LABORATORY FOR CHEMICAL TECHNOLOGY
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Supervisor(s)	**Period**	**Funding**
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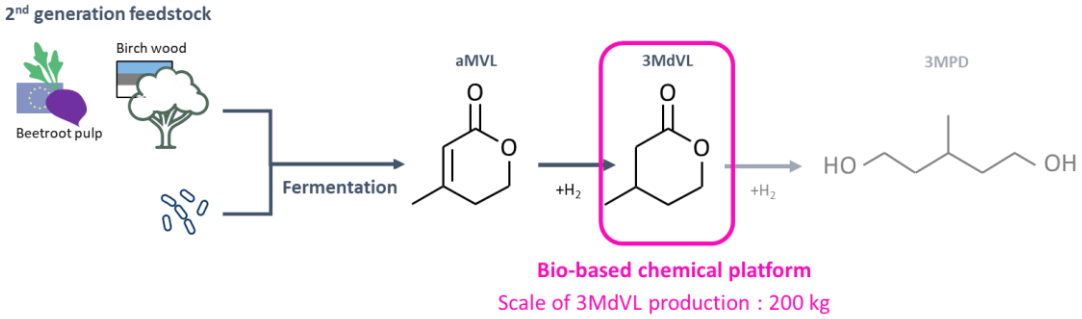
Catalytic production of biobased 3MdVL: experimental assessment, modelling and scale-up

Aim

Develop and validate a fundamental kinetic model to mechanistically describe the catalytic conversion of aMVL into 3MdVL and 3MPD. To that aim, a comprehensive experimental campaign using both in-house synthetized and commercial catalysts is foreseen.

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 NEXT-STEP. It is produced by the catalytic hydrogenation of aMVL as obtained from fermentation, see scheme above. Depending on the catalyst and operating conditions used, further reaction towards 3MPD may occur. 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 is to improve the sustainability and recyclability 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. Laboratory scale experimentation, comprising:
   - synthesis and characterization of different catalysts configurations, including a commercial benchmark CuCr catalyst;
   - evaluation of stability and reusability of the catalysts over time;
2. Kinetics determination in terms of elementary steps.
   - intrinsic kinetics data acquisition
   - microkinetic model development based on a fundamental understanding of the reaction.
3. Evaluate the scalability of the reactions of interest through the construction of a suitable multiscale reactor model, capable of predicting the performance at real operating conditions and, e.g., accounting for potential transport limitations.

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