uncover the potential of biomass as a sustainable carbon source. This development is crucial for the diversification of applications that go beyond conventional methods and have a transformative impact on the field of bio-based chemicals.

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Keywords
Biorefining; Modelling; Reaction Engineering; Catalysis.