LABORATORY FOR CHEMICAL TECHNOLOGY

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Coach	Supervisor(s)	Funding
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Dehydration of biomass-derived butanediols into green 1,3-butadiene: Single-Event MicroKinetic model construction and process design

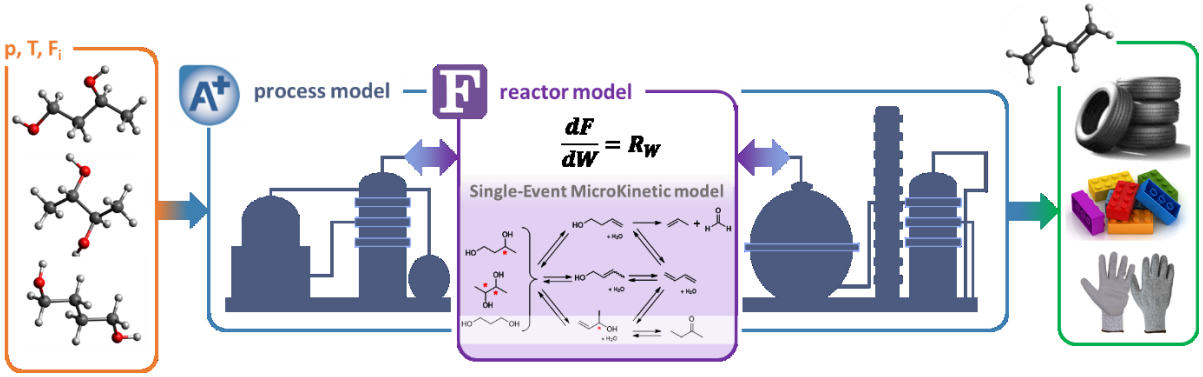
Aim

Development of a Single-Event MicroKinetic (SEMK) model for the dehydration of biomass-derived butanediols to green 1,3-butadiene using available kinetic data. The fundamental mechanistic insight obtained from the modelling effort will steer the design of next-generation dehydration catalysts. The SEMK model will then be used to optimize a process scheme for the production of green 1,3-butadiene.

Justification

1,3-Butadiene (BD) is a key building block for the polymer industry and is currently mainly produced as a byproduct of energy-intensive naphtha steam cracking. As there is a tendency to move towards lighter steam cracking feedstocks (e.g. ethane) less BD is produced through the latter process and novel (on-purpose) production processes are needed to meet the increasing BD demand. Moreover, the steam cracking process generates more than one ton of CO_2 per ton of BD. Both economic and environmental reasons, thus, plead for a diversification of butadiene production processes, preferably from renewable feedstock and with a reduced CO_2 footprint.

This master thesis will be carried out as part of the Moonshot GREEN-B2B project[1], which is a collaboration between UGent, KU Leuven and BBEPP. This project combines expertise in genetic engineering, catalyst design, reaction kinetics and process engineering and will pave to way to the circular production of green butadiene via the CO_2 co-processing fermentation of paper/cardboard waste into butanediols and subsequent acid-catalyzed dehydration into BD.



The dehydration model developed within this Master thesis will be a key tool to provide guidelines for the design of the optimal butanediol dehydration catalyst as well as for the overall process. The SEMK methodology is suggested here as an adequate way to describe the chemo-catalytic conversion of different reactants within a single family of components via complex reaction paths.[2] As such, the dehydration chemistry of a variety of biowaste-derived butanediol isomers (e.g., 1,3-butanediol, 2,3-butanediol and 1,4-butanediol) can be captured into a single fundamental kinetic model which allows to evaluate the impact of a highly variable feedstock on the overall process performance.

Program

- Literature survey: dehydration of biomass-derived butanediols
- Implementing the Single-Event methodology to yield a versatile microkinetic dehydration model.
- Linking the SEMK model to an Aspen Plus process scheme using an (already available) interface to develop a green process concept.

[1] https://moonshotflanders.be/mot1-green-b2b/

[2] Thybaut, J. W., *et al.* Single-Event MicroKinetics: Catalyst design for complex reaction networks. *J.Catal*, **2013**, *308*, 352-362.