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Optimal Learning Control Combined with Quality Inferential Control for Batch and Semi-batch Processes

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Abstract : An optimal control technique designed for simultaneous tracking and quality control for batch processes. The proposed technique is designed by transforming quadratic-criterion based iterative learning control(Q-ILC) into linear quadratic control problem. For real-time quality inferential control, the quality is modeled by linear combination of control input around target quality and then the relationship between quality and control input can be transformed into time-varying linear state space model. With this state space model, the real-time quality inferential control can be incorporated to LQ control problem. As a consequence, both the quality variable as well as other controlled variables can progressively reduce their control error as the batch number increases while rejecting real-time disturbances, and finally reach the best achievable states dictated by a quadratic criterion even in case that there is significant model error. Also the computational burden is much reduced since the most computation is calculated in off-line. The proposed control technique is applied to a semi-batch reactor model where series-parallelreactions take place.

Keywords : iterative learning control, quality inferential control, LQ control

1. Introduction

One of important objectives in operation of industrial batch process is maintain the quality of end-product. A major obstacle to achieving this objective is that on-line sensors for quality measurement are very often unavailable. The current industrial practice is to control the directly measured variables such as temperatures and pressures at various locations so that they track some pre-assigned trajectories, while eliminating the disturbances at the source. The product quality is analyzed in the laboratory after each batch run and the information is relayed back to the operator for adjusting the condition of upcoming batch runs -- based on some established guidelines (e.g., SQC charts) or, simply, experience.

Motivated by this industrial approach, the research on batch process control has thus far centered around the problem of tracking a given reference trajectory for nonlinear systems. Various nonlinear control methods have been suggested (Berber, 1996) while most industrial problems have been solved by ''gain-scheduling" PID controllers (Tan *et al.*, 1997). Besides the research on the conventional feedback control, a stream of recent research has focused on the notion of *iterative learning control*(ILC) (Bien and Xu, 1998; Chen, 1998; Moore, 1998), which seeks gradual run-to-run improvements by feeding back the error signals from previous batch runs.

This paper focuses on how the two approaches, the following of reference trajectories and inferential (as well as laboratory-analysis-based) control of quality variables, can be merged. An obvious and straightforward way to implement the two together is to have the quality controller determine the reference trajectories for the tracking controllers. On the other hand, by separating the two design, the trade-off between the two controls cannot be made systematically. For instance, if the process variables should be kept within certain bounds, it is not clear how to reflect this requirement in the quality controller design since the optimal design would depend on, among other things, the performance of the tracking controller. In addition, based on the economic considerations, one may wish to systematically trade off the quality control performance for a reduced deviation of relevant process variables from their economic target values (or trajectories). Motivated by this, we propose in this paper an integrated framework to design the two controllers as a single unit.

The tracking controls are there not only to assure a stable and economic operation but also to provide some protection against disturbances that would otherwise affect the final product quality. This strategy would work well if all the disturbances affecting the quality variables do so by first affecting the controlled process variables (such as the heat transfer disturbances affecting the temperature and thereupon the product quality through kinetics). On the other hand, practical evidences suggest that, due to often significant run-to-run changes in batch ingredients and process behavior, maintaining consistent temperature and/or pressure trajectories alone does not render consistent product quality. Feeding back the results of laboratory analysis helps to combat sustained changes but not those occurring on a run-to-run basis. As a way to improve the quality control aspect of a batch process operation, one may consider the option of *inferential control*, a strategy of predicting the final product quality using the correlation with on-line process measurements. The keystone in this approach is the correlation model (called "soft sensor"), which must reliably predict the final product quality. Suggested methods for developing the correlation model range from simple static linear regression, such as the least squares and its variants (e.g., partial least squares), to more elaborate optimal dynamic estimation methods like the Kalman filtering (Lee and Datta, 1994; Russell *et al.*, 1998) and methods based on nonlinear regression tools like the neural networks (Qin, 1997).

The starting point of our development is our previous work on Model Predictive Control for Batch Processes (BMPC) (Lee *et al.*, 1997), which was constructed by incorporating the feature of ILC into the regular model predictive control (MPC) algorithm (formulated based on a time-varying linear model description). This algorithm, however, handles only tracking control of measured process variables and has heavy computational burden because the input solution should be calculated at every sampling time.

Hence, the focus will be given here on how we can embed quality correlation models (established through a data regression) into the servo LQG algorithm combined with iterative learning control so that the objective of inferential quality control can be incorporated into the optimal control calculation.

2. Formulation

2.1 Modeling for process variable

The time-varying linear repetitive process can be generally modeled as follows.

$$\begin{aligned} x_k(t+1) &= A(t)x_k(k) + B(t)u_k(t) + w_k(t) \\ y_k(t) &= C(t)x_k(t) + n_k(t), \quad \text{for } t \in [0, N] \end{aligned} \tag{1}$$

where the subscript k is batch index.

Taking the difference between the k+1[th] and the k[th] for system (1), the state space model of batch-wise differenced can be obtained by

$$\begin{aligned} \Delta x_{k+1}(t+1) &= A(t)\Delta x_{k+1} + B(t)\Delta u_{k+1}(t) + \Delta w_{k+1}(t) \\ \Delta y_{k+1}(t) &= C(t)\Delta x_{k+1}(t) + \Delta n_{k+1}(t) \end{aligned} \tag{2}$$

where

$$\begin{aligned} \Delta x_{k+1}(t) &\equiv x_{k+1}(t) - x_k(t) \\ \Delta u_{k+1}(t) &\equiv u_{k+1}(t) - u_k(t) \\ \Delta w_{k+1}(t) &\equiv w_{k+1}(t) - w_k(t) \\ \Delta y_{k+1}(t) &\equiv y_{k+1}(t) - y_k(t) \\ \Delta n_{k+1}(t) &\equiv n_{k+1}(t) - n_k(t). \end{aligned} \tag{3}$$

2.2 Modeling for quality variable

The linear regression model around reference trajectory can be written as

$$\Delta q_{k+1} = \sum_{t=0}^{N-1} D(t)\Delta u_{k+1}(t) + d_{k+1}. \tag{5}$$

It can be written using the integrating state z(t) as

$$\begin{aligned} z_k(t+1) &= z_k(t) + D(t)\Delta u_k(t) + w_k^q(t) \\ \Delta q_k(t) &= z_k(t) + n_k^q(t) \\ \Delta q_k(N) &= z_k(N). \end{aligned} \tag{6}$$

Combining (2) and (5) yields

$$\begin{aligned} \begin{bmatrix} \Delta x_k(t+1) \\ z_k(t+1) \end{bmatrix} &= \begin{bmatrix} A(t) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \Delta x_k(t) \\ z_k(t) \end{bmatrix} + \begin{bmatrix} B(t) \\ D(t) \end{bmatrix} \Delta u_k(t) \\ &\quad + \begin{bmatrix} \Delta w_k(t) \\ w_k^q(t) \end{bmatrix} \\ \begin{bmatrix} \Delta y_k(t) \\ \Delta q_k(t) \end{bmatrix} &= \begin{bmatrix} C(t) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \Delta x_k(t) \\ z_k(t) \end{bmatrix} + \begin{bmatrix} \Delta v_k(t) \\ v_k^q(t) \end{bmatrix}. \end{aligned} \tag{7}$$

The above (6) can be rewritten as

$$\begin{aligned} \mathbf{x}_k(t+1) &= \mathbf{A}(t)\ \mathbf{x}_k(t) + \mathbf{B}(t)\Delta u_k(t) + \mathbf{w}_k(t) \\ \mathbf{y}_k(t) &= \mathbf{C}(t)\ \mathbf{x}_k(t) + \mathbf{n}_k(t) \end{aligned} \tag{8}$$

where

$$\begin{aligned} &\mathbf{x}_k(t) \equiv \begin{bmatrix} \Delta x_k(t) \\ z_k(t) \end{bmatrix}, \quad \mathbf{y}_k(t) \equiv \begin{bmatrix} \Delta y_k(t) \\ \Delta q_k(t) \end{bmatrix}, \quad \mathbf{w}_k(t) \equiv \begin{bmatrix} \Delta w_k(t) \\ w_k^q(t) \end{bmatrix} \\ &\mathbf{v}_k(t) \equiv \begin{bmatrix} \Delta v_k(t) \\ v_k^q(t) \end{bmatrix}, \quad \mathbf{A}(t) \equiv \begin{bmatrix} A(t) & 0 \\ 0 & I \end{bmatrix}, \quad \mathbf{B}(t) \equiv \begin{bmatrix} B(t) \\ D(t) \end{bmatrix}, \\ &\mathbf{C}(t) \equiv \begin{bmatrix} C(t) & 0 \\ 0 & I \end{bmatrix}. \end{aligned} \tag{9}$$

2.3 Input calculation

Unconstrained Case :

The optimal input can be obtained by solving the following servo-LQG problem:

$$\begin{aligned} \min \Big\{ \frac{1}{2} \Big[&\big(\mathbf{C}(N)\ \mathbf{x}_k(N) - \mathbf{r}_k(N) \big)^T \mathbf{P} \\ &\times \big(\mathbf{C}(N)\ \mathbf{x}_k(N) - \mathbf{r}_k(N) \big) \\ &+ \sum_{t=0}^{N-1} \Big(\big(\mathbf{C}(t)\ \mathbf{x}_k(t) - \mathbf{r}_k(t) \big)^T \mathbf{Q}(t) \\ &\quad \times \big(\mathbf{C}(t)\ \mathbf{x}_k(t) - \mathbf{r}_k(t) \big) \\ &+ \Delta u_k^T(t)\ R \Delta u_k(t) \Big) \Big] \Big\} \end{aligned} \tag{10}$$

where

$$r_k(t)=\begin{bmatrix} y_{ref}(t)-y_{k-1}(t) \\ q_{ref}-q_{k-1}\end{bmatrix},$$
$$Q(t)=\begin{bmatrix} Q(t) & 0 \\ 0 & Q^q(t)\end{bmatrix}, \tag{11}$$
$$Q^q(t)\begin{cases} =0 & \text{for } t=0,\cdots,N-1 \\ \neq 0 & \text{for } t=N \end{cases}.$$

The standard variational method or dynamic programming approach can be used for the solution. The resulting solution is given by

$$\Delta u_k(t) \;=\; -\; \boldsymbol{K}_{FB}(t)\;\; \boldsymbol{x}_k(t) + \;\boldsymbol{K}_{FF}(t)\;\; \boldsymbol{m}_k(t+1) \tag{12}$$

where

$$\begin{aligned} \boldsymbol{K}_{FB}(t) &= (\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{B}(t)+\boldsymbol{R})^{-1} \\ &\quad\times\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{A}(t) \\ \boldsymbol{K}_{FF}(t) &= (\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{B}(t)+\boldsymbol{R})^{-1}\;\boldsymbol{B}^T(t) \end{aligned} \tag{13}$$

and

$$\begin{aligned} \boldsymbol{S}(t) &= \boldsymbol{A}^T(t)[\;\boldsymbol{S}(t+1)-\boldsymbol{S}(t+1)\;\boldsymbol{B}(t) \\ &\quad\times(\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{B}(t)+\boldsymbol{R})^{-1} \\ &\quad\times\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)]\;\boldsymbol{A}(t) \\ &\quad+\;\boldsymbol{C}^T(t)\;\boldsymbol{Q}(t)\;\boldsymbol{C}(t) \\ \boldsymbol{m}_k(t) &= [\;\boldsymbol{A}^T(t)-\boldsymbol{A}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{B}(t) \\ &\quad\times(\;\boldsymbol{B}^T(t)\;\boldsymbol{S}(t+1)\;\boldsymbol{B}(t)+\boldsymbol{R})^{-1}\;\boldsymbol{B}(t)] \\ &\quad\times\;\boldsymbol{m}_k(t+1)+\;\boldsymbol{C}^T(t)\;\boldsymbol{Q}(t)\;\boldsymbol{r}_k(t). \end{aligned} \tag{14}$$

The boundary conditions for (13) are seen to be

$$\begin{aligned} \boldsymbol{S}(N) &= \boldsymbol{C}^T(N)\;\boldsymbol{P}\;\boldsymbol{C}(N) \\ \boldsymbol{m}_k(N) &= \boldsymbol{C}^T(N)\;\boldsymbol{P}\;\boldsymbol{r}_k(N). \end{aligned} \tag{15}$$

4. Numerical Example

We consider a discrete-time batch process of which the total run length is fixed at N sampling steps. Unlike in continuous processes, operational modes of a batch process can vary with time. For example, some input variables may be varied continuously over the entire batch run while others can be manipulated only at a specific time or during a specific time interval. The situation can be further complicated by the fact that some output variables are measured at every sampling instant while others only once every several sampling instances. Some measurements may even be gathered in an aperiodic manner. In addition, just as inputs, an output may be measured over the entire batch run or only during a limited interval. End-product quality can be measured only upon the completion of batch. Finally, some of the output variables are to be controlled along specified trajectories while others are measured only for monitoring purposes.

Figure 1 shows a hypothetical but conceivable pattern of a semi-batch reactor operation and demonstrates the potential complexity involved in representing a batch process operation.

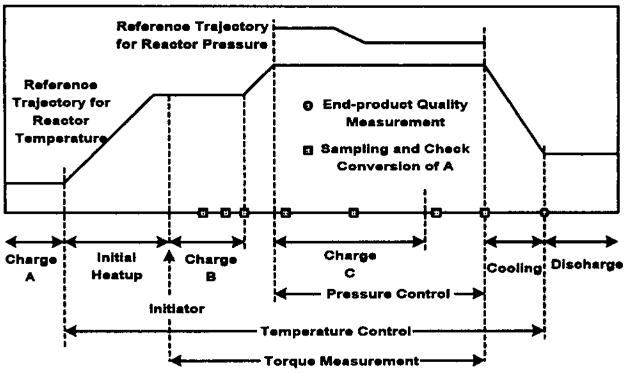

Figure 1. A typical operation pattern of a semi-batch reactor.

4.1 Process description

We consider a jacketed semi-batch reactor where an exothermic series-parallel first-order reaction (with respect to each reactant) takes place.

$$\begin{aligned} A+B &\overset{k_1}{\rightarrow} C \\ B+C &\overset{k_2}{\rightarrow} D. \end{aligned} \tag{16}$$

The following equations describe the reactor system:

$$\begin{aligned} \frac{d(VT)}{dt} &= -\frac{UA}{\rho C_p}(T-T_j)+Q_B T_B \\ &\quad -\frac{V\Delta H_1}{\rho C_p}k_{10}e^{-E_1/RT}C_A C_B \\ &\quad -\frac{V\Delta H_2}{\rho C_p}k_{20}e^{-E_2/RT}C_B C_C,\;\; T(0)=T_I \\ \frac{d(VC_A)}{dt} &= -Vk_{10}e^{-E_1/RT}C_A C_B,\;\; C_A(0)=C_{AI} \\ \frac{d(VC_B)}{dt} &= C_{BF}Q_B - Vk_{10}e^{-E_1/RT}C_A C_B \\ &\quad - Vk_{20}e^{-E_2/RT}C_B C_C,\;\; C_B(0)=0 \\ \frac{d(VC_C)}{dt} &= Vk_{10}e^{-E_1/RT}C_A C_B - Vk_{20}e^{-E_2/RT}C_B C_C, \\ &\quad C_C(0)=0 \\ \frac{dV}{dt} &= Q_B,\;\; Q_B(t)=\begin{cases} 0 & \text{for } t<31 \\ Q_B(t) & \text{for } t\geq 31 \end{cases} \end{aligned} \tag{17}$$

with

$$\begin{aligned} &UA/\rho C_p=0.375(\ell/\min) && T_I=25(^\circ C) \\ &T_B=35(^\circ C) && C_{AI}=1(mol/\ell) \\ &V_I=50(\ell) && C_{BF}=0.95(mol/\ell) \\ &\Delta H_1/\rho C_p=-28.50(^\circ K\cdot \ell/mol) && \\ &\Delta H_2/\rho C_p=-20.50(^\circ K\cdot \ell/mol) && \\ &k_{10}=5.0969\times 10^{16}(\ell/mol\cdot \min) && E_1/R=12,035(^\circ K) \\ &k_{20}=2.2391\times 10^{17}(\ell/mol\cdot \min) && E_2/R=13,450(^\circ K). \end{aligned} \tag{18}$$

The reactor operation is displayed in Figure 2. A is charged initially and the heat-up is followed until B starts to be fed at t=31 min. The reaction commences at this point and continues until the batch terminal time of t_f=100 min. During this period, the concentration of A is sampled at every 10 min and measured with a 5 min delay for analysis. The desired product is C and maintaining the final yield of C (which is $V(t_f)C_c(t_f)$) at a target value (42 mol) is the main objective of the operation. We considered two manipulated variables; jacket temperature and flow rate of B. The sample time for control was chosen to be 1 min. Target value for $V(t_f)C_c(t_f)$ was chosen as 42 mol.

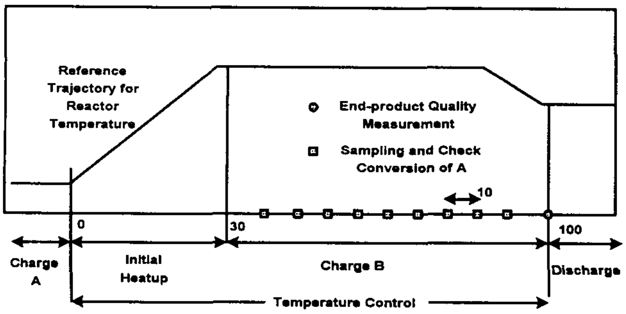

Figure 2. An overview of the operation of the reactor model.

References

[1] Berber, R., "Control of Batch Reactors: A Review," *Trans IChemE.*, *74*, 3-20, 1996,

[2] Bien, Z. and Xu, J.(eds.), *Iterative Learning Control*, Kluwer Academic Publisher, Boston, 1998.

[3] Chen, Y. A Bibliographical Library for ILC Research. *http://www.ee.nus.sg/~yangquan/ILC/ilcref.html*, 1998.

[4] Lee, J. H. and Datta, A. K., "Nonlinear Inferential Control of Pulp Digesters," *AIChE J.*, 40, 50, 1994.

[5] Lee, K. S. and Lee, J. H., "Model-based Predictive Control Combined with Iterative Learning for Batch or Repetitive Processes," In *Iterative Learning Control, Chapter 16, 313,* edited by Zeungnam Bien and Jian-Xin Xu, Kluwer Academic Publisher, Boston, 1998.

[6] Moore, K., "Iterative Learning Control-An Expository Overview," *Applied \& Computational Controls, Signal Processing, and Circuits,* 1, 1998.

[7] Qin, S. J., *Neural Networks for Intelligent Sensors and Control --- Practical Issues and Some Solutions. In Neural Systems for Control,* Chapter 8, 213, edited by Omid Omidvar and David L. Elliott, Academic Press, New York, 1997.

[8 Russell, S., Kesavan, P., Lee, J. H., and Ogunnaike, B., "Recursive Data-based Prediction and Control of Product Quality," *AIChE J.* 44, 2442, 1998.

[9] Tan S. H., Hang, C. C., and Chai, J. S., "Gain Scheduling - From Conventional to Neuro-fuzzy," *Automatica* 33, 411, 1997.