

Insights into Hydrodeoxygenation of Furfural and Guaiacol Mixture: Experimental and Theoretical Studies

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Abstract

Catalytic hydrodeoxygenations of furfural, guaiacol, and their mixture at different concentrations were carried out over a Ni/SiO₂ catalyst to study the kinetic and competitive effects. Anisole was also studied to compare with the effects of guaiacol. Additionally, kinetic parameters were adjusted through mathematical modeling to explain the mixture behavior, and density functional theory (DFT) simulations were carried out to study the effect observed in the present work. The use of guaiacol and anisole in the mixture produces an increase in the reaction rate of furfural. Furthermore, guaiacol slightly generates a change in the selectivity of furfural products, attributed to its hydroxyl group, as such a change was not observed with anisole. DFT studies showed that the hydrogen atom of the hydroxyl group of guaiacol migrated to furfural. Both effects would be enhanced by increasing the guaiacol concentration, which could act as a stabilizing agent inhibiting the coke formation in the furfural reaction.

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