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催化、动力学与反应器

Pd/C上松香催化歧化反应集总动力学

王琳琳[1]； 李丽明[2]；陈小鹏[3]； 蒲小东[2]；童张法[1]

广西大学化学化工学院[1]

广西大学化学化工学院精细化工教研室[2]

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摘要 以松香为原料、改性Pd/C为催化剂、200#油为溶剂及N 2为保护气，进行松香催化歧化反应集总动力学的研究。在消除内外扩散影响的条件下，在线跟踪48315～53315 K的反应产物并用毛细管柱气相色谱法测定反应体系组成随时间的变化关系。根据松香歧化反应机理和特点，借鉴集总思想和方法，按结构族组成和动力学相近原则划分该复杂反应体系的集总组分，构建了Pd/C上松香歧化集总反应网络，建立了枞酸型树脂酸、海松酸型树脂酸、氢化枞酸型树脂酸、氢化海松酸型树脂酸和脱氢枞酸五集总动力学模型；采用Levenberg-Marquart法，以Matlab编程和SPSS数理统计软件估算了模型参数，得到枞酸型树脂酸脱氢、加氢，海松酸型树脂酸加氢反应过程的活化能分别为11139 kJ·mol-1、10876 kJ·mol-1、9735 kJ·mol-1，结果表明，所建动力学模型与实验数据吻合良好，并能预测反应在54315 K的集总组分浓度分布。

关键词 松香 催化歧化 集总动力学

分类号

Lumping kinetic model for catalytic disproportionation of rosin on Pd/C

Abstract

The lumping kinetic model for catalytic disproportionation of rosin in 200# solvent naphtha on modified Pd/C was investigated in nitrogen atmosphereThe reaction products at 48315—53315 K were tracked by online analysis with capillary gas chromatographAccording to the reaction mechanism and characteristics of catalytic disproportionation of rosin，the lumped components of the complex reaction system were defined and a reaction network was proposedThe five lumping kinetic models of abietic type resin acid，pimarenoic acid type resin acid，hydrogenated abietic type resin acid，hydrogenated pimarenoic acid type resin acid and dehydroabietic acid were established based on structural group and approximate reaction kinetic theory according to the fundamental principles of lumping methodThe kinetic model parameters were estimated with the Levenberg-Marquart method by programming Matlab and SPSS statistics software，and the activation energies were 11139 kJ·mol-1，10876 kJ·mol-1，9735 kJ·mol-1 for abietic type resin acid hydrogenation and dehydrogenation and pimarenoic acid type resin [JP3]acid hydrogenation respectivelyThe final results demonstrated that the lumping model could characterize the kinetic behavior of the complex reaction and predict the concentration distribution of the multi-products at 54315 K.

Key words rosin catalytic disproportionation lumping kinetic model

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通讯作者 童张法 bioche@gxu.edu.cn;zhftong@sina.com