Parameter Optimization for Biphasic Depolymerization of Kraft lignin

Supervision: Saša Bjelić (group leader)

Research group: Advanced Analytics Platform

Time scope: 6–9 months

Start: as soon as possible

Work location: Paul Scherrer Institute, 5232 Villigen, Switzerland

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Prospective candidates should currently be enrolled in a Master's program in chemistry, chemical engineering, technical chemistry, or environmental science.

Scope of the Thesis

This thesis aims to optimize key process parameters in biphasic oxidative depolymerization (BPD) of Kraft lignin to maximize monomer yields and selectivity. The student will systematically vary reaction time, temperature, oxygen partial pressure, catalyst-to-lignin ratio, and phase ratio (aqueous/organic) to identify optimal conditions. The work will include kinetic studies as well as product identification and quantification by UHPLC-HRMS.

Scientific Background

Lignin is a significant natural resource – it is the most abundant naturally occurring aromatic polymer on Earth. Lignin is also a major side-product from the pulp and paper industry and cellulosic ethanol production, with about 50 million tons of lignin produced [1]. One of the promising approaches to its valorization is biphasic oxidative depolymerization. It combines oxidative depolymerization in an acidic aqueous phase with simultaneous extraction of aromatic monomers into an organic phase, protecting them from over-oxidation and repolymerization. Optimization of operational parameters is critical to improve efficiency and scalability for industrial applications.

[1] Omar Y. Abdelaziz et al., "On the Oxidative Valorization of Lignin to High-Value Chemicals: A Critical Review of Opportunities and Challenges," *ChemSusChem* 15, no. 20 (2022), https://doi.org/10.1002/cssc.202201232.

Objectives

1. Optimization of BPD conditions.

3. Quantification monomer yields (e.g. vanillin, 5-nitrovanillin) using UHPLC-HRMS.

4. Data analysis for identification of trends and interactions.

5. Validation of optimized conditions in larger-scale batch or continuous setup.

Key Learnings

You will learn how to:

- Design and execute systematic parameter screening experiments.
- Operate UHPLC-HRMS and interpret high-resolution mass spectrometry data.
- Apply advanced data analysis techniques for complex mixtures.
- Collaborate within a multidisciplinary team focused on sustainable fuel analytics.

General Tasks

During this project, you will:

- Develop experimental matrix for parameter screening (time, temperature, oxygen pressure, catalyst ratio, phase ratio).
- Perform BPD reactions under varied conditions using selected catalysts.
- Perform UHPLC-HRMS analysis.
- Analyze kinetic data and evaluate reaction efficiency.
- Document findings in a written thesis according to university guidelines.

  Your results will be reported in a written thesis conforming with the rules of the respective university you are enrolled in. Depending on the quality of the results, they could be included in future publications in scientific publications.