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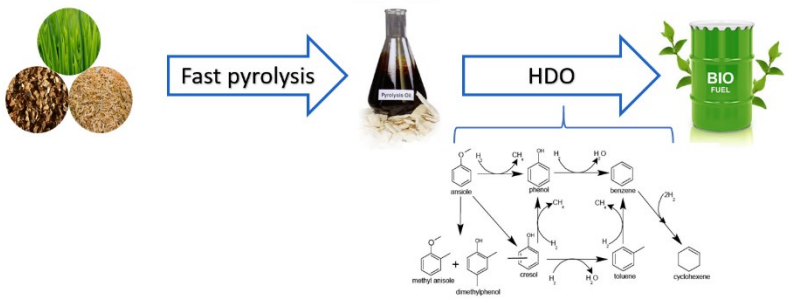
Kinetic modelling of anisole hydrodeoxygenation using NiCu catalysts

Aim

Kinetic modelling of anisole hydrodeoxygenation over NiCu catalysts. Ultimately a simulation tool should be developed that can provide guidelines on the reaction conditions and catalyst to be used in order to efficiently produce a desired product stream.

Justification



There is a strong and rising need for alternative feedstocks for fuel production, preferably renewable in nature. Lignocellulose is an example of a type of biomass that will not compete with food industry. There are several ways to valorise lignocellulosic biomass, such as pyrolysis and wet processing. These pathways ultimately produce a form of bio-oil that, because of unsaturated bonds and functional groups, lacks stability and has a low energy density. To improve the properties of this bio-oil, a hydrodeoxygenation (HDO) step is needed.

The current generation of HDO catalysts is still based on those used in the petroleum industry, while the molecules obtained from biomass are chemically different from petroleum-based molecules. Recent research has shown that supported NiCu catalysts may be a good alternative to perform HDO reactions in biorefineries. However, to make this catalyst industrially applicable for HDO reactions, the catalyst and reaction conditions need to be further optimized in terms of yield, selectivity and stability. The goal of this thesis is to assess the intrinsic kinetics and construct a comprehensive kinetic model for the HDO of anisole, as model compound for bio-oil, over NiCu catalysts. Development of such a model should allow for the optimization of both the catalyst, if adequate descriptors are identified, and the reaction conditions, and thus provide a valuable step towards the utilization of these bimetallic supported catalysts in HDO processes.

Program

1. Literature survey on the HDO over bimetallic catalysts / bio-oil HDO reaction mechanisms / biorefineries / …
2. Construction of an appropriate reaction mechanism and implementation in code (FORTRAN)
3. Parameter estimation using the acquired experimental data and sensitivity analysis
4. Development of an HDO simulation tool that is able to provide guidelines on both the reaction conditions and catalyst
5. Optimization of the catalyst and reaction conditions using the developed tool coupled with verification on the High-Throughput Kinetics Screening set-up

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