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Conversion Improvement for Catalytic Synthesis of Propylene Glycol Methyl Ether Acetate by Reactive Chromatography: Experiments and Parameter Estimation

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Abstract

As an industrial case study, esterification of acetic acid with 1-methoxy-2-propanol using a cation exchange resin has been investigated using a well-stirred batch reactor and chromatographic reactor. Well-stirred batch reactor experiments were conducted over different operating conditions to analyze the reaction equilibrium and kinetics. It was found that the final conversion was limited by equilibrium, and temperature had no significant effect on increasing the final conversion. Parameters in a reaction rate model were obtained at different temperatures (50°C-90°C). Since the well-stirred batch experiment alone was not enough to capture the adsorption behavior of the system, pulse injections of each component into the chromatographic column were conducted to obtain the adsorption parameters. The esterification reaction was performed systematically in a lab-scaled chromatographic reactor at different flow rates (0.2ml/min-1ml/min), injection volumes (0.05ml, 0.5ml), and temperatures (70°C-110°C). A mathematical model for isothermal equilibrium dispersive model was implemented and parameters were determined by fitting the model to the experimental data. It was observed that when the injection volume of single component was too large, two reaction sites were formed inside the column, resulting in a deformed peak shape of the product in the outlet chromatogram. Nearly 100% of conversion, which was infeasible in the well-stirred batch reactor, was achieved when the flow rate was low and the injection volume was small. The results indicate that the chromatographic reactor enhanced the reaction beyond the equilibrium by separating the products from the reaction sites.

Nomenclature

AA	acetic acid
b	constant in Langmuir isotherm (L/mol)
c	liquid phase concentration (mol/L)
E_a	activation energy (kJ/mol)

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