Optimization of Equilibrium-Limited Esterifications Using Heteropolyacids in Two-Phase SNISMs Systems

Intended for: Bachelor-/Master-Thesis/ Research Internship
Field: Technical Chemistry
Starting Date: Individual Agreement

Description:

The efficiency of chemical syntheses is determined by the interplay between the catalyst and the reaction medium. In homogeneous catalysis, high substrate solubility, fast kinetics, high yields, and the recyclability of both solvent and catalyst are desirable. Achieving all of these factors leads to a more sustainable chemistry.

In the DFG-funded project SNISMs (**S**trongly **N**on-**I**deal **S**olvent **M**ixture**s**), esterifications are investigated as model reactions limited by chemical equilibrium. The goal of the project is to shift the reaction equilibrium position through the use of different additives in order to increase product yield. By employing heteropolyacids (HPAs) as catalysts, the reactions can be carried out under mild reaction conditions (1 bar, 25–50 °C).

In the previous project phase, we achieved initial successes in single-phase systems. Within the scope of this thesis, the project will be extended to two-phase systems. This enables the equilibrium to be shifted further toward the products and allows for a direct separation of product and catalyst. For the model reactions of ethanol with formic acid and/or acetic acid, the equilibrium yield is intended to be improved, and the recyclability of the HPA catalyst and the solvent system will be systematically studied.

In this project you will

• conduct esterification experiments at the fourfold glass reactor setup and test various SNISMs additives that lead to two-phase systems
• determine the equilibrium position (and reaction kinetics) using ^{1}H NMR
• apply a wide range of analytical methods for catalyst characterization (e.g., NMR, IR, Raman, TGA, ICP-OES, etc.)
• separate catalyst, product, and solvent via extraction and membrane filtration
• evaluate the recyclability of the catalyst and the solvent system

You will be part of a cooperative and motivated team and make an important contribution to the success of the SNISMs project.

Requirements

• interest in fundamental research in technical chemistry
• knowledge in NMR spectroscopy