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过程系统工程

PET固相缩聚反应器动态模型

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摘要

PET固相缩聚过程涉及反应固体颗粒和反应器床层两个空间尺度的传质，是一个复杂的多维多相对象。以反应过程控制为目标，在已有的反应动力学模型基础上，同时考虑可逆化学反应和小分子产物内外扩散两个控制因素，并借用固定床拟均相模型的建模思想，将小分子产物在颗粒内外扩散形成的浓度梯度用一个有效系数来表示，从而建立了简化的PET固相缩聚反应器一维动态模型。在相关文献的实验条件下求解分布参数模型的数值解，并进行启动过程仿真和过程动态分析，计算反应器出口质量指标，与文献曲线和数据对照，验证了模型的正确性。

关键词 固相缩聚 分布参数 拟均相 动态模型

分类号

Dynamic model of PET solid-state polycondensation reactor

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Abstract

PET solid-state polycondensation process involves spatial mass transfer of both solid reaction particles and reactor bed, which is a multi-dimensional and multi-phase objective. Aiming at reaction process control, a simplified one-dimensional dynamic model of PET solid-state polycondensation reactor based on existing reaction kinetics models was developed. The model emphasized not only reversible reactions, but also the diffusion of small molecular products inside and outside the particles. It approximated the concentration gradient of small molecular products due to diffusion with an effective coefficient, which borrowed the idea of pseudo-homogeneous fixed bed reactor model. Finally with the experimental data reported in the literature the paper numerically solved the distributed parameter model, which were partial differential equations, and analyzed the dynamic reaction process to get concentration profiles and product quality indices values, which were compared with the data in the literature to show the effectiveness of the developed model.

Key words

solid-state polycondensation distributed parameter pseudo-homogeneous dynamic model

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