化工学报 2004 55 (4): 593-597 ISSN: 0438-1157 CN: 11-1946/TQ

催化、动力学与反应器

对硝基苯胺臭氧化反应动力学和吸收过程模拟

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收稿日期 2003-1-13 修回日期 2003-6-3 网络版发布日期 2008-9-1 接受日期

摘要 采用停流光谱法研究了T=298 K，pH=2.1～6范围内对硝基苯胺与臭氧在水溶液中的臭氧化反应动力学.研究结果表明，降解1 mol的对硝基苯胺需要4 mol臭氧，对硝基苯胺臭氧化总的反应是二级，对臭氧浓度和对硝基苯胺浓度分别为一级.臭氧化反应速率常数随溶液pH值的增大而加快:在T=298 K时，当pH值从2.1变化到6，总的反应速率常数从6.17×10^{4} (mol•L^{-1})$^{-1}$•s^{-1}增大到1.55×10^{6}(mol•L^{-1})$^{-1}$•s^{-1}.为了验证其适用性，进行了臭氧在搅拌釜中在对硝基苯胺溶液中吸收过程的模拟.采用Matlab软件求解吸收过程的质量平衡方程，模拟了吸收过程中臭氧和对硝基苯胺浓度的变化，并与实验值进行了比较.结果表明，在80%的对硝基苯胺降解之前，模拟值和实验值能很好地一致.

关键词 臭氧化 对硝基苯胺 反应动力学 反应速率常数 模拟

分类号

KINETICS AND SIMULATION OF OZONATION OF *p*-NITROANILINE IN AQUEOUS SOLUTIONS

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Abstract

The stopped-flow spectrophotometric method was used to study the kinetics of the ozonation between dissolved ozone and *p*-nitroaniline in aqueous solutions of pH values varying from 2.1 to 6 at 298 K. It was found that four moles of ozone were required for conversion of each mole of *p*-nitroaniline in the aqueous solution containing a limited amount of dissolved ozone. The overall ozonation reaction of *p*-nitroaniline was of second order, but of first order for each reactant.The overall ozonation rate constant increased with solution pH value in the range of 2.1 to 6 investigated. As pH value increased from 2.1 to 6, the overall rate constant increased from 6.17×10^{4}(mol•L^{-1})$^{-1}$•s^{-1} to 1.55×10^{6}(mol•L^{-1})$^{-1}$•s^{-1} at 298 K. To validate its applicability, the absorption process was simulated as ozone absorption in *p*-nitroaniline solution in stirred-tank. The mass balance equations about absorption process for the complete mixing model were solved by utilizing the Matlab ODE program. The concentration of ozone and the concentration of *p*-nitroaniline during an absorption experiment were simulated. The simulated concentrations of *p*-nitroaniline agreed well with the measured concentrations up to 80% consumption of *p*-nitroaniline.

Key words ozonation *p*-nitroaniline reaction kinetics rate constant simulation

DOI:

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