

Solution-phase Adsorption of Furan and Carboxylic Acid in Hierarchical Zeolites: Insights from Molecular Simulation

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ABSTRACT

Oleo-furans¹ are a novel class of bio-renewable surfactants with superior hard-water stability compared to petroleum-derived surfactants. During their synthesis, sugar-derived furans react with triglyceride-derived fatty acids via acid-catalyzed acylation. Their synthesis is promoted by hierarchical zeolites, such as self-pillared pentasil (SPP) zeolites², which combine microporous and mesoporous functionalities to perform selective catalysis and accommodate diffusion of large molecules.

To improve fundamental understanding and enable improvements in catalyst and process design, the co-adsorption of furan, hexanoic acid, and various solvents from solution into SPP was investigated using Monte Carlo simulations in the Gibbs Ensemble. Solution composition and reaction conditions significantly affect adsorption selectivity, as well as the distribution of species in the meso- and micropores of SPP. Silanols on the surface of SPP strongly hydrogen bond with hexanoic acid, promoting selective adsorption of acid from the solution phase onto the mesopore walls, while furan and hexane solvent are more evenly distributed throughout the mesopore and micropore volumes. The influence of several process variables on the adsorption selectivity and spatial distribution in the zeolite was also investigated, including solution composition, pressure, and the chain length and degree of branching of the solvent,.

References

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