LABORATORY FOR CHEMICAL TECHNOLOGY

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Coach	Supervisor(s)	Funding
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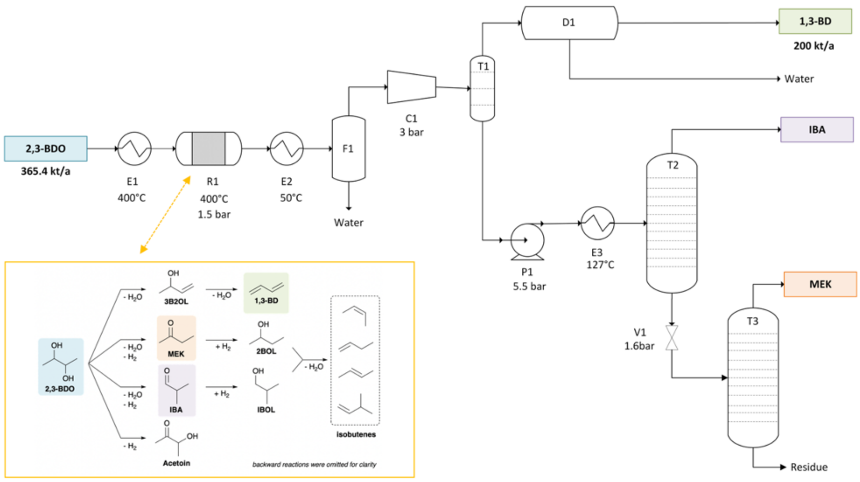
Industrial-scale process design and techno-economic assessment of bio-based 2,3-butanediol dehydration into green 1,3-butadiene

Aim

Development of an integrated process concept in Aspen Plus linked to a detailed kinetic model for the dehydration of biomass-derived 2,3-butanediol to green 1,3-butadiene. The process will be analyzed and optimized guided by the process economics to yield an economically and environmentally viable alternative to the current fossil-based production routes.

Justification

1,3-Butadiene (BD) is a key building block for the polymer industry (17 Mt/a representing 19 billion EUR) and is currently mainly produced as a byproduct of the energy-intensive steam cracking. As there is a tendency to move towards lighter steam cracking feedstocks (e.g., ethane instead of naphtha) 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 BD production processes, preferably from renewable feedstock and with a reduced CO_2 footprint.



2,3-butanediol (2,3-BDO) is a versatile compound and its dehydration into methyl-ethyl ketone (MEK) has been researched extensively [1]. Directing its dehydration pathway towards BD has proven to be quite challenging due to the vast amount of side products which complicate its downstream purification and thereby limit the process' economic viability. However, **recent reports on novel phosphate-based catalysts have changed the scene**, as favorable selectivity profiles (i.e., BD + high-value and easy-to-remove side product(s)) were obtained [2]. To evaluate its industrial potential, a preliminary 200 kt/a process flowsheet (see figure) and a detailed kinetic model are currently being developed in our group.

This master thesis will take the development and optimization of a realistic industrial-scale total process concept to the next level for which the above flowsheet could serve as a basis, if desired. The overall design will contain a user-defined reactor block which links an (external) kinetic model into the process flowsheet and, as such, allows to evaluate the impact of operating conditions and/or alterations of the reactor recycles based on fundamental physicochemical laws. The ambition of this thesis is to **benchmark the overall CO_2 footprint and energy consumption with respect to conventional methods, as well as to determine the minimum butadiene selling price for of a 200 kt/a dehydration plant**.

Program

- Literature study: dehydration of biomass-derived 2,3-BDO to BD
- Overall process design in Aspen plus, steered by integrated kinetic and process simulations to pinpoint the optimal configuration and operating window.
- TEA of the developed process, specifically focused on the industrial viability of the technology

[1] e.g., Nikitina et al. *ChemCatChem* **2016**, 8 , 1346-1353; Penner et al. *Ind. Eng. Chem. Res.* **2017**, 56, 14, 3947-3957.

[2] e.g., Nguyen et al. *Catalysis Today* **2019**, 323, 62-68; Tsukamoto et al, *Chem. Lett*. **2016**, 45, 831-833.

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