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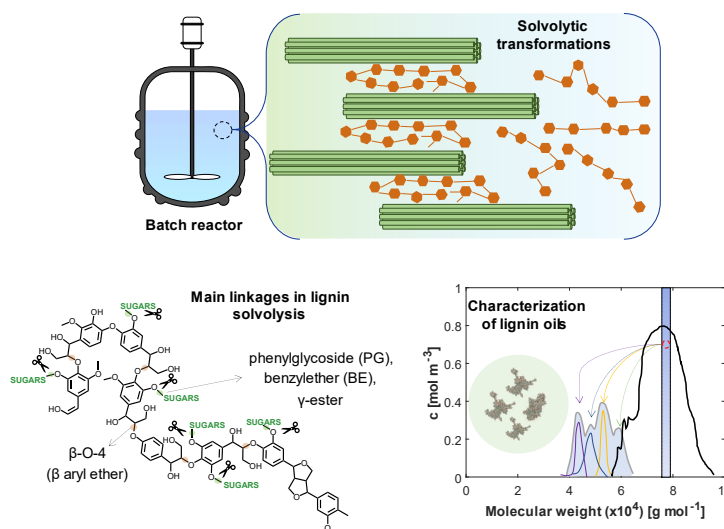
Experimental and kinetic investigation of lignin solvolysis: a first step in lignin biorefining

Aim

This thesis aims to investigate the solvolytic transformations of lignin, the initial step in the reductive catalytic fractionation (RCF) of lignocellulose, under several operating conditions, ultimately acquiring intrinsic kinetic data for the validation of a kinetic model.

Justification

Due to resource scarcity and CO₂ emissions associated with the use of fossil feedstocks, non-edible biomass such as lignocellulose is becoming one of the most promising alternative resources. Lignin, the aromatic fraction of lignocellulosic biomass, is the most abundant renewable source of aromatics on earth. RCF of lignocellulose combines biomass fractionation, by solvolytic transformations, with heterogeneously catalysed lignin depolymerization and stabilization. The ultimate goal is the production of aromatic building blocks from biomass which can be further converted into novel materials or chemicals. Developing a comprehensive kinetic model to assess the solvolytic transformations and catalytic depolymerization of lignin is challenging due to the heterogeneity of the feedstock, and the large number of reactions involved. To tackle this, both phenomena can be described separately through a continuous lumping model to account for catalysed and non-catalysed reactions.



Solvolytic reactions are typically conducted in a batch reactor where different types of lignocellulosic biomass are used as feedstock. Organic solvents, e.g. methanol and ethanol, as well as water will be considered to evaluate the effect on the product distribution. Reaction temperatures will range from 150 to 300 °C. In principle, lignin solvolysis generates a wide range of products which usually involves a low monomer selectivity¹. The impact of different operating conditions and biomass type in the resulting range of products will be assessed via molecular weight (MW) characterization of the lignin oil through analytical methods such as gel permeation chromatography (GPC) or gas chromatography combined with mass spectroscopy (GCxMS)². Moreover, since solvolytic reactions and diffusion of lignin products compete at similar time scales, preliminary experiments should assess on the degree of delignification in order to identify intrinsic kinetics regimes, using an already developed reaction-diffusion model.

Program

- Literature survey on lignin chemistry, lignin solvolysis and analytical methods to characterize lignin oils;
- Experimental work in a batch reactor for different solvolytic systems in terms of type of biomass, e.g. hardwood and softwood, and solvent environments at different temperatures;
- Characterization of lignin oils in terms of its MW distribution, e.g. via GPC, for the construction and validation of a kinetic model;

- Evaluate the reaction conditions that lead to a high monomer/light-oligomer selectivity.

References

- (1) Hashmi, S. F.; Meriö-Talvio, H.; Ruuttunen, K.; Sixta, H. Influence of reaction conditions on solvolysis of organosolv lignin using water and green organic co-solvents as reaction medium. *Fuel Processing Technology* **2020**, 197. DOI: 10.1016/j.fuproc.2019.106200.
- (2) Tolbert, A.; Akinosho, H.; Khunsupat, R.; Naskar, A. K.; Ragauskas, A. J. Characterization and analysis of the molecular weight of lignin for biorefining studies. *Biofuels, Bioproducts and Biorefining* **2014**, 8 (6), 836-856. DOI: 10.1002/bbb.1500.