Iterative Learning Control of a Batch Cooling Crystallization Process based on Linear Time-Varying Perturbation Models

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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 optimization methodology is based 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 approach was evaluated for a batch cooling crystallization process with the aim to control the mean crystal size by manipulating the reactor temperature profile. The simulated temperature trajectories resulting from the iterative measurement-based optimization approach converged to the theoretically optimal trajectory obtained using model-based optimization. These results demonstrate the potential of the ILC approach for controlling batch processes without rigorous process models.

Keywords: Batch process, Iterative learning control, LTV perturbation model.

1. Introduction
Batch chemical processes are essential for the production of high value added products, such as 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 et al., 2004), since it does not require within batch measurements and can rely on the 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 et al., 2007), but it can also be applied to find the transient setpoint to achieve a desired end-point performance. 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. Additionally, developing a first principle model is usually very complicated, time consuming and hence expensive for industrial batch processes (Xiong et al., 2010). This paper introduces a data-driven ILC approach to automate recipe updating to improve product quality from batch to batch in the case of a batch cooling crystallization process.
2. Iterative Learning Control (ILC) in Batch Chemical Processes

In the batch-to-batch control approach variations must be considered on two time-scales. As shown on Figure 1, variations within and between batches can be considered leading to an optimization problem on two time scales (Nagy, 2009). However, during a batch, within batch measurements are often unavailable or adjustment to the operating conditions cannot be made due to limited online sensors or actuators. Hence, batch-to-batch improvement is still dependent on learning from the information obtained usually from after-batch laboratory analyses. In this situation the within batch measurements (if available) are used to estimate model based parameters and states. The updated model is then used in an ILC framework to improve the future operating recipe (see Figure 2).

2.1. Linear Time Varying (LTV) Perturbation Model

The methodology applied is based on the approach proposed by Xiong et al., (2003) which is an ILC scheme based on linear time varying (LTV) perturbation models. Typically the input/output trajectories in batch processes are inherently nonlinear and time varying. However, the concept of using perturbation variables removes process nonlinearity by subtracting time varying nominal trajectories from the batch operation trajectories. If we consider the following nonlinear function between input \( X_b(t) \) and output \( Y_b(t) \) in the matrix form,

\[
Y_b = \Psi(X_b) + n_b
\]

where, \( \Psi(\cdot) \) is the nonlinear static function between the input and output and \( n_b \) is the vector of measurement noise. For the system (1), an LTV perturbation model \( L_b \) is developed by linearizing the nonlinear model along the nominal trajectories. Initially several sets of historical process operating data are collected and the input-output data matrices, \( \Omega'_b = [X_b, X_{b-1}, ..., X_0]^T \) and \( \Omega''_b = [Y_b, Y_{b-1}, ..., Y_0]^T \) respectively, are constructed, where, \( H \) is the number of historical batches. From these data, the best performing trajectories are selected as the nominal trajectories \( (X_b, Y_b) \). At any time \( t \), the perturbation variables for the \( b^{th} \) batch are calculated as \( \bar{X}_b = X_b - X_s \) and \( \bar{Y}_b = Y_b - Y_s \).

Linearizing the nonlinear model (1) around the nominal trajectories gives,

\[
Y_b = Y_s + \left. \frac{\partial \Psi(X_b)}{\partial X_b} \right|_{X_s} (X_b - X_s) + m_b + n_b
\]

Figure 1: Schematic representation of the dynamic two-time scale variations in batch control (Nagy, 2009).

Figure 2: Structure of the ILC framework (Nagy, 2009).
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where, \( \mathbf{m}_b = [m_b^1(1), m_b^1(2), \ldots, m_b^1(N)]^T \) is the sequence of model errors of \( N \) observations due to linearization. The LTV perturbation model and corresponding absolute model prediction of Equation (2) are,

\[
\mathbf{Y}_b = \mathbf{L}_b \mathbf{X}_b + \mathbf{d}_b \\
\mathbf{Y}_b^* = \mathbf{Y}_b^* + \mathbf{L}_b \mathbf{X}_b^* 
\]

The tracking errors of the actual process and of the predicted perturbation model are \( \mathbf{e}_b = \mathbf{Y}_b - \mathbf{Y}_b^* \) and \( \hat{\mathbf{e}}_b = \mathbf{Y}_b - \hat{\mathbf{Y}}_b^* \), respectively. The transfer function \( \mathbf{L}_b \) is predicted according to the steps of Equation (5), for \( b = 1, 2, \ldots, B \), number of observations per batch and \( h = 1, 2, \ldots, H \) is the number of historical batches,

\[
\mathbf{x}_b(i) = x_b(i) - x_b(i), \quad \text{and} \quad \mathbf{u}_b(i) = [x_b(i), x_b(i), \ldots, x_b(i), x_b(i)]^T
\]

If, \( \mathbf{Y}_0^* = \begin{bmatrix} \mathbf{y}_1^T(i) \\
\mathbf{y}_2^T(i) \\
\vdots \\
\mathbf{y}_H^T(i) \end{bmatrix} \) and \( \mathbf{U}_0^* = \begin{bmatrix} \mathbf{u}_1^T(i) \\
\mathbf{u}_2^T(i) \\
\vdots \\
\mathbf{u}_H^T(i) \end{bmatrix} \)

then, the system, \( \hat{\mathbf{i}}_b \), is estimated at each observation by the least squares method as, \( \hat{\mathbf{i}}_b = (\mathbf{U}_0^* \mathbf{U}_0^*)^{-1} \mathbf{U}_0^* \mathbf{y}_0^* \) and \( \hat{\mathbf{L}}_b \) is obtained as, \( \hat{\mathbf{L}}_b = [\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \ldots, \hat{\mathbf{i}}_H]^T \). After completion of the \( b \)th batch run, prediction errors between off-line-measured or analyzed product qualities and their model predictions can be calculated as, \( \mathbf{e}_b = \mathbf{Y}_b - \hat{\mathbf{Y}}_b^* \). The absolute modified model prediction is defined as, \( \mathbf{Y}_b = \mathbf{Y}_b^* + \mathbf{Y}_b \). In ILC, it is desired that, \( \lim_{b} \| \mathbf{e}_b \| \rightarrow \min \| \mathbf{e}_b \| \). Finally, the following quadratic objective function is formulated based on the minimization of the predicted tracking errors,

\[
J_{b+1} = \min_{\Delta \mathbf{x}_{b+1}} \frac{1}{2} [\mathbf{e}_{b+1}^T \mathbf{O} \mathbf{e}_{b+1} + \Delta \mathbf{x}_{b+1}^T \mathbf{P} \Delta \mathbf{x}_{b+1}]
\]

where, \( \mathbf{O} \) and \( \mathbf{P} \) are weighting matrices based on output performance and input change, respectively. This objective function should be solved upon completion of the \( b \)th batch to update the input trajectory for the \((b+1)\)th batch as, \( \mathbf{X}_{b+1} = \mathbf{X}_b + \mathbf{K}_b \mathbf{e}_b \), where, \( \mathbf{K}_b = [\hat{\mathbf{L}}_b^T \mathbf{O} \hat{\mathbf{L}}_b + \mathbf{P}]^{-1} \hat{\mathbf{L}}_b^T \mathbf{O} \), is the calculated control action.

3. ILC of a Batch Cooling Crystallization Process

In this study an unseeded batch cooling crystalliser was considered for the heart drug component (Propanolol base), with a batch time of 300 minutes. The kinetics of the system is given by the following set of ordinary differential equations,

\[
d\mu_s / dt = B \\
d\mu / dt = i G \mu_{i-1} + Br_i \quad i = 1, 2, \ldots \\
dC / dt = -k \rho (3G \mu + Br_i)
\]

where, \( B \) and \( G \) are the nucleation and growth rates respectively, \( S = C - C_s(T) \) is the absolute supersaturation, \( C \) is concentration, \( C_s \) is the solubility as a function of the temperature \( T \), \( \mu_0, \mu_1, \mu_2, \) and \( \mu_3 \) are the moments defining total number, length, area, and volume of crystals in the system respectively, \( r_n \) is the size of the nuclei. The initial
and final temperatures were 41 °C and 21 °C respectively. The model parameters are shown in Table 1.

Table 1: Parameters of the crystallization model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility in water (T in K)</td>
<td>$C_s = 1.58 \times 10^{-4} T^2 - 9.057 \times 10^{-7} T + 1.31$</td>
</tr>
<tr>
<td>Growth rate (cm/sec)</td>
<td>$G = \begin{cases} 1.64(S)^{1.54} &amp; \text{if } S &gt; 0 \ -1.64(S)^{1.54} &amp; \text{if } S \leq 0 \end{cases}$</td>
</tr>
<tr>
<td>Nucleation rate</td>
<td>$B = \begin{cases} 7.8529 \times 10^{06}(S)^{2.25} &amp; \text{if } S &gt; 0 \ -7.8529 \times 10^{06}(S)^{2.25} &amp; \text{if } S \leq 0 \end{cases}$</td>
</tr>
<tr>
<td>Density of crystal (g/cm³)</td>
<td>$\rho = 1.296$</td>
</tr>
<tr>
<td>Volumetric shape factor $k_v$</td>
<td>0.24</td>
</tr>
<tr>
<td>Initial concentration (g/g solvent)</td>
<td>$C_0 = 0.0254$</td>
</tr>
</tbody>
</table>

A simulation program was developed using MatLab to be used as the real process. The objective was to achieve a desired mean crystal size by manipulating the reactor temperature $T$. The batch length was divided into $N = 10$ equal stages. Eleven batches considering different temperature profiles were simulated using the model. From these eleven data sets ten were used as the historical data and the data with the best result was selected as the nominal data set, $X_n, Y_n$ used to create the LTV model. The first principles model was also used to generate the desired product reference trajectory $Y_d$ and the theoretical optimum temperature profile. Using the historical data sets and the selected nominal trajectories $(X_n, Y_n)$, the parameters of $L_n$ was re-identified using process measurements. The weighting matrices were set as, $O = 10^5 \text{diag}(1,2,5,2,5,2,5,2,5,2,5,1.5,1)$ and $P = 0.5I$. According to the ILC algorithm, after the completion of each iteration the new data is added to the historical data set to update $L_n$. The forgetting factor was, $\beta = 0.8$. The temperature profile resulting from each step of the ILC scheme was applied to the mechanistic model (i.e. real process) and the corresponding mean crystal size was obtained.

Figure 3: Trajectories for the a) mean crystal size and b) input temperature at different batches.
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The input/output data obtained after each batch during the ILC was again included in the historical data sets and the LTV model re-identified and used in a model-based optimization to determine the temperature profile for the next batch. The results of the ILC approach are shown in Figure 3, indicating that the mean size of crystals converged to the desired trajectory and the resulting final temperature profile was very close to the theoretically optimum trajectory.

Figure 3: Tracking performance

Figure 4 shows the root mean square error (RMSE) values of the desired and the real mean crystal size trajectories. It took about 34 batches to arrive at final trajectories without the need of any process model. However, the results were almost converged from the 5th batch onwards, and practically all subsequent batches after the 5th would produce crystals with very similar size to the desired target.

4. Conclusions

In this paper, an operating data based iterative learning control (ILC) algorithm is presented. The proposed method was evaluated using a simulated pharmaceutical crystallization process. The results demonstrated that the approach is able to converge to the theoretically optimal operating profiles without the need of a detailed mechanistic process model. The convergence of the approach can be improved by using nonlinear data-driven models in the ILC scheme, such as artificial neural networks or polynomial chaos expansions.

References


