

Operando spectroscopy to study the deactivation of molecular catalysts in flow and its application for process control

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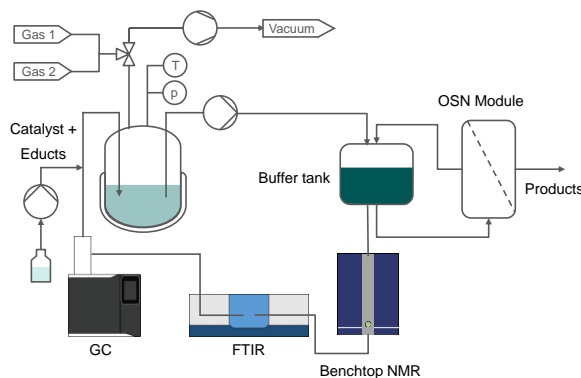
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Abstract

High catalyst stability is an important property necessary for good catalytic performance, especially when continuous processes with physical separation steps are considered.^[1] Catalyst deactivation greatly affects the catalyst performance leading to reduced conversion and selectivity. This can result in varied product streams, reduced reaction, and higher process costs, and in general a reduced process performance.^[2] Studying the catalytic system and understanding the deactivation mechanisms, to then control the reaction conditions before the product quality actually declines, could result in more stable product qualities. Operando spectroscopy is an emerging tool for studying the catalytic system, which utilizes real-time analytical techniques, carried out under reaction conditions.^[3]

In our work, operando spectroscopic techniques are used to investigate the catalytic cycle of hydroformylation of 1-decene, catalyzed by a Rh catalyst complex. For this purpose, a miniplant is set up in which the reaction mixture from the reactor is pumped through the NMR, FTIR and GC. With this operando setup, it is possible to detect unstable intermediates formed during the reaction and thus analyze the catalytic cycle. In this work, the hydroformylation of 1-decene was successfully monitored. In addition, methods for prolonging and restoring catalytic activity are to be developed and used for process control, in order to obtain more stable product streams.



- [1] J. M. Dreimann, E. Kohls, H. F. W. Warmeling, M. Stein, L. F. Guo, M. Garland, T. N. Dinh, A.J. Vorholt, *ACS Catalysis*, 2019, 9 (5), 4308–4319.
- [2] R. H. Crabtree, *Chem. Rev.*, 2015, 115, 127–150.
- [3] K. Köhnke, N. Wessel, J. Esteban, J. Jin, A. J. Vorholt and W. Leitner, *Green Chem.*, 2022, 24, 1951–1972.

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