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High-throughput screening under demanding conditions: Cu/ZnO catalysts in high pressure methanol synthesis as an example

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Abstract

High-throughput experimentation is by now an established technology for the synthesis and evaluation of catalysts. However, so far most of the systems described in the literature for the study of gas-phase reactions have been restricted to less demanding reaction conditions, i.e., atmospheric pressure. We have developed a 49-channel parallel flow reactor for use under elevated pressures up to 5 MPa and used this system to screen methanol synthesis catalysts based on the Cu/ZnO system. The catalysts have been prepared by co-precipitation under various preparation conditions. Catalysts obtained from the same precursors, but showing vastly different performance, were then selected for a more detailed study. Differences in performance could be traced back to differences in phase composition and reduction behavior. This study demonstrates that high-throughput experimentation not only is a suitable tool to screen catalysts, giving little scientific insight—as it is often perceived—but can also be used as a first step to obtaining more fundamental insight by rapidly identifying those compositions which are most suitable for detailed study.

Keywords: High-throughput experimentation; Catalysis; Methanol synthesis; Combinatorial catalysis; Cu/ZnO; Catalyst synthesis; Parallel reactor; EXAFS