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Quantitative Design of Seed Load Based on Model Identification of Nucleation and Crystal Growth Stages without Transmittance Data

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¹ Department of Pharmaceutical Engineering, China Pharmaceutical University, Nanjing 210009, P. R. China ² Department of Energy and Mechanical Engineering, Nanjing Normal University, Nanjing 210042, P. R. China Abstract: How to quantitatively design the loading time and amount of seed is a critical problem in the seeded crystallization process. In this study, correlations for different moment of crystal size distribution (CSD) function were established by subsection induction. By using the established different moment of CSD function, a new algorithm for kinetic model that can estimate the nucleation and growth kinetic parameters was proposed. Compared with kinetic model based on the conventional moments method, the new algorithm has a great significance since the overall heat transfer coefficient U is no longer necessary in the entire calculation. Using experimental data from literature, kinetic parameters of crystallization of KNO₃ aqueous solution and xylene solution were estimated by the new algorithm, which are in good accordance with those fitting with moments method. This agreement shows the feasibility of the new algorithm. Finally, since it is difficult to measure transmittance data r of some systems, a criterion K that can identify nucleation and crystal growth stages without transmittance data was established. By means of the K curve of para-xylene (PX) and vitamin C, which is based on kinetic simulation results from the new algorithm and different moment of CSD function established by subsection induction, the single step seed load and two steps seed load were designed, respectively.

Keywords: Seeded crystallization; Crystal size distribution (CSD); Kinetic analysis; Different steps seed load; Unknown transmittance data

1. Introduction

Solution cooling crystallization is a widely used separation technique in many chemical, pharmaceutical, petrochemical and food industries. However its operation is difficult to optimize due to the complicated process mechanism. The main difficulty in solution cooling crystallization is to produce a uniform and reproducible CSD. It has been addressed by the approaches proposed in the literature such as optimized cooling profile and controlled supersaturation degree of system [1-3]. Among these solutions, the method of loading seeds is highly effective and thus broadly applied in the industry. Unlike unseeded crystallization, the seeded crystallization process usually has lower nucleation rate and better CSD of products [4, 5], because most of solute molecules in solution can be precipitated on the seed surfaces when seeds are loaded.

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