Mechanism and kinetic modeling of the liquid-phase cinnamaldehyde hydrogenation

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Abstract

The liquid-phase hydrogenation of cinnamaldehyde (CAL) on copper-based catalysts was studied using pseudo-homogeneous and heterogeneous Langmuir-Hinshelwood-Hougen-Watson (LHHW) kinetics. Three catalysts were used: Cu/SiO_2, which was prepared via incipient wetness impregnation, and Cu-Al and Cu-Zn-Al, which were obtained by coprecipitation. The pattern observed for the activity and selectivity to cinnamyl alcohol (COL) was as follows: Cu-Zn-Al > Cu-Al > Cu/SiO_2. The best fitting using LHHW models was obtained, in all the cases, by assuming total surface coverage. However, and consistent with pseudo-homogeneous analysis, the best fitting for the Cu/SiO_2 and Cu-Al was achieved by considering that CAL is much more strongly adsorbed than products on metal copper sites to yield essentially hydrocinnamaldehyde (HCAL). In contrast, the best model for the Cu-Zn-Al catalyst considers that (i) the adsorption strength values of CAL, HCAL, and COL on the catalyst surface are similar; and (ii) CAL is adsorbed on two different types of active sites (specifically, CAL adsorbs on Cu^0 to form HCAL and on the $Cu\text{-}Zn^{2+}$ interface sites to produce essentially COL). The modeling of catalytic data using LHHW kinetics and the estimated parameters allowed for interpretation of the reasons for the higher COL formation rate observed on Cu-Zn-Al catalyst, in comparison to Cu/SiO_2 and Cu-Al catalysts.

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