114d Alkylation of Deactivated Aromatic Compounds Using Zeolites

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Currently, Friedel-Crafts alkylations are performed with corrosive Lewis acids such as AlCl3 or BF3. The inconveniences encountered with these homogeneous catalysts are a difficult catalysts recovery, corrosion of the working apparatus and toxic wastes. Therefore, substitution of these homogeneous catalysts with cleaner heterogeneous catalysts such as zeolites is desirable. However, use of heterogeneous catalysts invokes, besides a different catalytic behavior, important adsorption and deactivation effects. In the present work, a study is made of adsorption, kinetic and deactivation effects in the liquid phase alkylation of deactivated aromatic compounds on zeolites. Such reactions produce important intermediates for the chemical and pharmaceutical industry. The alkylation of bromobenzene with allyl acetate was studied on a range of faujasite zeolites with different Si/Al ratio, using a high-throughput frontal analysis setup. The effect of reaction temperature, feed composition and contact time was determined. The reaction products could be divided into 3 fractions: (1) light components, formed in side reactions of the alkylating agent (2) primary alkylation products, resulting from the alkylation of bromobenzene or toluene and subsequent rearrangement reactions (3) a heavy fraction, consisting of secondary alkylation products and polyaromatics. Significant catalyst deactivation occurred in these reactions, which is attributed to pore blocking by very strong adsorption of side products in the zeolite micropores. Based on the experimental data, several molecular kinetic models were proposed, and implemented in a reactor model, accounting for axial dispersion, mass transfer into the catalyst crystals, competitive adsorption effects and catalyst deactivation. Model discrimination revealed the underlying reaction mechanisms. Based on the reaction model, reaction conditions were optimized for the best performing catalyst.