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Dynamic Simulation and Optimization for Batch Reactor Control Profiles

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Abstract. Batch crystallization is one of the most important chemical separation unit operations. Due to the complex mechanism and dynamic nature of this process the mathematical model research is a challenging task. In this paper, the authors present research achievement on batch crystallization modeling, simulation, optimization and parameter estimation. Within the proposed control strategy, a dynamic optimization is first preformed with the objective to obtain the optimal cooling temperature policy of a batch crystallizer, maximizing the total volume of seeded crystals. Next, owing to the complex and highly nonlinear behavior of the batch crystallizer, the nonlinear control strategy based on a generic model control (GMC) algorithm is implemented to track the resulting optimal temperature profile.

Keywords : Optimal control, Batch crystallization, Dynamic simulation, Parameter estimation.

1. Introduction

Crystallization process plays an important role in many industries. It is widely used for separation and purification in the petrochemical and fine-chemical, pharmaceutical, and semiconductor industries. Crystallization can generally be operated in continuous and batch operation modes. Since the temperature of solution in crystallizer has direct influence on the super saturation, it is employed as a manipulated variable to control these processes[1,2]. Various cooling methods such as linear cooling and natural cooling have been widely investigated in the past years[4-7].

The study of the paper is focused on the implementation of a dynamic optimization to find an optimal operation policy in terms of crystallizer cooling temperature for maximizing the total volume of the final crystal product. Then, the resulting optimal temperature policy is implemented as set-point in closed-loop control studies. In this work, a generic model control (GMC), one of the nonlinear model-based control algorithms that is successfully applied to a number of chemical processes[8-13] is applied to track the crystallizer temperature following the desired profile. The crystallization process for the production of potassium sulfate is studied. Comparison of GMC and conventional PI control techniques is also presented.

2. Mathematical Model of a Batch Crystallization Process

The driving potential for both nucleation and growth rates is the nonequilibrium state of the system measured by the relative supersaturation (S) as expressed in Eq. (1) in the formation of a crystal:

$$S = \frac{C - C_S(T)}{C_S(T)} \tag{1}$$

The mass balance describing the change of solute concentration in continuous phase is given as shown below.

$$\frac{dC}{dt} = f(L, G(t), t) \tag{2}$$

The energy balances for a batch crystallizer and jacket are as follows.

$$\frac{dT}{dt} = f(\Delta H_c, G(t), L, T(t), T_j(t)) \tag{3}$$

$$\frac{dT_j}{dt} = f(T_j(t), T(t)) \tag{4}$$

The crystallization model is completed by the definition of the kinetic processes that relate the dynamics of the crystal population to the state of the bulk system. This involves the specification of rate expressions for the nucleation and growth of crystals (Eqs. 5- 6) .

$$B(t) = f(S, L(t), t) \tag{5}$$

$$G(t) = f(S, T) \tag{6}$$

It is noted that since the crystal breakage or agglomeration model was not considered in the proposed crystallizer model, a total number of the crystals growing from seeds remain s constant which is determined by the initial seed size distribution.

3. Dynacim Optimization Strategy

In batch crystallization processes, a large volume of seeded crystals favors product quality. On the other hand, fine crystals obtained from nucleation should be kept in possible lower limit as they may cause difficulties in downstream operations e.g. filtration and drying.

In this work, two optimization problems with different objective functions are considered.

Problem 1 (OPT1)

$$\min_{T(t)} \mu_3^n(t_f) - \mu_3^s(t_f) \tag{7}$$

Subject to the crystallizer model equations

$$C_s \le C \le C_m, \qquad T_{\min} \le T \le T_{\max}, \qquad \left\|\frac{dT}{dt}\right\| \ge k$$

Problem 2 (OPT2)

$$\min_{T(t)} \mu_3^n(t_f) \tag{8}$$

Subject to the crystallizer model equations

$$C_s \le C \le C_m, \qquad T_{\min} \le T \le T_{\max}, \qquad \left\|\frac{dT}{dt}\right\| \ge k$$

In regard to its infinite-dimensional nature, the direct use of PBE in optimization and design of controllers should be avoided[12]. Recently, the development in the method of moments leads to reduced order models in which the key dynamics of crystallization processes is taken into account. Following this approach, the PBE is transformed to a set of ordinary differential equations (ODEs).

In principle, the method of moments defines the ith moment in terms of the population density function by

$$\mu_i = \int_0^\infty f(L,t) L^i(t) dL \tag{9}$$

The rate equation of moments is derived by deter mining separately the moments of the seed and nuclei classes for the CSD as in Eqs. (10) and (11),

$$\frac{d\mu_0^n}{dt} = B(t)$$

$$\frac{d\mu_i^n}{dt} = iG(t)\mu_{i-1}^n(t) \qquad i = 1,2,3 \tag{10}$$

$$\mu_0^n = cons\tan t$$

$$\frac{d\mu_i^s}{dt} = iG(t)\mu_{i-1}^s(t) \quad i = 1,2,3 \tag{11}$$

4. Simulation Results

4.1. Dynamic optimization

Since the dynamic optimization computes the optimal control trajectory by optimizing the objective function, defining such a function for best process optimization is important. Here, the effect of different choices in the objective function of the dynamic optimization problem is first investigated. To obtain the solution of the optimization problems via the sequential approach, the optimal temperature profile is discretized by using a piecewise constant function with 60 time interval.

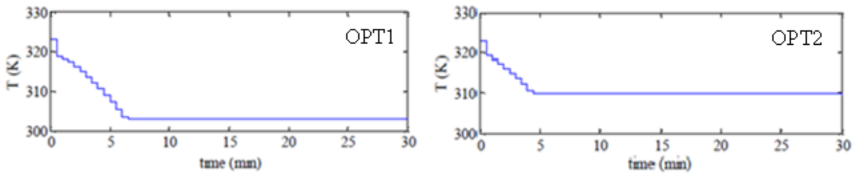
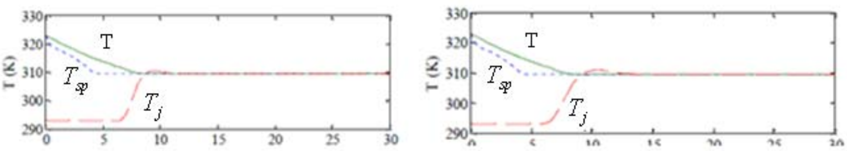


Fig.1. The optimal temperature profiles

Fig. 1 shows the optimal cooling temperature profiles obtained by solving the optimal control problem with different optimization problems (OPT1 and OPT2). It can be seen that OPT1 provides greater total number of crystals with larger average crystal size at the final batch time than OPT2. It is also observed that by comparing with the result of OPT2, the total volume of seeded crystals obtained from OPT1 is larger by 28.6% satisfying the desired product quality whereas the total volume of fine crystals is excessively larger by 152.2% which is undesirable not only for the product quality but also for the subsequent process operations. These results indicate that the product quality in terms of μ_3 obtained at the end of batch run is sensitive to the optimization formulations and therefore, the objective function should be selected carefully.

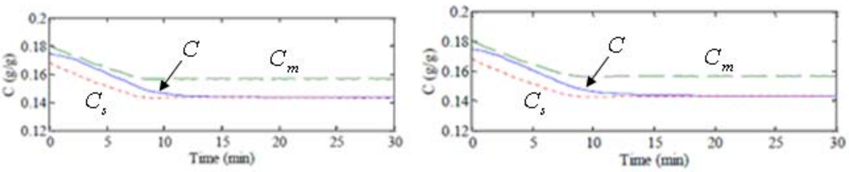
4.2. Cooling temperature control

Once the optimal temperature profile is computed, the feedback controller based on GMC and PI is used to control the crystallizer temperature to follow the desired profile by manipulating the jacket temperature. It is noted here that only the optimal cooling temperature profile obtained from OPT2 in which the μ_3 (t_f) is minimized, is considered since such a temperature policy provides less fine crystals leading to efficient operation in downstream processes whereas the volume of seeded crystal (μ_3) is still satisfy the product quality requirement.



(a) GMC control (b) PI control

Fig.2. Control response



(a) GMC control (b) PI control

Fig.3. Concentration profile

Fig.2 and Fig.3 show the response profiles of crystallizer temperature and the solution concentration under GMC and PI controllers in the nominal case where all parameters are known exactly. It can be seen that the control responses of both GMC and PI controllers show a similar trend leading to comparable product qualities. However, it is noted that at the initial time period, the temperature set point of the crystallizer cannot be perfectly tracked since water as coolant has lower limit of temperature at 293K with the usage of other coolants of which the lower bound on the temperature can be determined below 293K, the temperature set point could be tracked rap idly; however, it might lead to higher operating cost.

5. Summaries

A dynamic optimization and a nonlinear model-based control of a seeded batch crystallizer for the production of potassium sulfate have been considered in this work. To achieve the desired product quality in terms of the total volume of fine and seeded crystals, two dynamic optimization problems are formulated and solved by using a sequential approach. It is found that different choices in selecting objective function have an effect on the optimization solution. When the optimal temperature set point is determined, a generic model control (GMC) is implemented to control the crystallizer temperature and compared with a conventional PI control. Simulation results show that both the GMC and PI controller give good control performance in the nominal case where they were designed; the final product quality of crystals satisfy all the requirements as well. However, in the presence of plant parameter mismatch i.e. in the overall heat transfer coefficient, the GMC is found to be more robustness than the PI control.

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