LABORATORY FOR CHEMICAL TECHNOLOGY
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Coach	**Supervisor(s)**
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Thesis subject for Chemical Engineering Technology (Industrieel Ingenieur Chemie)

Design of a separation process for biomass molecules via computational chemistry

Aim

Design of separation processes for lignin-derived mixtures based upon interaction parameters and equilibria predictions determined via computational chemistry and the COSMO-RS model.

Justification

Biorefineries in which inedible feedstock biomass or biogenic waste is converted into platform molecules are an important contribution to the development of a circular economy. In these plants, a wide range of products are synthetized to serve as alternative building blocks for more complicated chemicals, which are usually produced from fossil feedstocks using environmentally harmful processes. Lignocellulose (e.g. hard and soft wood, wheat straw, switchgrass, etc.) is the most abundant and cheapest inedible biomass source, potentially being the most scalable and economically viable bio-source. Moreover, lignocellulosic biomass is mainly composed of three major biopolymers, i.e., cellulose, hemicellulose and lignin, which via depolymerizations and further chemical treatments can be transformed into building blocks for many different industries, e.g. the polymer, pharmaceutical, cosmetic, agrochemical, food, etc. Depolymerisation of these biopolymers inevitably results in a mixture of a multitude of components with all very similar structures and properties. Further separation processes are indispensable to achieve the necessary requirements for the market. For example, pharmaceutical or food applications require high purities for specific components.

For the design of accurate separation processes, regardless of whether they are flash separations, distillations, liquid-liquid extractions, etc, adequate predictions of the thermodynamic parameters of the specific bio-molecules involved are required. Classic thermodynamic models are based upon experimental data to provide the necessary parameters to simulate the separations, but the determination of experimental data for all possible compounds is a very time consuming and costly procedure. Also, many of the functional groups in typical biomass derivatives are not well described by the existing thermodynamic models, which are usually developed for fossil-oil based products. Computational chemistry methods have become better and better in recent years, also for liquid phase mixtures. Therefore, computational chemistry could assist in predicting the vapour-liquid and liquid-liquid equilibria and binary interaction parameters that are required to model the separation of these biomass streams.

Program

- The candidate will be taught from zero on simple ab initio methods and on COSMO-RS theory for obtaining the knowledge required for the rest of the thesis (geen voorkennis vereist)
- Acquisition of V/L and L/L equilibria and binary interaction parameters via computational chemistry and COSMO-RS
- Assessment of the obtained parameters in comparison with the available experimental data
- Simulation and design of a separation processes in Aspen utilizing the previously calculated parameters
- Comparison of the designs with thermodynamic models available in the Aspen package