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Real Condition High Throughput Screening of $Cu/ZnO/Al_2O_3$ Catalysts for Methanol Synthesis

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Abstract

Ternary $Cu/ZnO/Al_2O_3$ catalysts were systematically prepared via the co-precipitation route under strict control of parameters such as pH, precipitation temperature and calcination temperature. All catalysts were tested with respect to their methanol activity in a 49-fold multitubular high-throughput experimentation setup under conditions similar to the commercial methanol production route, using a syngas mixture of CO, CO_2 and H_2.
Statistically representative catalysts were chosen for more detailed structure and morphology analysis in order to study correlations between the catalyst “preparation history” and the methanol productivity.
The highest catalyst performance was observed for catalysts obtained in the pH range from 6 to 8 at 70 °C. XRD measurements allowed the “groupi ng” of catalysts based on their composition. It was found that a group of best-performance catalysts exhibited the characteristic XRD pattern of non-calcined Cu/Zn hydroxycarbonate residues, leading to the assumption that carbonate species in the final catalyst structure may enhance its productivity. Further investigations of these hydroxycarbonate containing catalysts gave more detailed insights into the dynamic aging process and its influence on the catalytic performance. Highest methanol activitiy was observed for catalysts aged between 20 and 60 minutes after an initial phase formation time. The optimum calcination temperature was found to be in the range from 250 to 300 °C. Under these conditions the resu lting Cu/Zn/Al hydroxycarbonates remained stable.
Additionally, the syngas feed composition was varied under reaction conditions and correlated to catalytic activities. Highest methanol productivity over $Cu/ZnO/Al_2O_3$ catalysts was observed for the following gas concentrations; H_2: 50 – 60 %, CO: 30 – 40 % and CO_2: 5-10 % at 4.5 MPa and 245 °C.