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Iterative learning control for the systematic design of supersaturation controlled batch cooling crystallisation processes

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ABSTRACT

The paper presents an approach to improve the product quality from batch-to-batch by exploiting the repetitive nature of batch processes to update the operating trajectories using process knowledge obtained from previous runs. The data based methodology is focused on using the linear time varying (LTV) perturbation model in an iterative learning control (ILC) framework to provide a convergent batch-to-batch improvement of the process performance indicator. The major contribution of this work is the development of a novel hierarchical ILC (HILC) scheme for systematic design of the supersaturation controller (SSC) of seeded batch cooling crystallizers. The HILC is used to determine the required supersaturation setpoint for the SSC and the corresponding temperature trajectory required to produce crystals with desired end-point property. The performance and robustness of these approaches are evaluated through simulation case studies. These results demonstrate the potential of the ILC approaches for controlling batch processes without rigorous process models.

1. Introduction

Batch chemical processes are essential for the production of high value added products like biochemical, pharmaceuticals, microelectronics, and specialty chemicals. Generally in the case of batch processes controlling the operating conditions to improve the final product quality from batch-to-batch is often the most practically achievable control strategy (Xiong & Zhang, 2004), since it does not require within batch measurements and can rely on generally more frequently available results of laboratory analyses at the end of the batches. This batch-to-batch control approach exploits the repetitive nature of batch processes to update the process operating trajectories using process knowledge obtained from previous batch runs. This is the main idea of iterative learning control (ILC), which has been successfully applied from industrial robots to autonomous vehicles (Moore, 1998). ILC improves transient tracking performance of a system that executes the same task repeatedly over a fixed time interval (Lee & Lee, 2007), but it can also be applied to find the transient setpoint to achieve a desired end-point performance. The supplementary requirements are that, the reference trajectories (to be followed by the outputs) remain the same from run-to-run and the process starts from the same state during each operation. In practice, there are many processes repeating the same task in a finite interval including a batch reactor in the chemical industry. Hence, it is a natural approach to apply ILC in tracking control of product quality in agile batch manufacturing processes. In fact, in batch chemical processing ILC applications have increased significantly after its introduction in late 90s (Lee, Kim, & Lee, 1996).

During the last decade, researchers have studied several ILC approaches for batch crystallisation processes (Forgione, Mesbah, Bombois, & Van den Hof, 2012; Hermanto, Braatz, & Chiu, 2006a; Hermanto, Braatz, & Chiu, 2006b; Hermanto, Braatz, & Chiu, 2011; Lee, Lee, Fujiwara, & Braatz, 2002; Su, Braatz, & Chiu, 2012; Zhang, Nguyan, Xiong, & Morris, 2009a; Zhang, Nguyan, Xiong, & Morris, 2009b; Zhang, Wang, Dakuo, & Jia, 2012). However, being complete or hybrid model based ILCs, almost all approaches are dependent on a first principle model of the system and sometimes based on complex mathematics which are also computationally intensive (Lee et al., 2002). A run-to-run C-control (Hermanto et al., 2006a) and a run-to-run temperature control (Hermanto et al., 2006b) were studied for a model of polymorphic transformation of L-Glutamic acid from metastable α-form to stable β-form. These approaches utilise the available concentration–temperature profile at every sampling time to calculate the required input. Zhang et al. (2009a, 2009b) proposed an ILC strategy that uses linearised models identified from process operational data (Xiong & Zhang, 2005) to maintain a desired supersaturation profile in a simulated crystallisation system. The work was mainly focused on the comparison between PCR (principal component regression) and MLR (multiple linear regressions) models in presence of unknown disturbances. A similar type of supersaturation tracking problem was

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studied by Forgione et al. (2012). They developed a first principles model based ILC + PI control scheme in master-slave configuration. The slave PI configuration used to reject the system disturbances requires knowledge of the transfer function of the system. In order to minimise the requirement of a detailed mathematical model and to overcome the poor extrapolative capability of data based LTV models, researchers have focused on hybrid models by combining the simplified model and data-driven model (Hermanto et al., 2011; Zhang et al., 2012). The hybrid model based ILC enables good performance by complementing both strategies. However, the authors studied the approaches only for systems with well-established mathematical models and still it is a challenge to adopt these approaches for completely unknown or new processes.

This paper introduces a data-driven approach based on using the linear time varying (LTV) perturbation model in an iterative learning control (ILC) framework to automate recipe updating to improve product quality from batch-to-batch. Development of a first principle model is usually very complicated and difficult to obtain for industrial batch process (Xiong, Xu, Dong, & Zhang, 2010). In addition, due to the limited availability of robust on-line sensors in the industrial practice of batch process operations, typically only off-line quality measurements are available. On the other hand, batch processes are inherently nonlinear which makes the whole control scenario even more complicated. Under these circumstances, it is more useful and convenient to develop and practice operating data based control strategies which are applicable within conventional linear modelling frameworks (Russell, Kesavan, & Lee, 1998). The main concept of linear time varying (LTV) perturbation model is to remove process nonlinearities by using perturbation variables instead of using the actual process variables (Xiong & Zhang, 2003).

The work is focused on controlling batch cooling crystallisation to produce crystals with desired end-point property. Batch crystallisation is important in the pharmaceutical industry as a separation process for the intermediates and often serves as the final step in the manufacture of active pharmaceutical ingredients (APIs) (Chen, Sarma, Evans, & Myerson, 2011). It is crucial that crystalline products should exhibit consistent properties throughout the batches, especially in the pharmaceutical industries, which handle high value-added products with strong regulatory constraints (Hounslow & Reynolds, 2006; Wibowo, Chang, & Ng, 2001). Batch cooling crystallisers are often subject to a cooling strategy determined by model-based optimisation, resulting in a trajectory that generally decreases slowly in the beginning and then rapidly at the end of the batch (Rawlings, Miller, & Witkowski, 1993). Optimal cooling has been extensively studied by the researchers during the last four decades (Banga, Irizarry, & Seider, 1998; Jones, 1974; Mayrhofer & Nyvlt, 1988; Miller & Rawlings, 1994; Shen, Chiu, & Wang, 1999). Although efficient, these kinds of model based techniques and the resulting performances are often susceptible to the accuracy of the model (Nagy, Fujiwara, Woo, & Braatz, 2008b). Other control strategies involve either simple linear temperature control or supersaturation control (or concentration control, i.e. C-control) when the solute concentration is controlled to follow a supersaturation profile in the phase diagram, using a concentration feedback control (Fujiwara, Nagy, Chew, & Braatz, 2005; Xie, Rohani, & Phoenix, 2002). Simple temperature control cannot guarantee reproducible results from one batch to the other since temperature is not directly related to the crystallisation dynamics. Supersaturation control is able to produce much better product consistency as it controls directly the main driving force for the crystallisation mechanisms. However, the need for high accuracy of concentration measurement makes C-control often unfeasible in industrial scale (Forgione et al., 2012). As an alternative Su et al. (2012) experimentally extended the concentration control strategy to pH-shift reactive crystallisation of L-glutamic acid based on a nonlinear model of the system. However, this approach is still in development stage due to some performance limitation and beyond the scope of this paper.

In this study, simulated batch cooling crystallisers were used to evaluate the performance and robustness of the proposed ILC strategies. Computer simulations were performed using an unseeded batch cooling crystallisation system of Paracetamol in water. In the first phase, the mechanistic model was used to solve an open loop optimal control problem, where the objective was to maximise the mean crystal length within a fixed batch time. The resulting nonlinear programming problem was solved using standard sequential quadratic programming yielding the optimal temperature trajectory. Subsequently the first principles model was treated as the real processes to generate historical data and LTV model based ILC was applied using this data to generate required temperature profile to produce crystals with desired mean length. The results from the simulation case studies show that the simulated temperature trajectories resulting from the iterative measurement-based optimisation approach converged to the theoretically optimal trajectory obtained using model-based optimisation. The results offer substantial modification over the existing ILC strategies of batch crystallisation processes, which are merely set-point tracking control strategies (Forgione et al., 2012).

The main contribution of this work is the development of a novel hierarchical ILC (HILC) scheme for the systematic design of the supersaturation control (SSC) of a seeded batch cooling crystalliser. SSC drives the process within the metastable zone to avoid nucleation (Fujiwara et al., 2005). Although applying SSC improves the quality of the product CSD, and can produce consistently high quality crystals, until now there is no systematic design approach to select the set-point operating profiles. In practice, the supersaturation profile is often chosen by trial-and-error experimentation or based on a series of supersaturation controlled experiments at different constant supersaturation levels that cover the entire potential operating zone and then selecting a the setpoint that can lead to near optimal results (Aamir, Nagy, & Rielly, 2008; Fujiwara et al., 2005). Zhou et al. (2006) investigated an automated approach to design a nearly optimal supersaturation profile by applying different const. supersaturation (CSS) profiles and observing the related counts/sec over time. Due to unsatisfactory results, they ended up with constant relative supersaturation instead of CSS to avoid secondary nucleation. However, it was not mentioned in the paper how the specified constant relative supersaturation was selected.

In this situation, the proposed HILC can be a convenient tool to select the operating profile. This model free control approach is implemented in a hierarchical structure. On the upper level, a data-driven supersaturation controller determines the extent of optimal supersaturation needed to produce the desired end-point property of crystals. On the lower level, the corresponding temperature trajectory is determined by time domain experiments to generate necessary supersaturation. The proposed approach is evaluated in the case of a simulated seeded batch cooling crystallisation system of Paracetamol in water.

2. Iterative learning control (ILC) in batch chemical processes

Traditionally batch process industries were based stably on methods by following a recipe, leading to consistent and successful products. Usually the recipe is arrived at over a long period through a continuous, iterative improvement based on some analysis of products. Although such a recipe is usually adjusted based on perception and heuristics instead of a rigorous model and optimisation, such a practice can indeed be interpreted as feedback