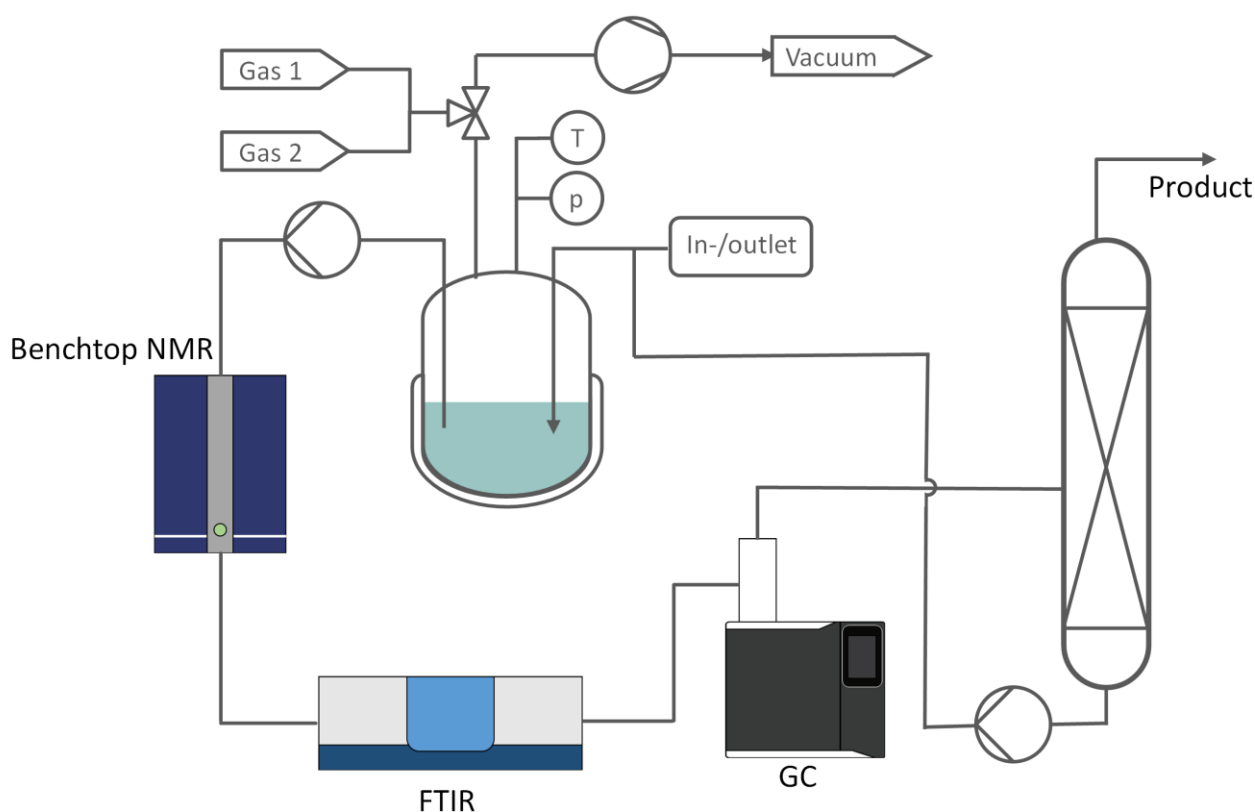


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Operando spectroscopy to investigate molecular catalysts in flowR. Medhekar¹, A. Sobolev², M. Gerlach², C. Hamel², W. Leitner^{1,3}, A. J. Vorholt¹¹MPI Chemical Energy Conversion, Mülheim an der Ruhr, Germany, ²Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany, ³RWTH Aachen, Aachen, Germany

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 Rhodium 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.[4]

**Flowsheet of operando miniplant**

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, different start-up methods were investigated to study their effect on the conversion and selectivity obtained, while simultaneously correlating these effects with the observed catalytic species. Furthermore, the effect of mass transfer limitations on the formed catalytic species, and the resulting selectivity was studied.

In addition, the effect of downstream processing, such as distillation, on the catalyst system are to be investigated, and methods for prolonging and restoring catalytic activity are to be developed and used for process control in order to obtain a stabler continuous process.

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