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Improvement of batch crystallization control under uncertain kinetic parameters by model predictive control

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ABSTRACT

As the widespread use of a batch crystallization process in many industries, finding an optimal operating condition and effective control strategy are significant for improving product quality and downstream operations. To achieve these, an accurate model is required to predict the process behavior and to design an effective and robust controller. However, due to unknown disturbances and batch-to-batch variations, the kinetic parameters obtained from experimental study may not represent the real process resulting in poor control and estimation performances. In this work, improvement of batch crystallization control of a potassium sulfate production under uncertain kinetic parameters has been proposed. An extended Kalman filter (EKF) has been designed to estimate uncertain parameters and un-measurable states. An optimization model based feedback controller known as Model Predictive Control (MPC) technique has been implemented to achieve the desired crystal size distribution (CSD) subject to a product quality constraint i.e., the requirement of seeded crystal size. Simulation results demonstrate that the robustness of the batch crystallizer control satisfying the requirement of crystal quality has been improved by the MPC control integrated with the EKF in the presence of un-measurable states and uncertain parameters.

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1. Introduction

Batch crystallization is one of widely used process for separation and purification with high purity in the production of fine and specialty chemicals, food, and pharmaceutical products. A batch crystallizer can provide a large mean crystal size and narrow crystal size distribution (CSD) which directly affects final product qualities. Therefore, effective control of desired CSD crystals is needed to improve the batch crystallization process and product qualities.

In any crystallization process, the first step is to achieve supersaturation which is driving force for crystallization. After that, formation of nuclei occurs and finally the subsequent growth of these nuclei to form large crystals. There are the common techniques to generate supersaturation such as evaporating the solvent from solution, salting that change the solubility of the solute and cooling a solution below its saturation temperature. Among these techniques, cooling crystallization is the most common method of achieving supersatuation because the operation and control is simple; the solubility increases dependent with temperature. For this method, the initial temperature is reduced gradually to the final temperature; a solvent shows high solubility at high temperature and low solubility at low temperature. As the nucleation and growth rates depend on the supersaturation level which is a function of temperature, the control of crystal products is usually performed by manipulating the solution temperature. The effect of different cooling policies such as linear, natural, and controlled cooling on the supersaturation level in batch crystallizers can be found in the literature [1–2].

Recently, an optimization of batch crystallizers has received considerable attention to determine optimal operating profiles for improving final product qualities [3–5]. With an optimal open-loop profile, a controlled system is carefully driven in an optimal way. However, the effectiveness of the optimal profile is usually degraded in real applications due to inadequate instrumentation to measure all states, uncertainty in an initial condition, batch to batch variations, plant/model mismatches, and the occurrence of the unmeasured disturbances. In addition, constraints regarding physical limitations on the capacity of actuators and/or the state variables, i.e., temperature and concentration for safety and/or product quality requirement are inevitably considered. As a result, a robust feedback control is needed to deal with these problems [6–7].

A model predictive control (MPC), one of model-based feedback controllers, has been found to be a successful control strategy in several industrial applications because of its ability to handle

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Nomenclature

A	total heat transfer surface area (m^2)
b	nucleation rate exponent
B	nucleation rate (no. crystal s^{-1} g solvent^{-1})
C	solution concentration (g solute g solvent^{-1})
C_m	metastable concentration (g solute g solvent^{-1})
C_p	heat capacity of the solution (kJ kg^{-1} K^{-1})
C_{pi}	heat capacity of cooling water (kJ kg^{-1} K^{-1})
C_s	saturation concentration (g solute g solvent^{-1})
E	activation energy
f	population density of crystals (no. of crystals μm^{-1} g solvent^{-1})
F_j	cooling water flow rate (m^3 s^{-1})
g	growth rate exponent
G	growth rate (μm s^{-1})
ΔH_c	heat of crystallization (kJ kg^{-1})
k_b	birth rate coefficient (s^{-1} μm^{-3})
k_g	growth rate coefficient (μm s^{-1})
k_v	volumetric shape factor
K	Kalman gain metrix
L	characteristic crystal length (μm)
M	mass of solvent in the crystallizer (kg)
R	gas constant
t	time (min)
T	reactor temperature (K)
T_j	cooling jacket temperature (K)
T_{jsp}	set point of the jacket temperature (K)
U	overall heat transfer coefficient (kJ m^{-2} h^{-1} K^{-1})
u	the control vector
V_j	jacket volume (m^3)
v	the measurement noise
w	the process noise
x	the system state vector
y	the observation vector

Greek symbols

ρ	density of crystals (g μm^{-3})
ρ_j	density of cooling water (kg m^{-3})
μ_0	zeroth moment of the CSD (no. of crystals g solvent^{-1})
μ_1	firth moment of the CSD (μm g solvent^{-1})
μ_2	second moment of the CSD (μm^2 g solvent^{-1})
μ_3	third moment of the CSD (μm^3 g solvent^{-1})

Superscripts

n	nucleation
s	seeded crystal

nonlinear processes, multivariable interactions, constraints, and optimization requirements [8]. For a batch process, a key control objective is to achieve the desired size distribution of a product in the presence of appropriate constraints.

The MPC controller has been applied to control a batch crystallizer [9]. The control objective is to achieve a desired particle size distribution under control and product quality constraints. Simulation results have shown that the MPC controller gives much less total volume of fine crystals compared to a linear cooling strategy does.

In this work, the implementation of the MPC algorithm is proposed to achieve the desired crystal size distribution (CSD) subject to a product quality constraint. For the batch crystallizer, not all states are available on-line; only concentration and temperature can be measured directly. Hence, an extended Kalman filter (EKF), an on-line estimator, is incorporated in the MPC formulation to estimate un-measurable states: the quality of crystals in terms of the ith moments. Furthermore, as the MPC requires an accurate model to predict exact process behavior and design the controller maximizing product quality the EKF is also designed to on-line estimate uncertain kinetic parameters.

2. Modeling of a batch crystallization process

Crystallization is a dispersed phase, heterogeneous system that poses many difficulties. Not only environmental variables (concentration, temperature) affect the rate of crystal growth, but other characteristics of each crystal such as crystal defects can influence the growth rate of a crystal as well. A mathematical framework for modeling a batch crystallization process consists of the population balance equation (PBE) describing a conservation equation for a number of crystals in a population.

To simplify mathematical models of the process, the PBE is developed based on a few assumptions: well mixed condition, neglecting the suspension volume change in the system, size independent crystal growth and the agglomeration and breakage of crystals. With these assumptions, the PBE for the CSD of the process can be written as:

$$\frac{\partial f(L,t)}{\partial t} + G(t)\frac{\partial f(L,t)}{\partial L} = 0 \tag{1}$$

With initial and boundary conditions for the evolution of the CSD:

$$f(0,t) = \frac{B(t)}{G(t)} \tag{2}$$

$$f(L,0) = f_{\text{seed}}(L) \tag{3}$$

The mass balance describing the change of solute concentration in continuous phase is as follows:

$$\frac{dC}{dt} = -3\rho_c k_v G(t)\int_0^\infty f(L,t)L^2 dL \tag{4}$$

The energy balances for the batch crystallizer and the jacket are

$$\frac{dT(t)}{dt} = -3\frac{\Delta H_c}{C_p}\rho_c k_v G(t)\int_0^\infty f(L,t)L^2 dL - \frac{UA}{MC_p}(T(t) - T_j(t)) \tag{5}$$

$$\frac{dT_j(t)}{dt} = \frac{F_j}{V_j}(T_{jsp}(t) - T_j(t)) + \frac{UA}{\rho_j V_j C_{p_j}}(T(t) - T_j(t)) \tag{6}$$

The kinetic phenomena that influence the formation of crystals are nucleation and growth rates. The driving force for both phenomena is the non-equilibrium state of the system measured by a relative super-saturation (S) as in Eq. (7):

$$S = \frac{C - C_s(T)}{C_s(T)} \tag{7}$$

The rate of nucleation and growth are simplified by assuming an empirical functional form as given in Eqs. (8) and (9):

$$B(t) = k_b \exp\left(\frac{-E_b}{RT}\right)S^b \int_0^\infty f(L,t)L^3(t)dL \tag{8}$$

$$G(t) = k_g \exp\left(\frac{-E_b}{RT}\right)S^g \tag{9}$$

The solution of the model equations of the crystallization process is determined based on the conservation of a numbers of crystals. The

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