催化、动力学与反应器

用于甲苯歧化与C$_9$芳烃烷基转移过程先进控制的反应动力学模型

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摘要　　针对某实际工业装置，建立了甲苯歧化和C$_9$芳烃烷基转移反应简化机理模型，用于反应过程的监控、优化及大型轴向流反应器内各物料组成分布的预测；采用四-五阶Runge-Kutta法对模型方程进行了数值求解，并基于多套稳态平衡数据，采用Broyden-Fletcher-Goldfarb-Shanno(BFGS)优化算法对动力学模型参数进行了估计；针对不同的进料组成和操作条件，对工业装置进行模拟仿真。结果表明，模型估计值与工业标定值相当吻合，达到了工业应用的模拟精度要求。所建立的模型形式简单、参数估计方便，适用于工业装置的离线仿真和在线软测量。

关键词　　甲苯；C$_9$芳烃；歧化；烷基转移；机理模型；离线拟合；在线软测量

分类号

A kinetic model for advanced process control of toluene disproportionation and transalkylation with C$_9$-aromatics

Abstract

To monitor and optimize the operation and to predict the concentration profiles of the components in commercial units for toluene disproportionation and transalkylation with C$_9$-aromatics, a kinetics-based mathematical model was developed and solved by the widely used Runge-Kutta algorithm.Based on several sets of operation data obtained from a commercial unit at steady state, the reaction kinetic parameters involved were estimated by the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method.The kinetic model was also validated by the data from the commercial-scale unit operated with different feedstock compositions and operation variables.The results showed good agreement between the model predictions and plant observations, signifying that the proposed model could be applied to both offline simulation and online soft sensors.

Key words　toluene　C$_9$-aromatics　disproportionation　transalkylation　kinetic model　offline simulation　online soft sensors

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