

RESEARCH PAPERS

7-氨基去乙酰氧基头孢菌素半间歇反应结晶过程

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摘要 Semi-batch crystallization of 7-amino-desacetoxycephalosporanic acid (7-ADCA) is a complicated process, in which agglomeration occurs together with nucleation and crystal growth. To systematically study such a process, experiments were conducted to estimate the crystallization thermodynamics and kinetics, and then the process was simulated by a numerical method. The application of Monte Carlo concept in the algorithm to describe agglomeration event offers an alternative approach of solving the population balance, the intrinsic simplicity of which allows us to investigate several mechanisms and include several internal coordinates in the analysis. Furthermore, present study may be a valuable paradigm for other semi-batch crystallization processes.

关键词 [7-ADCA](#) [thermodynamics](#) [kinetics](#) [agglomeration](#) [Monte Carlo simulation](#)

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Semi-batch Crystallization of 7-Amino-Desacetoxycephalosporanic Acid

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Abstract Semi-batch crystallization of 7-amino-desacetoxycephalosporanic acid (7-ADCA) is a complicated process, in which agglomeration occurs together with nucleation and crystal growth. To systematically study such a process, experiments were conducted to estimate the crystallization thermodynamics and kinetics, and then the process was simulated by a numerical method. The application of Monte Carlo concept in the algorithm to describe agglomeration event offers an alternative approach of solving the population balance, the intrinsic simplicity of which allows us to investigate several mechanisms and include several internal coordinates in the analysis. Furthermore, present study may be a valuable paradigm for other semi-batch crystallization processes.

Key words [7-ADCA](#); [thermodynamics](#); [kinetics](#); [agglomeration](#); [Monte Carlo simulation](#)

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