Upstream purification, Catalyst Development and Kinetic Modeling for the Production of Lignocellulosic Bio-based Furanics

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Lignocellulosic biomass is a highly abundant, non-edible and sustainable source of carbon. Its (hemi)cellulose fraction can be efficiently utilized for the production of targeted bio-based furanics [1]. BioSPRINT project, funded by BBI EU H2020, focuses on the valorisation of the rather underutilized hemicelluloses (HMC). Aiming towards applicability of the customer ready products, the project addresses various areas such as upstream purification, catalytic conversion, followed by downstream purification and polymerization.

For the upstream purification step, both evaporative lignin precipitation and antisolvent HMC precipitation were investigated using thin film spinning disc reactors. Up to 70 % of lignin recovery was achieved with well under 10 seconds disc residence times highlighting the intensified solvent evaporation rates from the thin films. Intense mixing of antisolvent with the HMC feed stream enabled to attain sugar recoveries of up to 40 % in a fraction of the second. Current work is focusing on the solvent evaporation rates improvement and mixing intensification by using textured disc surfaces. In complementary research, sugars were concentrated using nanofiltration membranes in order to maximize the process efficiency. Aiming towards sufficient sugar retention and small-chain acid removal, the membrane selection was based on a screening study performed with synthetic (HMC) mixtures. For the validation of the best performing membrane(s), multiple streams of European bio-refineries were subjected to nano-membrane filtration. Additionally, the activities also aim to diminish the known membrane fouling issues with HMC streams by taking advantage of multi-scale simulations. Future work will comprise of hybridization of the upstream processing steps.

Focusing on the establishment of sustainable and scalable process, heterogeneous catalysis in aqueous media was selected for catalytic conversion of hemicellulose derived saccharides [2]. Acid catalysed dehydration of xylose and glucose, the most prevalent HMC sugars, enabled the production of value-added furanics: hydroxymethylfurfural and furfural [3]. Both bio-based products have an immense potential of further valorisation and can be converted into various renewable chemicals, contributing to a carbon-neutral economy. Modified heteropolyacids on different supports were used as a solid acid catalysts, for the catalytic conversion of multiple C5 and C6 sugars. To systematically test the catalytic activity, libraries of HPA have been synthesised using easy-to-scale methods. Formulation and design of heteropolyacid (HPA) catalysts was guided by machine Learning (ML) to accelerate the optimisation of 5-HMF and furfural selectivity. It has been possible to establish correlations between the catalyst properties and key performance indicators. This approach enabled the prediction of formulations for novel catalytic materials that will be investigated for the conversion of complex sugar mixtures and real HMC streams.

Subsequently, a kinetic model was developed and a precise reaction network was established, which helped to identify reaction intermediates and rate-determining steps. Focusing on the catalytic conversion of sugar model compounds, dehydration of individual saccharides was conducted. Calculated kinetic parameters allowed to optimise the process conditions and transfer the model towards more complex and previously purified real biomass streams. The mentioned actions will help to successfully complete future steps of downstream purification and polymerisation to final products.

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