### 传递现象

# 基于Simha-Somcynsky状态方程的高分子-溶剂体系扩散系数模型

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摘要 将Simha-Somcynsky状态方程引入到Vrentas-Duda扩散系数模型,建立基于状态方程的溶剂在高分子中扩散系数模型。与原模型相比,改进的模型避免进行高分子的黏弹性实验测定,模型中高分子的相关参数仅由状态方程的特征温度和特征体积确定,提高了模型的预测能力。对苯、甲苯、乙苯、氯仿在聚苯乙烯、聚异丁烯和聚醋酸乙烯酯中的扩散系数计算结果表明,改进模型的预测值与实验值吻合较好。

关键词 高分子 溶剂 扩散系数 状态方程

分类号

# A diffusion coefficient model for polymer-solvent systems based on Simha-Somcynsky equation-of-state

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#### **Abstract**

With the introduction of the Simha-Somcynsky (SS) equation-of-state (EOS) into the Vrentas-Duda model, a modified diffusion coefficient model based on the EOS was developed for polymer-solvent systems. In the modified model, the measurement of polymer viscoelasticity was not required, and the parameters related to the polymer could be determined solely by the characteristic parameters of temperature and volume in the SS EOS. Therefore, it has better predictive capability compared with the original model. The calculated diffusion coefficients of benzene, toluene, ethylbenzene and chloroform in polystyrene, polyisobutylene and poly (vinyl acetate) indicated that predictions of the modified model were consistent with the experimental results.

Key words polymer solvent diffusion coefficient equation-of-state (EOS)

DOI:

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