

Sustainable Aviation Fuels from Biomass: Understanding of Catalysts with Model Compounds

Supervision: Prof. Dr. Frédéric Vogel (group leader), Dr. Joshua Csucker & Dr. David Baudouin

Research group: Catalytic Process Engineering (<https://www.psi.ch/de/cpe>)

Time scope: 6-9 months

Start: as soon as possible

Work location: Paul Scherrer Institute, 5232 Villigen, Switzerland

Contact: frederic.vogel@psi.ch

Prospective candidates should currently be enrolled in a university in a Masters program in chemistry, chemical engineering, technical chemistry or materials science.

Scope of the Thesis

You will primarily work on catalytic hydrodeoxygenation (HDO) of oxygenated aromatics, such as vanillin, under supercritical hydrothermal conditions. Focus will be placed on how different catalysts impact product distribution, conversion, degree of deoxygenation, and catalyst stability in model HDO procedures. Potential catalysts will be commercially sourced or tailor-made as part of your laboratory work. HDO reactions will be primarily investigated by qualitative and quantitative gas chromatography (GC-MS and GC-FID) analysis. A catalyst of interest should fully deoxygenate phenolic or poly-oxygenated aromatics while remaining stable under hydrothermal conditions. This project is part of SWEET reFuel.ch (<https://www.sweet-refuel.ch/>).

Scientific Background

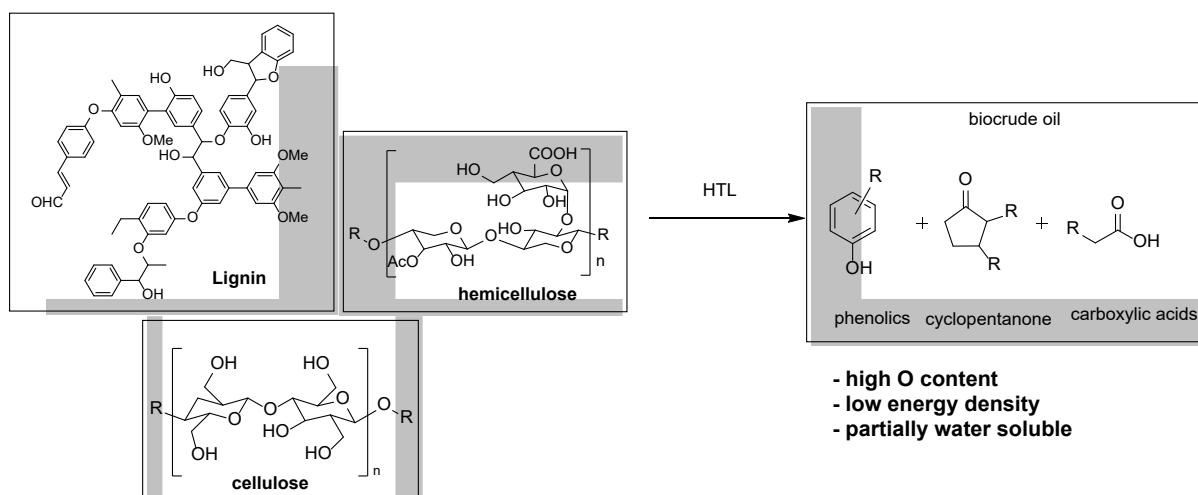


Figure 1: Schematic illustration of HTL reaction partners and products.

Hydrothermal liquefaction (HTL) is an attractive technology for the direct conversion of wet biomass into high-energy, high-quality fuel precursors and platform chemicals. This process enables the synthesis of complex, value-added chemicals from renewable rather than non-renewable fossil petrochemical sources. During HTL, biopolymers such as lignin, cellulose, and hemicellulose are broken down into oligomers or small-molecule monomers (Figure 1). The underlying chemical reactions are complex, and many occur simultaneously. The liquid resulting from HTL typically

contains phenolics, cyclopentanone derivatives, and carboxylic acids. The relatively high residual oxygen content of these breakdown products results in a low energy density of the so-called biocrude oil (the organic liquid product of HTL). Therefore, catalytic upgrading of HTL (cHTL) aims to reduce the oxygen content of biocrude oils through hydrogenation and hydrodeoxygenation (HDO). During catalytic HDO, carbon–oxygen bonds are reduced, typically with molecular hydrogen (H_2). New C–H bonds are formed while oxygen is removed as water or methanol. Such reactions have been studied on biomass and model compounds, but usually under anhydrous or subcritical water conditions. We aim to demonstrate that supercritical water is an equally suitable medium for HDO catalysts. Initial experiments will focus on the deoxygenation of vanillin to creosol, p-cresol, and toluene (Figure 2).

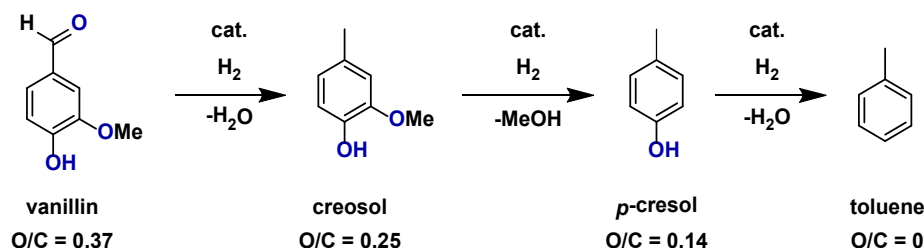


Figure 2: stepwise hydrodeoxygenation of vanillin to toluene.

Catalytic performance will be judged based on the O/C ratio of the reaction products. The ultimate goal of this project is to identify stable catalysts that facilitate complete HDO (O/C = 0) of model feeds such as vanillin with high conversion and high selectivity. Catalyst candidates will consist of highly dispersed transition metal nanoparticles on support materials (e.g., platinum on activated carbon).

Key Learnings

You will learn how to:

- Prepare, analyze, and handle supported metal catalysts.
- Safely conduct high-pressure, high-temperature hydrogenation reactions.
- Perform robust qualitative and quantitative analyses of model HDO reactions.
- Critically interpret chemical transformations and optimize them toward a clearly defined target.

General Tasks to be Accomplished

During this project, you will:

- Screen HDO catalysts on model reactions with vanillin and other oxygenated aromatics in batch procedures.
- Synthesize and analyze (N_2 physisorption, powder XRD, TEM) supported metal catalysts with transition metals.
- Develop standardized analytical procedures for quantitative product analysis with GC-FID.
- Investigate catalyst stability under supercritical water conditions.
- Engage in regular scientific exchange with mentors and group members.

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 scientific publications.