Kinetics, Mechanism and Simulation of Hydrogen Transfer Reaction of α, β-Unsaturated Aldehydes to Allylic Alcohols

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Abstract

Homogeneous hydrogen transfer reactions of methacrolein (MAL) and isopropanol (IPA) to methallyl alcohol (MAA) were investigated in batch reactor (Conv.89%, Select 93.1%) and tubular reactor (Conv.88.1%, Select 95%) using aluminum isopropoxide (Al(OPri)3) as catalyst. Kinetic experiments on hydrogen transfer reactions and reaction order were investigated in batch reactor and tubular reactor. Response surface methodology (RAM) was applied to optimize the optimum reaction conditions of hydrogen transfer reaction. Purification process of MAA from product mixture after hydrogen transfer reaction was simulated with Aspen Plus software, theoretical stages, reflux ratio and feed stage of distillation tower were optimized. Density Functional Theory (DFT) was used to investigate viable reaction pathway and to probe the catalytic mechanism between reactants and catalyst, including dehydrogenation, coupling and hydrogenation reaction. Microscopic mechanisms of hydrogen transfer reaction from MAA to MAL were acquired in detail and could be easily extended to other series of hydrogen transfer reaction.

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