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Optimal control of batch cooling crystallizers by using genetic algorithm

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ABSTRACT

The formation of crystals from solutions plays a key role in various industrial applications. In this study, a new approach is presented into the optimal control of batch cooling crystallizers through a genetic algorithm. The Population balance is formularized for a typical batch crystallizer. The objective functions considered here are related to quality of products at the end of the batch. These functions are objective function of maximum mean weight size, closeness to the specified value and minimum coefficient of variation. By using an optimization algorithm (genetic algorithm), the minimum and maximum values of the objective function the input temperature parameter are obtained. The obtained results show that various trajectories can be used for cooling batch crystallizer based on objective functions. This method is applied for the potassium-nitrate system.

1. Introduction

Crystallization of organic and inorganic substances in solutions is one of the essential processes in different industrial applications including chemical, electronics and pharmaceutical industries [1–3]. This process provides highly purified products that are highly demanded by a noticeable fraction of industrial markets. In addition, crystallization presents a practical method for obtaining pure chemical substances in a satisfactory condition for packing and storing [4,5]. In the chemical engineering process, this method gains great advances except in some aspects such as the overall control on the temperature of crystallites to obtain the appropriate shape and size of particles [6,7]. Although high purity of products seems an important objective in the crystallization, the appearance and size of a crystalline product is also significant parameters. The reasonable size and size uniformity are desirable for filtering, washing, reacting, transporting and storing of the crystals [8]. As the crystals are processed further in optimized temperature, the size of the particles becomes uniform in the whole solution [9]. If the crystals are a final product of marketing, crystals with strong, non-aggregated, uniform in size, and non-caking is highly important in the packing. For these reasons, crystal size distribution (CSD) must form under a precise temperature control. In fact, the appropriate temperature control plays a significant role in the design and operation of crystallizers [10].

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Nomenclature

A	hear transfer surface
B	nucleation rate, number/g-solvent min
b	nucleation power
C	concentration of solute, g/g-solution
C_{0i}	nitial concentration
C_{sat}	saturated solution, g/g-solution
C_p	heat capacity of solution J/(kg. K)
f	population density function
G	growth rate, m/min
g	growth power
$\hat{H}_*$	partial molar enthalpy
$\hat{H}$	specific enthalpy
H_{ext}	exited heat flux
K_E	kinetic energy
k_b	nucleation coefficient
k_g	growth coefficient
k_v	volumetric shape factor
L	crystal size (m)
L_{wm}	mean weight size
m	crystal mass
n	number of moles
P	pressure
P_E	potential energy, J
Q	volume floe rate
S	super saturation
t	time
T	temperature
U	heat transfer coefficient
V	volume of crystallizer, m^3
w	Gaussian function weight

Greek symbols

ρ	density (g/ cm3)
δ	*Dirac function*
μ_j	j-th moment of the CSD
σ	standard deviation
σ^2	variance

Subscripts

k	index of flow
c	crystal

To obtain these goals, the batch reactors (crystallizers) have to be operated optimally in a precise condition. Hence, the main problem on the control of batch crystallizer is the optimization strategies. To overcome in this problem, some researchers have expressed the procedures to find a temperature that optimizes the final distribution of particle sizes [11–15]. In fact, due to the experimental limitations, simulation and theoretical optimization possess the greatest value to achieve the optimal control of the batch reactor. Simulation and theoretical optimization, as a research tool, can complete the results of experimental studies by calculating the desired parameters at regions or situations in which experimental work is expensive or impossible [16–27]. In the past few decades, iterative model development, and experimental designs have been employed in some crystallization processes. Gunawan et al. [28] have reported a model for different growth rates of crystallites in the batch reactor. In the other investigations, Ma and Braatz [29,30] have used the overall closed loop crystal product as the objective of the experimental design. Furthermore, various efforts have been performed on the optimal control of the batch cooling crystallizers that are reported in various literatures [31–33]. The influence of the crystal size distribution and degree of freedom on the performance of crystallization was studied by Chang and Brate [34]. Since the main goal is achieved large crystals, the optimization should avoid seeding in order to get a crystal with large size. Therefore, Moulin [35] provided a temperature control route to fix the seeding in a low level. Because of the non-linear dependency of seeding and the growth rate of super-saturation, it is essential to continue the growth and seeding by keeping the super-saturation in a low level. This is a suitable and desired trend which is followed by Jones and Moulin [36]. Ray and Ajinkya [37] used the functional optimization of the sulfate ammonium model to maximize the mean crystal size and obtain the optimal temperature profile. Moreover, Moulin [36] investigated the role of temperature control on the liquid solution of potassium and sulfate ammonium to maximize the final size of the crystals. In addition, the researchers found that the speed of the primary cooling is too slow in this curve while the cooling rate is much greater at the end of the cooling [38].

Jones and Moulin [36] used the optimal control theory to find an optimized cooling profile by using the momentum way for independent population balance. This research confirmed that the optimized cooling profile is achieved when the mean crystal size increases in contrast to cooling linear strategies. Hu et al. [39] worked to find a temperature profile in order to obtain the objective functions of the product in the final time. By using population balance idea, a new method is presented to solve the population balance in the crystallization process. Moreover, optimized algorithm finds the quantified value of the objective function for an input temperature parameter. Finally, they presented the results for the natural cooling, linear cooling and optimal cooling.

In this work, the batch cooling crystallization procedure is investigated to develop an appropriate optimization strategy. The influence of solubility is studied to characterize the temperature of batch cooling crystallization. In order to produce a product with high purity, parameter size distribution and suitable shape crystal, the temperature profile should be optimized for the crystallization process. Temperature control policy is necessary in the batch cooling crystallization to provide a suitable crystal size distribution for the product through the optimization. Hence, batch cooling crystallization is initially modeled. Then, objective functions are used to optimize the temperature of crystallization by the genetic algorithm. Maximum mean size, closeness to the desired value (desired mean weight size) and the minimum coefficient of variation