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Model-based Optimal Control of Industrial Batch Crystallizers

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Abstract

This paper presents a model-based control and optimization approach for real-time improved operation of industrial batch crystallization processes, which is successfully tested on a pilot as well as on a full-scale industrial crystallizer. The core component of the control and optimization framework is a nonlinear model predictive controller or a nonlinear dynamic optimizer that utilizes a reduced-order nonlinear process model for on-line computation of the optimal input profiles of the batch crystallizer. The control approach uses an observer to keep the process model aligned with the real process and to estimate the unmeasured process variables.

The proposed model-based control and optimization strategy is devised to maximize the batch throughput, while satisfying requirements on the product quality. Optimal control of the crystal growth rate is the key to fulfilment of this objective. It is demonstrated that real-time application of the control strategy leads to a substantial increase, i.e. up to 30%, in the batch productivity, while preserving the product quality. The model-based control approach also facilitates the control of the process to its equilibrium conditions at the batch end. This is essential for industrial applicability of any control strategy.

Keywords: Batch process, Crystallization, Real-time control, Dynamic optimization, Nonlinear model predictive controller

1. Introduction

A substantial amount of materials in the pharmaceutical, food, and fine chemical industry is produced in crystalline form. Batch crystallization is a key separation and purification step in these industries, with a significant impact on the efficiency and profitability of the overall process.

In view of the fierce economic competition between the companies manufacturing high value-added crystalline products, there is an ever-increasing interest in optimal operation of batch crystallization processes in order to boost the process productivity, while satisfying the stringent product quality and batch reproducibility requirements. Currently, batch crystallizers are often operated by tracking predetermined recipes, e.g. temperature, feed flow and/or heat input trajectories, which are largely based on operator's experience. The standard PID controllers used to implement the batch recipes however lack the ability to push the process to its most optimal operating trajectory, while various operational and quality constraints are honoured.

In recent years, the development of computationally powerful modelling and optimization tools has greatly facilitated the use of first principle models in devising optimal batch recipes. Application of the off-line optimized profiles to a batch crystallizer however results in sub-optimal operation as plant-model mismatch, measurement errors, unmeasured process disturbances and irreproducible start-ups, i.e. unknown initial conditions, often worsen the effectiveness of the off-line optimized operating policies. This performance deterioration can be effectively alleviated by on-line optimization of the process based on feedback from system states that are estimated by an observer, i.e. soft sensor, using the process model and available in-situ process measurements (Nagy 2009; Mesbah et al. 2009). The real-time control approach continuously optimizes the system on the basis of its current status and, therefore, drives the process to its most optimal operation at any time throughout the batch.

This paper presents a model-based control and optimization approach for the optimal operation of industrial batch crystallizers. The controller aims to optimally operate the batch process within the meta-stable zone such that the production capacity is maximized, while fulfilling the product quality requirements. This is realized by manipulating the supersaturation to control the crystal growth rate during the batch run. In addition to the batch productivity, the crystal growth rate has a close relation with various product quality attributes, namely the purity of crystals, crystal habit and crystal size distribution. A trade-off between the achievement of sufficient product quality and the maximization of batch throughput however has to be sought as better product quality is typically achieved at low crystal growth rates, whereas increase in the batch productivity requires the highest possible crystal growth rate. This problem is therefore well suited for a model-based control approach where conflicting operational considerations can be traded off against each other by satisfying various constraints defined on process inputs and outputs.

The model-based control and optimization approach proposed in this work utilizes either a Nonlinear Model Predictive Controller (NMPC) or a nonlinear dynamic optimizer for on-line computation of the optimal input profiles that govern the supersaturation in the crystallizer. The optimal control problem is formulated such that the crystal growth rate is continuously kept at a predetermined maximum rate throughout the batch in order to realize a compromise between the fulfilment of product quality requirements and the maximization of batch throughput. An observer is used to keep the process model aligned with the real process in the presence of model imperfections and process uncertainties. The observer also enables us to estimate the unmeasured process variables, e.g. crystal growth rate, that are to be controlled. The real-time performance of the NMPC and the dynamic optimizer is examined by several implementations on a semi-industrial evaporative 75-liter draft tube crystallizer. The application of the proposed model-based control and optimization approach to industrial crystallizers is also investigated by testing the NMPC on a full-scale industrial evaporative 14 m^3 forced circulation crystallizer.

In what follows, section 2 discusses the crystallization process model. The description of the control framework is given in section 3. Section 4 presents the experimental results of implementation of the model-based control approach on the two processes, followed by the concluding remarks outlined in section 5.

2. Crystallization Model

The cornerstone of any model-based control and optimization strategy is its dynamic process model, describing the dynamic relation between the relevant inputs and outputs of the system to be controlled. These control strategies utilize the model to continuously explore the degrees of freedom in the process in order to achieve the maximum performance in accordance with an optimization criterion.

The dynamic behaviour of a crystallization process can be rigorously captured by the population balance equation, along with the conservation equations and kinetic relations. The population balance equation is a hyperbolic partial differential equation, which describes the evolution of the crystal size distribution in time. The population balance equation is numerically solved by approximating the original equation with a finite number of ordinary differential equations through discretization of the crystal size distribution. Accurate numerical solution of the population balance equation often requires a large number of discretization points that may render real-time application of the model-based control strategy computationally too expensive.

In this work, the method of moments (Randolph and Larson, 1971) is applied to the population balance equation in order to recast it into a reduced-order set of computationally affordable ordinary differential equations. The method of moments reduces the information on the crystal size distribution such that only relevant properties of the total crystal population required for the intended control application are calculated. Batch crystallizers can therefore be represented by a set of nonlinear differential algebraic equations of the general form

$$\begin{aligned} &\dot{x} = f(t,x,z,y,u,\theta)\ ; \qquad x(t_0)=x_0 \\ &0 = g(t,x,z,y,u,\theta) \\ &y = h(t,x,z,y,u,\theta) \end{aligned} \tag{1}$$

where f and g denote the system of explicit model state and algebraic equations, respectively; h is the system of explicit model output equations; x is the state vector; z is the vector of algebraic variables; y is the vector of process outputs; u is the vector of process inputs; θ is the model parameter set and t is the time. In this model, the state vector contains the leading moments of the crystal size distribution, the solute concentration and the crystallizer temperature, whereas the vector of algebraic variables is comprised of the kinetic variables, namely the crystal growth rate and the total nucleation rate. On the other hand, the inputs of the system are the mechanisms to influence the supersaturation and, consequently, govern the crystallization kinetic phenomena. It is worth noting that the model parameters are estimated based on a set of historical data of normal batch operation.

3. Model-based Control Framework

The proposed model-based control and optimization approach is depicted in Figure 1. As can be seen, the control framework consists of various blocks, namely the model-based controllers, the observer and the scheduler. The internal communication as well as the communication between the framework and the real process (plant) is based on the OPC (OLE for Process Control) protocol, which has become the standard communication protocol used in process industry nowadays. The heart of the framework is an OPC server (IPCOS DataServer), containing all variables that have to be exchanged between the different tasks present in the framework. The execution sequence of different tasks at each sampling instant is determined by the scheduler.

The core component of the framework is the model-based controller, i.e. the nonlinear model predictive controller (INCA-NLMPC, IPCOS, The Netherlands) or the dynamic optimizer. These optimization-based control strategies utilize the nonlinear moment

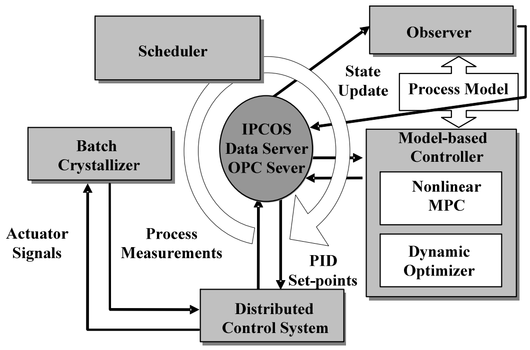

Figure 1. Block diagram of the model-based control framework.

model for on-line computation of the optimal control actions over the future control horizon N_c given a certain performance index that is subject to various equality, i.e. process model, and inequality constraints evaluated over the prediction horizon N_p. The optimal control problem is stated in its most general form as

$$\begin{aligned}&\min_{u_k,\dots,u_{k+N_c-1}} \sum_{i=1}^{N_C} \left\|u_{k+i} - u_{k+i}^{ref}\right\|_R^2 + \sum_{i=1}^{N_P} \left\|y_{k+i} - y_{k+i}^{ref}\right\|_Q^2 + \sum_{i=1}^{N_C} \left\|\Delta u_{k+i}\right\|_W^2 \\ &\text{s.t. Eq. (1)} \\ &u_{k+i}^{\min} \le u_{k+i} \le u_{k+i}^{\max}, \quad \Delta u_{k+i}^{\min} \le \Delta u_{k+i} \le \Delta u_{k+i}^{\max}, \quad y_{k+i}^{\min} \le y_{k+i} \le y_{k+i}^{\max} \qquad i \in (1, N_p).\end{aligned} \tag{2}$$

This performance index allows us to weigh deviations on the process inputs and outputs with respect to their reference trajectories, while minimizing the control effort, i.e. Δu, put into the system.

The primary difference between the NMPC and the dynamic optimizer lies in how the process model is exploited to determine the optimal control actions. The dynamic optimizer computes the control actions using the nonlinear process model in one stage, whereas the NMPC first utilizes the nonlinear process model to forecast the system behaviour over the prediction horizon. Subsequently, a local Linear Time-Variant (LTV) model extracted from the original nonlinear model at each operating point is used for optimization of the performance index (Landlust et al., 2008).

In real-time applications, the optimal control problem is continuously solved on-line in a receding horizon mode (Maciejowski, 2002). An observer, namely an extended Kalman filter or an extended Luenberger-type observer, is therefore employed to estimate the system states in order to initialize the controller recursively at regular time intervals when process measurements, e.g. solute concentration, crystal content, crystal size distribution, become available.

4. Experimental Results

4.1. Case 1: Semi-industrial Crystallization of Ammonium Sulphate

The dynamic optimizer and the NMPC are applied to a seeded fed-batch evaporative crystallization process producing ammonium sulphate in a 75-liter draft tube crystallizer equipped with a Yokogawa Distributed Control System (CENTUM CS3000, Japan). Seeding is exercised according to the procedure proposed by Kalbasenka et al. (2007) to ensure the reproducibility of the batch runs. The crystal size distribution is measured on-line by means of a laser diffraction instrument (HELOS-Vario, Sympatec, Germany).

An in-line solute concentration measuring probe is also used to monitor the supersaturation till the seeding point; the probe enables us to insert the seed crystals at a predetermined supersaturation. The evolution of the solute concentration throughout the batch is estimated by the extended Luenberger-type observer.

Figure 2 shows the experimental results. Three different batch runs are shown, namely the reference experiment DT_c81 and the experiments DT_c68 and DT_c82 in which the NMPC and the dynamic optimizer are applied, respectively. As the crystal growth rate predominantly determines the product quality in seeded batch runs, variations of the crystal growth rate in relation to different heat input profiles, i.e. the supersaturation generation mechanism, are investigated in the various experiments. When the heat input is kept constant at 4.5kW in experiment DT_c81, the crystal growth rate gradually decays towards the end of the batch without following its maximum admissible value of 2.5×10^{-8} m/s. Real-time implementation of the controllers on the other hand facilitates effective tracking of the maximum crystal growth rate limit till the heat input hits its upper limit of 13 kW that renders further optimal control of the process impossible. It is also shown that the application of the controllers leads to a substantial increase, i.e. up to 30 %, in the crystal content at the batch end as a result of higher crystal growth rates, while the mean crystal size remains almost intact due to the optimal seeding procedure.

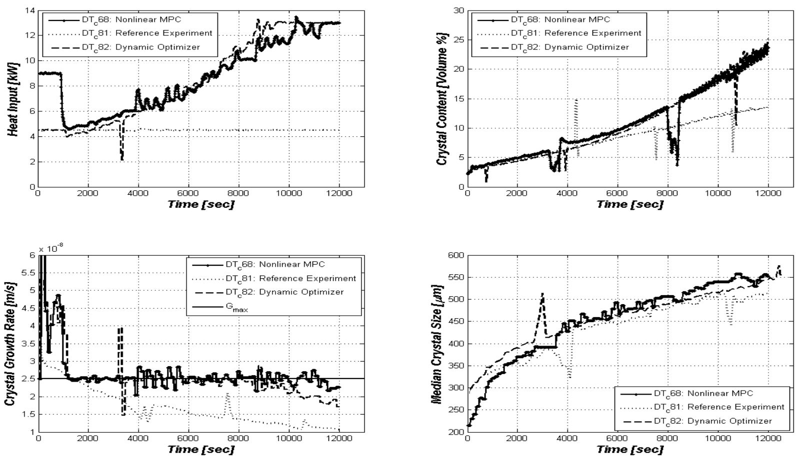

Figure 2. Experimental results of the nonlinear model predictive controller and the dynamic optimizer applied to the semi-industrial ammonium sulphate crystallization process.

4.2. Case 2: Industrial Crystallization of Lactitol Monohydrate

In this case study, the NMPC is implemented on a full-scale industrial crystallizer at PURAC Biochem BV; a seeded fed-batch evaporative forced circulation crystallizer equipped with a Siemens Programmable Logic Controller (PLC, Siemens S7, Germany). The crystal size distribution and the volumetric crystal content are measured together with an ultrasound measurement device (OPUS, Sympatec, Germany).

Figure 3 shows a comparison between the two batch runs to which the NMPC is applied and the original batch recipe; the detailed figures cannot be disclosed due to confidentially issues. As can be seen, the crystal growth rate is continuously pushed to its predefined maximum value by increasing the supersaturation to alleviate the adverse impact of impurities on the crystal growth rate. On the other hand, an upper limit is defined on the volumetric crystal content to enable automatic stabilization of the process

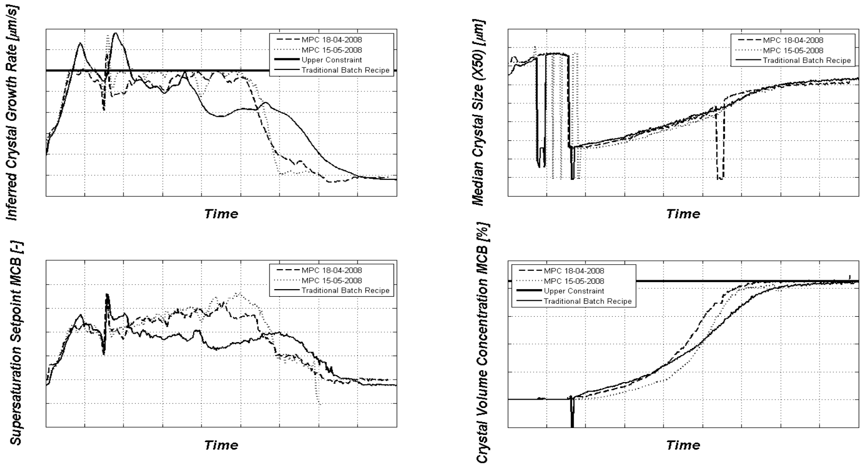

Figure 3. Experimental results of the nonlinear model predictive controller applied to the industrial Lactitol Monohydrate crystallization process.

at the batch end, which is essential for proper slurry handling in the downstream units. The supersaturation therefore decreases towards the batch end to obtain a solution close to equilibrium conditions with constant crystal content. In the controlled experiments, the final crystal content is achieved 10% faster than the original batch run.

5. Conclusions

A model-based control and optimization approach for optimal operation of batch crystallizers is proposed and experimentally validated on different scales. The underlying optimal control problem is formulated to maximize the overall batch throughput by defining an upper limit on the crystal growth rate in order to circumvent degradation of the product quality. The control strategy also ensures process stabilization at the batch end by bringing the solution to its equilibrium conditions using an upper bound defined on the crystal content.

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