LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Olivier Said-Aizpuru Jeroen Poissonnier	Joris Thybaut	Moonshot GREEN-B2B

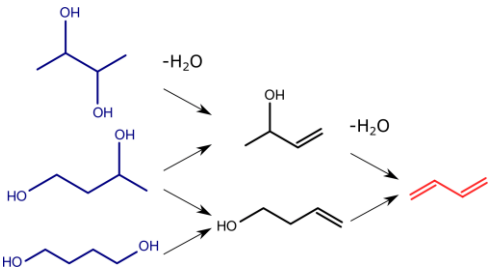
Butanediol dehydration into green 1,3-butadiene: microkinetic model construction and reactor design

Aim

Development of a microkinetic model for the dehydration of different butanediol isomers to 1,3-butadiene based on available kinetic data. The fundamental insight obtained from the modelling effort will clarify the reaction mechanism(s) and enable explaining the experimental observations obtained with a variety of innovative catalysts. This tool can be further applied to the design of industrial reactors and the optimization of catalytic systems.

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 steam cracking. The fluctuations of cracking feedstock supply (naphtha, shale gas…) are responsible for tensions on BD production and consequently pronounced BD price volatility. In addition, this process has a substantial CO_2 footprint of more than one ton of CO_2 per ton of butadiene. 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 GREEN-B2B project, which is a collaboration between research institutes (UGent, KU Leuven and BBEPP) followed up by the chemical industry on the Flemish level as part of the Moonshot Flanders program. This project will pave to way to the sustainable acid catalysed production of green butadiene from waste biomass. It combines expertise in genetic engineering, catalyst design, reaction kinetics and process engineering. GREEN-B2B pursues different objectives: (i) development of CO_2 co-processing fermentation pathways towards butanediols, (ii) butanediols conversion to butadiene[1], including dehydration catalysts conception and performance testing (iii) overall process concept development.
The model developed within this Master thesis will be a key tool to rationalize GREEN-B2B experimental observations and to provide guidelines for the design of the optimal butanediol dehydration catalyst and reactor. The Single-Event MicroKinetic (SEMK) methodology is suggested here as an adequate way to describe the chemocatalytic conversion of different reactants within a single family of components via complex reaction paths. In addition, it will allow determining the kinetic and catalytic descriptors in a kinetic model enabling catalyst and reactor design and optimization[2].

Program

- Development of a Single-Event Microkinetic (SEMK) butanediol isomers dehydration model
- Estimation of the kinetic parameters: kinetic and catalytic descriptors
- Exploitation of the kinetic model aiming at catalyst design, reactor dimensioning and development of a green process concept

[1] Sun, D., Li, Y., Yang, C., Su, Y., Yamada, Y., & Sato, S. (2020). Production of 1, 3-butadiene from biomass-derived C4 alcohols. *Fuel Processing Technology*, *197*, 106193.

[2] Thybaut, J. W., & Marin, G. B. (2013). Single-Event MicroKinetics: Catalyst design for complex reaction networks. *Journal of catalysis*, *308*, 352-362.