Hydrodeoxygenation of Acetic Acid Using Monometallic and Bimetallic Catalysts Supported on Carbon

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Abstract

Heterogeneous catalytic hydrodeoxygenation (HDO) of biomass-derived feeds is a deoxygenation process that is of highly interest. Carboxylic acids are one of the main components of bio-oils and acetic acid (AA) is one of the most abundant of these carboxylic acids. This acid is rich in oxygen, therefore there is a lot of research for to produce fuel and other valuable chemicals such as ethanol.

We investigated heterogeneous catalysis for the HDO of AA using supported group noble metals. Temperature-dependence selectivity and activity were evaluated in a conventionally continuous plug-flow reactor operated between 200-400°C under atmospheric pressure with concentrations of 1.1% AA/20% H₂/balance in He. The activity and kinetics involving the reaction rate orders with respect to AA and H₂ and apparent activation energies were discussed in detail. Several pathways were found when using monometallic catalysts such as: decarbonylation, decarboxylation, hydrogenation and ketonization. For the bimetallic catalyst the main pathways at low temperatures was hydrogenation. Also, on a different project phosphorous nickel phosphide (Ni₂P) is investigated. This material is being used in the HDO reaction of different carboxylic acids. The focus of this work is to investigate (P) diffusion in bulk Ni₂P by density functional theory (DFT) to find the origin of the low temperature P diffusion into the surface.

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