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Evaluation of Alkyl Levulinate Valorization Routes Using Parallel Fixed Bed Reactor Systems and Data Driven Catalyst Development

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PURPOSE OF THE ABSTRACT

Levulinic acid and its ester derivatives are important building blocks arising from the use of carbohydrate feedstocks in biorefineries of the future.[1] They are both inherent to the production process and potentially valuable as a precursors to other molecules of value.[2]

Hydrogenation of levulinic acid into γ -valerolactone (GVL) has been the subject of numerous studies and patent as a straightforward valorization route.[3] Indeed, GVL has been identified as both a promising bulk chemical, intermediary towards other bulk chemicals or solvent for further biomass valorization.[4]

Hydrogenation of levulinic acid or methyl levulinate involves a complex network of intermediates and side products (scheme). On the other hand, hydrogenation of methyl levulinate has been much less studied.

In this talk, we will present the results of an extensive catalyst screening campaign aimed at optimizing the conversion of a pure side-stream of methyl levulinate into GVL,[5] while keeping key techno-economic considerations in mind such as reactor configuration (fixed-bed, trickle-flow), process conditions, target selectivity (for both GVL and methanol recovery) and catalyst productivity and stability.

Methyl levulinate hydrogenation typically proceeds via the methyl 4-hydroxyvalerate intermediate, instead of the angelica lactone or γ -hydroxyvaleric acid components which are known to be responsible for metal leaching (together with levulinic acid) and coke or tar formation on some supports -- responsible for deactivation and reactor fouling.[6] This means that while the reaction is similarly a two step mechanism, calling for a bi-functional catalyst to perform the hydrogenation and the cyclization, the range of metals and supports, as well as operating conditions (in particular temperature) could be optimized to the use of ML as a reactant, to maximize productivity without negatively affecting the selectivity or the stability (as evidenced in experiments of up to 300 hours on stream).

We will present how parallel, miniature fixed bed catalyst-testing can be used to simultaneously evaluate up to 64 catalysts or process conditions per experiment.[7] High-throughput catalyst testing was combined with an extensive experimental design, to generate valuable screening data which was used in turn to make sequential improvements in catalyst composition. This approach, which has been successfully used in the past to develop and optimize a large variety of catalytic processes, ranging from refining applications, gas-to-liquids and chemicals is applied here as a continuation of our efforts on biomass valorization.[8]

FIGURES

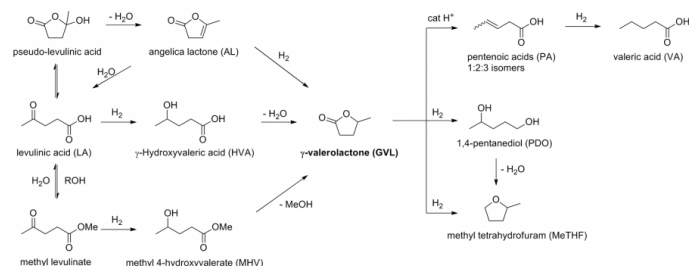


FIGURE 1

reaction scheme

Reaction routes from levulinic acid and methyl levulinate towards g-valerolactone and further side-products

FIGURE 2

KEYWORDS

heterogeneous catalysis | high-throughput experimentation | valerolactone | alkyl levulinate

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