Microkinetic modeling of CO TPD spectra using coverage dependent microcalorimetric heats of adsorption

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CO adsorption on the ternary methanol synthesis $Cu/ZnO/Al_2O_3$ catalyst was studied in detail by means of adsorption microcalorimetry and flow temperature-programmed desorption (TPD). Based on these experimental data, we established a microkinetic analysis method, which provides information about the adsorption kinetics of CO on the catalyst surface. Experimentally derived microcalorimetric heats of adsorption were applied in a microkinetic model to simulate TPD curves with varying initial coverage. Two approaches were used: an integral approach based on evaluation of the integral heats of adsorption which predicts the experimental TPD curves roughly and provides first approximations for the preexponential factors. The second, more detailed approach was based on the simulation of the adsorption isotherm taking the experimentally determined coverage-dependence of the heat of adsorption into account. This approach led to a significantly improved agreement between experimental and simulated TPD curves. Moreover, it was possible to derive the standard entropy of adsorption. The general applicability of our approaches is demonstrated by analyzing the CO TPD and microcalorimetry data obtained with a binary ZnO-free Cu/Al_2O_3 catalyst.