

催化、动力学与反应器

## 长链烯烃与苯烷基化外扩散影响的数学模拟

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摘要

在一定粒度的固体酸催化剂上进行不同反应原料质量流速的烷基化反应实验, 通过模型参数估值及模型预测分析, 建立评价外扩散阻力影响程度的外扩散有效因子数学模型。在此基础上考察外扩散阻力对烷基化反应的影响规律, 确定消除外扩散阻力影响的实验条件。模型预测结果表明, 计算值与实验值吻合较好。在一定的反应条件下, 随着流体质量流速的增大, 外扩散有效因子先快速增大然后缓慢趋于1; 随着烷基化反应时间的延长, 外扩散有效因子持续增大; 随着烷基化反应速率的提高, 消除外扩散阻力影响的流体质量流速相应有所增大。当流体质量流速达到 $4.0 \text{ g} \cdot \text{cm}^{-2} \cdot \text{h}^{-1}$ 时可消除外扩散阻力影响。

关键词

[固体酸催化剂](#) [烷基化](#) [数学模拟](#) [外扩散阻力](#)

分类号

## Mathematical simulation of external diffusion effect on benzene alkylation with long-chain olefins

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### Abstract

A kinetic model involving effectiveness factor of external diffusion was proposed based on the experimental data on the benzene alkylation with long-chain olefins over solid acid catalyst at different mass flow velocities. The model can be used for the determination of experimental conditions at which the resistance of external diffusion was eliminated. The model parameters were evaluated, and the model was justified by variance analysis and residual analysis. The agreement between the prediction values by the kinetic model and experimental data was satisfactory. The results showed that the external diffusion factor went up with increasing mass flow velocity sharply at first, then approached 1 slowly. When the reaction time was prolonged, the external diffusion factor increased continuously. If the alkylation rate increased, the weight hourly space velocity required for eliminating the influence of external diffusion raised. The results indicated that the effect of external diffusion for the benzene alkylation with long-chain olefins over solid acid catalyst could be eliminated when the mass flow velocity was  $4.0 \text{ g} \cdot \text{cm}^{-2} \cdot \text{h}^{-1}$ .

### Key words

[solid acid catalyst](#) [alkylation](#) [mathematical simulation](#) [external diffusion](#)

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