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催化、动力学与反应器

# TS-1催化环己酮氨氧化反应本征动力学模型

赵虹, 周继承

湘潭大学化工学院,湖南 湘潭 411105

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摘要 由TS-1催化环己酮氨氧化反应机理出发，分析了反应过程的特点及反应规律，根据推测的机理，建立了反应本征动力学模型. 结合搅拌釜中测得的动力学数据，对动力学模型进行了参数估值及模型筛选. 结果表明，假设反应合乎羟胺机理、双氧水吸附、表面反应为控制步骤时所导出的模型能较好地拟合实验数据，并满足统计检验. 根据该动力学模型，通过模拟计算对部分操作条件进行了分析和优化.

关键词 钛硅分子筛 环己酮 反应机理 本征动力学

分类号

# KINETIC MODEL OF CYCLOHEXANONE AMMOXIMATION CATALIZED BY TITANIUM SILICALITE-1

ZHAO Hong,ZHOU Jicheng

**Abstract**

The intrinsic kinetics of TS-1 catalyzed cyclohexanone ammoximation with hydrogen peroxide in water was studied. The kinetic reaction was carried out in a semi-batch stirred-tank reactor at 333.15—348.15 K. Two models from proposed mechanisms were regressed. The results obtained showed that the hydroxylamine mechanism fitted the experimental data better. The hydroxylamine mechanism proposes that hydrogen peroxide molecule is absorbed on the catalytic sites and reacts with ammonia first, and surface reaction is the rate-controlling step. Hydrogen peroxide can also decompose and compete with cyclohexanone ammoximation. So it is advisable to take measures to restrain hydrogen decomposition. After parameters estimation and model discrimination, a rational model, which showed good agreement with the experimental data,was obtained. Based on the model, some operation parameters were analyzed and optimized through simulation and calculation.

**Key words** titanium silicalite-1 cyclohexanone reaction mechanism intrinsic kinetics

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通讯作者 赵虹 yehongzh@yahoo.com.cn