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Coach	Supervisor(s)	Funding
Katrien De Gusseme	Joris Thybaut, Alexandra Bouriakova	NEXT-STEP project

Anhydrous mevalonolactone (aMVL) hydrogenation: experimental investigation and modelling of the production of new biochemical platform molecule

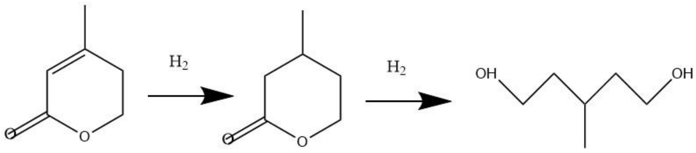
Aim

The aim of the thesis is to investigate and model the kinetics of the hydrogenation reaction of aMLV to 3MdVL and/or the subsequent hydrogenation of 3MdVL to 3MPD based on experimental work in a continuous flow reactor.

Justification

To compete with well-established fossil-based chemicals, research efforts are being directed towards biobased platform chemicals production. The latter not only have to comply with environmental and societal performance but must also be economically viable on an industrial scale. Moreover, key properties with respect to existing petroleum-derived compounds must be maintained, if not exceeded, by potential biobased candidates.

A new chemical platform molecule, i.e. 3-methyl-d-valerolactone (3MdVL), will be investigated within the European NEXT-STEP-project. 3MdVL is produced by the catalytic hydrogenation of aMVL as obtained from fermentation, see scheme below. Depending on the catalyst and operating conditions used, further reaction towards 3MPD may occur. The development of techno-economic and life cycle analyses of 3MdVL and processing routes in which it is involved, requires a profound understanding of the chemical kinetics and catalysis. The overall goal of the NEXT-STEP project is to improve the sustainability of polyurethane (PU) products and unlock new plastic applications for Polylactic acid (PLA) co-polymers. Together with its derivate 3-methyl 1,5-pentanediol (3MPD), 3MdvL can also be used as a biobased polyol in the traditional PU and other plastic production processes



Program

1. Literature survey on (i) the production processes of bio-based platform chemicals, focussing on the current advancements and challenges, and (ii) catalytic hydrogenation of cyclic chemicals
2. Lab-scale experimentation: (i) characterization of selected commercial catalysts (including Pd/C, Ru/C and Pt/C) (ii) assess the long-term performance (and reusability) of catalysts in a continuous flow reactor, (iii) catalyst screening to identify the optimal catalyst achieving a joint selectivity of 95% for 3MdVL and 3MPD.
3. Preliminary kinetic model development

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