315h Choosing an Objective Function for Seeded Batch Crystallization

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Determination of the optimal temperature (or supersaturation) trajectory for a seeded batch crystallizer is one of the most extensively studied continuous optimization problems in chemical engineering. Beginning with the pioneering work of Jones (1974), more than a dozen researchers have used a variety of techniques (including sequential quadratic programming, optimal control, and stochastic methods) to determine the optimal trajectory.

The majority of researchers have found that the optimal temperature trajectory is one which leads to an increase in supersaturation near the end of the batch (here termed "late growth"), and this has been suggested as a generally valid heuristic (Wibowo et al., 2001). However, a significant minority of researchers has found a result which in some sense is almost exactly opposite: that the optimal policy is to have an increased supersaturation at the beginning of the batch (here termed "early growth"). Still other researchers have indicated that, at least to a first approximation, the optimal way to operate a seeded batch crystallizer should be with constant supersaturation. In spite of the large number of publications in this field, these discrepancies apparently remain unresolved.

In this work we show that these discrepancies result from the different objective functions considered by different researchers. We further demonstrate that the qualitative nature of the optimal supersaturation trajectory (early growth or late growth) can be predicted for any given objective. Specifically, objectives that involve low moments (0-2) of either the nucleus-grown crystals or the total crystal population lead to early growth policies, whereas objectives involving only properties of the seed-grown crystals or the higher moments of the total crystal population (3-5) lead to late growth operating polices.

To support our conclusions, we present (1) a concise and comprehensive literature review, (2) results obtained by driving the population balance model with a series of pre-determined supersaturation trajectories, and (3) results obtained from the optimization of a case study process with a variety of different objective functions. The mathematical model used in (2) and (3) is based on a case study adapted from Chung, et al. (1999) on the crystallization of potassium nitrate from water.

References:

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