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From sugars to polymers: microkinetic analysis of 2,3-butanediol dehydration into butadiene over Sc-based catalysts

Aim

Understanding and quantifying the dominant reaction pathways in 2,3-butanediol dehydration into butadiene, providing, thereby, guidelines for catalyst and operating conditions optimization.

Justification

Due to the continuously increasing demand for energy and chemicals, while minimizing environmental impact, the search for alternative resources to fossil fuels is more urgent than ever. For instance, consumer goods incorporate significant amounts of polymers which are mainly yielded from light olefins (e.g. ethylene, propylene, butadiene) produced by steam cracking of light naphtha. Furthermore, the shift to lighter feedstock in steam crackers has also reduced the availability of butadiene. Therefore, new alternative production strategies for butadiene need to be investigated.

A highly promising route consists of 2,3-butanediol dehydration to butadiene via 3-buten-2-ol. High butadiene yields (ca. 85%) at full 2,3-butanediol conversion can be achieved over treated Sc_2O_3 , but the catalyst does not seem to be stable [1]. On the other hand, a recent study also showed that an amphoteric alumina is capable of selectively forming butadiene from 2,3-butanediol [2]. According to the authors, kinetics and the presence of water were essential in the conversion to avoid surface condensation (and catalyst deactivation) [2]. The goal is, hence, to understand and quantify the dominant reactions in 2,3-butanediol dehydration into butadiene and provide, thereby, guidelines for catalyst and operating conditions optimization.

Program

Experimental data on 2,3-butanediol dehydration into butadiene at different operating conditions will be first acquired over a Sc_2O_3 benchmark catalyst. These operating conditions will be carefully determined aiming at the acquisition of intrinsic kinetics, i.e. in absence of mass or heat transfer limitations. These data will allow quantifying the dominant factors for high butadiene yield and catalyst stability. A well selected set of complementary screening experiments will be performed on newly synthesized catalysts by the project partner at KU Leuven (e.g. $\text{Sc}_x\text{Al}_y\text{O}_z$ and Sc-doped alumina catalysts).

A detailed kinetic model will be developed, in terms of both physically meaningful and significant kinetic and catalytic descriptors, and then used to determine critical information such as the rate-limiting step, dominant surface species and a reaction pathway analysis [3]. This information will be used to enhance the butadiene yield and ultimately, the reaction system performance can then be further optimized by adapting the reactor process configuration.

[1] H.L. Duan, Y. Yamada, S. Sato, Appl. Catal. A 491 (2015), 163.

[2] D. Sun, S. Arai, H.L. Duan, Y. Yamada, S. Sato, Appl. Catal. A 531 (2017) 21.

[3] K. Toch, J.W. Thybaut, G.B. Marin, Appl. Catal. A 61 (2015) 880.