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催化、动力学与反应器

001×7（732）阳离子交换树脂催化醋酸甲酯水解反应过程模拟与优化

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摘要

在充分搅拌和可忽略粒度影响条件下，测定了间歇搅拌反应釜中001×7（732）阳离子交换树脂催化醋酸甲酯水解反应动力学数据，建立了其拟均相与非均相反应动力学模型，进行了模型筛选和参数估值。结果表明，醋酸甲酯与水均吸附，表面反应为控制步骤的非均相反应动力学模型能较好地拟合实验数据，并满足统计检验。根据优选的反应动力学模型，对醋酸甲酯水解过程进行了模拟计算，考察了反应温度、树脂浓度、水酯摩尔比对水解过程的影响，得到的优化反应条件为：反应温度55℃、树脂浓度260 $g \cdot L^{-1}$ 、水酯摩尔比1.5∶1。此时反应90 min接近醋酸甲酯平衡水解率34.8%。

关键词

阳离子交换树脂 醋酸甲酯 水解 反应动力学模型 模拟与优化

分类号

Simulation and optimization of methyl acetate catalytic hydrolysis with 001×7(732) cation-exchange resin

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Abstract

The hydrolytic kinetics experiments for methyl acetate with 001×7(732) cation exchange resin were carried out in a batch fully stirred reactor in the ranges of 40—55℃ of reaction temperature, 100—600 $g \cdot L^{-1}$ of catalyst concentration and 0.5∶1—9.0∶1 of molar ratio of water to MeOAc, while the effect of resin particle size was neglected Based on some experimental phenomena and absorption characteristics of some components on catalytic sites in the process of hydrolysis reaction, one pseudo homogeneous and two heterogeneous hydrolytic kinetic models were established, and the parameters were estimated based on experimental data An optimal heterogeneous hydrolytic kinetic model, which showed good agreement with the experimental data, was obtained The optimal model was based on the proposed mechanism that both methyl acetate and water were absorbed on catalytic sites and the surface reaction was the rate controlling step Some operational parameters of methyl acetate catalytic hydrolysis with 001×7(732) cation exchange resin were optimized through the simulation calculations based on this model The obtained optimal values were as follows: 55℃ of reaction temperature, 260 $g \cdot L^{-1}$ of catalyst concentration and 1.5∶1 of molar ratio of water to MeOAc Under the conditions of the optimized operation parameters, the hydrolytic conversion of methyl acetate reached 34 8% close to the equilibrium hydrolytic conversion after 90 min of the hydrolysis reaction.

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Key words

cation-exchange resin methyl acetate catalytic hydrolysis kinetic model simulation and optimization

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