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Influence of solvent, functional groups and operating conditions on the reaction rates of typical lignin bond cleavage during the organosolv process

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## PURPOSE OF THE ABSTRACT

Lignin is a natural polymer composed of aromatic monomeric units. It represents a very promising renewable source for chemicals production considering its aromatic, highly-functionalised structure and abundance. Moreover, economic operation of biorefinery requires valorisation of all three components of lignocellulosic (LC) biomass cellulose, hemicellulose and lignin into more valuable products<sup>1-3</sup>.

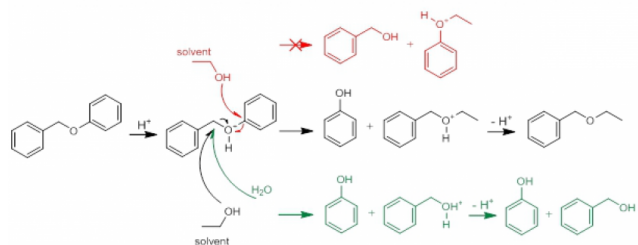
Lignin conversion into value-added chemicals usually involves three steps: isolation from other LC biomass components, depolymerisation and upgrading of obtained platform chemicals. Lignin isolation is a crucial one as it defines the structure and thus reactivity of isolated lignin. An organosolv process is recognised as one of the most environmentally friendly among other chemical treatments for biomass fractionation which provides a 'closer-to-native' lignin structure, i.e. preserves more ether bonds. It allows clean and safe fractionation of LC biomass and production of high-quality lignin due to the absence of sulphur and no impregnation of alkali/alkaline metals.

In this study, the organosolv treatment of several lignin dimer model compounds in different solvent systems, such as ethanol, ethanol/water,  $\gamma$ -valerolactone and  $\gamma$ -valerolactone/water, was performed. The aim of this study was to examine the influence of solvent, lignin functionalities and acidity of the reaction media on the rate and course of typical lignin bond cleavage. Operating conditions influence on product distribution as well as the rate of cracking was additionally investigated.

Experiments were performed in a six parallel batch high-pressure autoclave system. Lignin model compound (benzyl phenyl ether) was dissolved in a solvent or solvent system and sulfuric acid (0.5 - 1.5 wt%) was added as a catalyst. Experiments were performed in an inert atmosphere of N<sub>2</sub> with pressure of 1.0 MPa at 160 - 200 °C for 4 hours. Liquid samples were collected during the reaction time and analysed by using GC-MS analysis.

The detailed decomposition pathway of the benzyl phenyl ether (typical lignin model compound) in conventional solvents or solvent systems such as ethanol, ethanol/water,  $\gamma$ -valerolactone and  $\gamma$ -valerolactone/water was purposed. Once the ether bond was cleaved, the reaction proceeded in two different ways, depending on the solvent reactivity. This resulted in the addition of new functional groups to the molecule. Ethanol was found to be reactive, acting as a capping agent and terminating the possible coupling/condensation reactions, which were found to be characteristic in the case of  $\gamma$ -valerolactone (non-reactive reaction media). Additionally, operating conditions strongly affected the distribution of products.

## FIGURES



### FIGURE 1

Figure 1

Decomposition pathway of the benzyl phenyl ether in conventional solvent system such as ethanol/water in the presence of sulfuric acid.

### FIGURE 2

## KEYWORDS

Lignin | Organosolv | Added-Value Chemicals | Model Compounds

## BIBLIOGRAPHY