Modeling of Temperature-Programmed Desorption (TPD) Flow Experiments from Cu/ZnO/Al2O3 Catalysts

Abstract:
Different procedures to extract the kinetics of hydrogen desorption from a Cu/ZnO/Al2O3 catalyst for methanol synthesis were studied by performing temperature-programmed desorption experiments under atmospheric pressure. The four methods include (i) heating rate variation, (ii) analysis using a fixed pre-exponential factor, (iii) lineshape analysis and (iv) full analysis. Before extracting the parameters, transport limitations could be excluded for all experiments and a criterion for inner particle mass transfer limitations could be extended in the case of activated re-adsorption. All methods could be valid in the whole range of experiments, with only one exception for the lineshape analysis at full coverage of hydrogen. However, each method requires different input to extract physically meaningful parameters. The best modeling results were obtained when repulsive interactions of adsorbed species were accounted for. This led to a k (des) = 3.75 $\times$ 10^10 s^-1 centered dot exp (-(75 kJ centered dot mol^-1)-5.5 kJ centered dot mol^-1) center dot I similar to (H) (2.6) )/RT in good agreement with the literature. Moreover, it was found that there is no difference, when extracting the kinetic parameters from a fresh or deactivated catalyst at full coverage.