

Real Condition High Throughput Screening of CuO/ZnO/Al₂O₃ Catalysts for Methanol Synthesis

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Introduction

Methanol is an important bulk commodity in the chemical industry which is usually manufactured from synthesis gas. Ternary Systems of CuO/ZnO/Al₂O₃ are the most commonly used catalysts in the heterogeneously catalyzed commercial production of methanol.

In order to study the preparation-structure-activity relationship, various CuO/ZnO/Al₂O₃ catalysts were prepared under strictly controlled and defined conditions using the precipitation route.

All catalyst systems were tested in a 49 channel parallel flow reactor setup operating under “real” conditions close to the industrial production of methanol.

Experimental

The CuO/ZnO/Al₂O₃ catalysts were prepared by co-precipitation from aqueous solutions of Cu(NO₃)₂, Zn(NO₃)₂ and Al(NO₃)₃ using Na₂CO₃ as precipitation agent under strictly controlled conditions (pH, temperature, duration of precipitation, aging time and flow rate of the solutions). Corresponding to their activity, some representative selected catalyst samples were studied in detail (TEM, XRD, TG-MS, N₂O-chemisorption and TPR).

The precipitation procedure parameters were changed systematically in order to obtain data for representative plots showing the correlation between catalyst productivity and preparation conditions.

Results

Several sets of co-precipitated catalysts showed strong differences in catalytic productivity corresponding to the changes in the preparation conditions. Especially a substantial correlation between changes in temperature and pH and catalytic performance could be observed. We found an optimal range for preparation conditions to obtain catalysts providing productivities exceeding one of the most commonly used commercial catalyst (*ICI Katalco 51-8*) that was always used as standard benchmark catalyst. The highest catalyst performance (> 130 % of commercial catalyst productivity) was obtained under slightly acid and neutral pH conditions at precipitation temperatures above 60 °C.

XRD measurements of the precipitated precursor phases (hydroxycarbonates and carbonates) and the calcined catalysts were performed. A comparison reveals that residues of non-decomposed carbonates seem to improve the catalyst productivity in methanol synthesis.

TEM pictures of some selected catalysts have revealed the influence of structural properties (particle size and crystallite shape) on the productivity during all periods of catalyst preparation and reaction history.