Batch-to-Batch Control of Crystallization with a measurement-based model update

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31st Benelux Meeting on Systems and Control
27 March 2012

Outline

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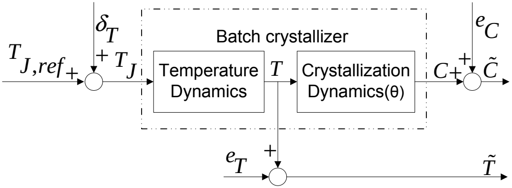
Process Description

Batch Crystallization

Separation and purification process of industrial interest.
A solution is cooled down, solid material (crystals) is produced.

Process described by

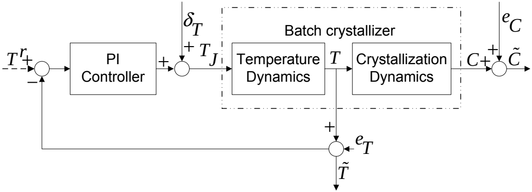
- Temperature Dynamics (linear, known or easy to estimate)
- Crystallization Dynamics (nonlinear PDE, parametric + structural uncertainties)
- Process disturbance, measurement noise on the outputs



Process Description

Control Strategies

- Only the crystallizer temperature is on-line measured and controlled.



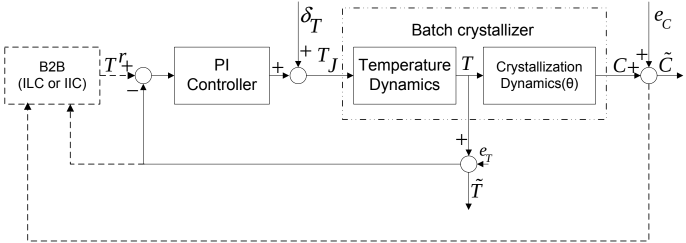
- Advanced strategies proposed. They require additional on-line measurements.

Outline

Batch-to-Batch Strategies

Overview

Additional measurements available at the end of a batch.
For this reason, B2B control strategies. $\mathbf{T}_k^r$ updated from batch to batch.



- Objective for batch k: tracking of supersaturation profile $\bar{\mathbf{S}}_k$.
- $\mathbf{S}_k$ is a static function of the measured output $\mathbf{T}_k, \mathbf{C}_k$.

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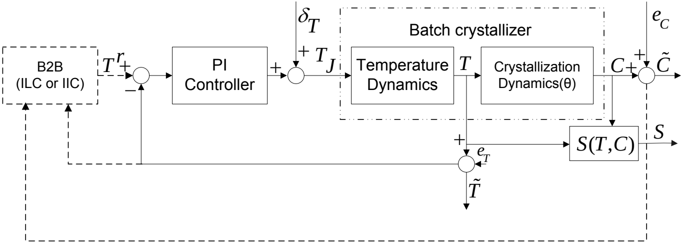

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Batch-to-Batch Strategies

Iterative Learning Control

ILC uses an additive correction offf a nominal model from $\mathbf{T}^r$ to $\mathbf{S}$.

$$\hat{S}(\mathbf{T}^r) \triangleq F_{ST^r}(\mathbf{T}^r;\hat{\theta}) \qquad \textit{nominal model}$$
$$\hat{S}_k(\mathbf{T}^r) \triangleq \hat{S}(\mathbf{T}^r) + \boldsymbol{\alpha}_k \qquad \textit{corrected model}$$

Note: $\mathbf{T}^r, \boldsymbol{\alpha}, \mathbf{S}$ vector of samples $\in \mathbb{R}^N$ ($N =$ batch length).
We describe the system in discrete, finite time (static mapping).

α can compensate the nominal model for

- model mismatch (along the particular trajectory)
- effect of repetitive disturbances

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$\boldsymbol{\alpha}$ can compensate the nominal model for

- model mismatch (along the particular trajectory)
- effect of repetitive disturbances

How to estimate the correction vector?

- Correction vector should "match" the previous measurement.

$$\boldsymbol{\alpha}_k = \tilde{\mathbf{S}}_k - \hat{S}(\mathbf{T}^r) \qquad = \qquad \text{model error}$$

Due to the effect of disturbances on $\tilde{\mathbf{S}}_k$, might not be a good solution.

- Take into account the deviation from α_{k-1}.

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}^N} \|\tilde{\mathbf{S}}_k - (\hat{S}(\mathbf{T}^r) + \alpha)\|^2_{Q_\alpha} + \|\alpha - \alpha_{k-1}\|^2_{S_\alpha}$$

However, tuning of Q_α, S_α not intuitive.

Batch-to-Batch Strategies

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Batch-to-Batch Strategies

Iterative Learning Control

- We model the real system as a stochastic process evolving in the iteration domain (batch number)

$$
\begin{aligned}
\boldsymbol{\alpha}_k &= \boldsymbol{\alpha}_{k-1} + \boldsymbol{\Delta\alpha}_k, & \boldsymbol{\Delta\alpha}_k &\sim \mathcal{N}(0, \Sigma_\Delta) \\
\tilde{\mathbf{S}}_k &= \hat{S}(\mathbf{T}^r) + \boldsymbol{\alpha}_k + \mathbf{v}_k, & \mathbf{v}_k &\sim \mathcal{N}(0, \Sigma_v)
\end{aligned}
$$

- Estimate $\boldsymbol{\alpha}_{k|k}$ using the Kalman Filter. Equivalent to the Q.C.
- $\boldsymbol{\alpha}_k$: output deviation that will reappear at $k+1$
- $\mathbf{v}_k$: output deviation that will not reappear at $k+1$

We model the expected amplitude and frequency content of the disturbances and the correction vector with Σ_Δ, Σ_v.

Batch-to-Batch Strategies

Iterative Learning Control

Steps of the ILC algorithm. At each k:

1. $\mathbf{T}^r_k$ is set as the input to the PI controller, the batch is executed. $\tilde{\mathbf{S}}_k$ is estimated from measurements.
2. An additive correction of the nominal model is performed: $\hat{S}_k(\mathbf{T}^r) \triangleq \hat{S}(\mathbf{T}^r) + \boldsymbol{\alpha}_{k|k}$.
3. The corrected model is used to design $\mathbf{T}^r_{k+1}$ for the next batch to track a set-point $\overline{\mathbf{S}}_{k+1}$

$$\mathbf{T}^r_{k+1} = \arg \min_{\mathbf{T}^r \in \mathbb{R}^N} \|\overline{\mathbf{S}}_{k+1} - \hat{S}_k(\mathbf{T}^r)\|^2$$

Batch-to-Batch Strategies

Iterative Identification Control

IIC is based on a parametric correction assuming a certain model structure

$$\hat{S}(\mathbf{T}^r) \triangleq F_{ST^r}(\mathbf{T}^r;\theta) \qquad \textit{model structure}$$
$$\hat{S}_k(\mathbf{T}^r) \triangleq F_{ST^r}(\mathbf{T}^r,\hat{\theta}_k) \qquad \textit{corrected model}$$

Recursive estimation of $\hat{\theta}_k$ in a Bayesian framework.
Given a measurement $\tilde{\mathbf{y}}_k = (\tilde{\mathbf{T}}_k \; \tilde{\mathbf{C}}_k)^\top$:

- The *a posteriori* distribution $p_{\theta|\tilde{\mathbf{y}}_k}(\theta|\tilde{\mathbf{y}}_k)$ is computed (Bayes rules)
- $\hat{\theta}_k$ is taken as the max over θ of the distribution (MAP estimate)

In our case (under simplifying assumptions)

$$\hat{\theta}_k = \arg\min_{\theta} \left(\|\tilde{\mathbf{C}}_k - F_{CT}(\tilde{\mathbf{T}}_k, \hat{\theta}_k)\|^2_{\Sigma_e^{-1}} + \|\theta - \hat{\theta}_{k-1}\|^2_{\Sigma^{-1}_{\theta_{k-1}}} \right)$$

A Nonlinear Least Squares problem with a regularization term.

Batch-to-Batch Strategies

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Batch-to-Batch Strategies

Iterative Identification Control

Steps of the IIC algorithm. At each k:

1. $\mathbf{T}_k^r$ is set as the input to the PI controller, the batch is executed. $(\tilde{\mathbf{C}}_k, \tilde{\mathbf{T}}_k)^\top$ are measured.
2. The updated parameter $\hat{\theta}_k$ is computed and the corrected model is defined as $\hat{S}_k(\mathbf{T}^r) \triangleq F_{ST^r}(\mathbf{T}^r, \hat{\theta}_k)$.
3. The corrected model is used to design $\mathbf{T}_{k+1}^r$ for the next batch to track a set-point $\overline{\mathbf{S}}_{k+1}$

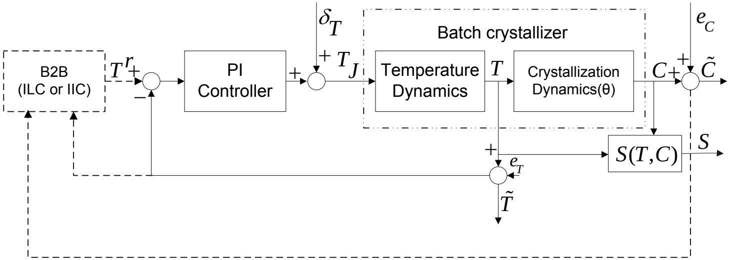
$$\mathbf{T}_{k+1}^r = \arg\min_{\mathbf{T}^r \in \mathbb{R}^N} \|\overline{\mathbf{S}}_{k+1} - \hat{S}_k(\mathbf{T}^r)\|^2$$

Outline

Simulation Results

Scenario

- Objective: tracking of a set-point $\overline{\mathbf{S}}_k$
- $N_{it} = 30$ iterations (batches)
- Set-point change in batch 11
- $\mathbf{T}^r_k$ updated from batch to batch using ILC and IIC

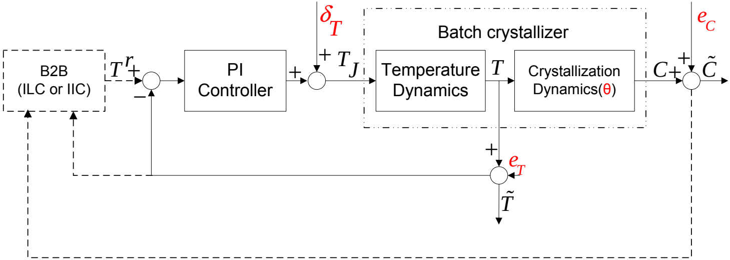


Simulation Results

Cases

Simulation study in two different scenarios

Case 1: Disturbances + parametric model mismatch



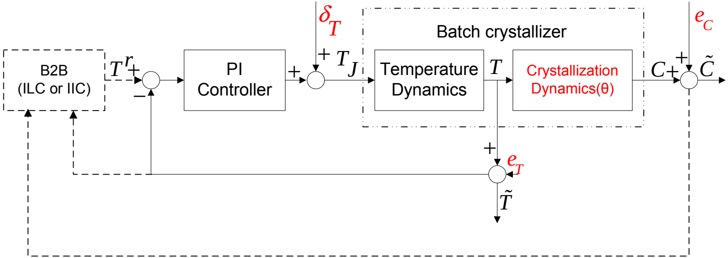
- White measurement noise on C and T
- Low-frequency disturbance on the jacket temperature T_J

Simulation Results

Cases

Simulation study in two different scenarios

Case 2: Disturbances + structural model mismatch



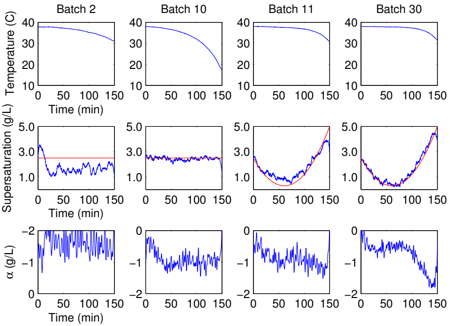
- Common situation in practice

Simulation Results

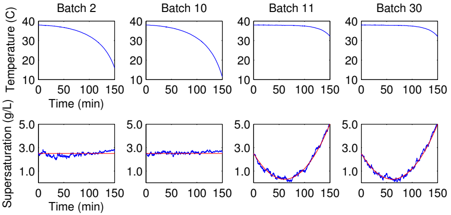
Case 1

Results for Case 1

Iterative Learning Control



Iterative Identification Control



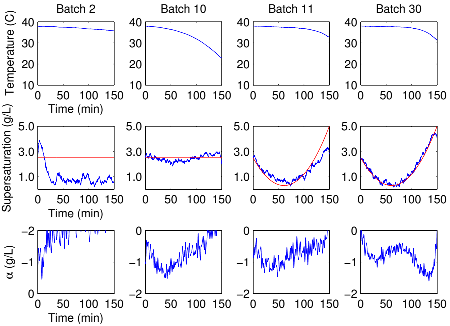
- IIC: faster convergence

Simulation Results

Case 2

Results for Case 2

Iterative Learning Control



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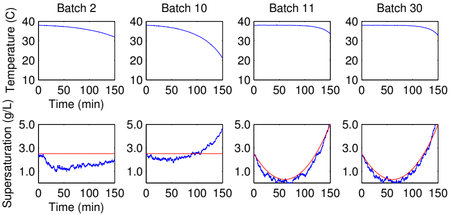


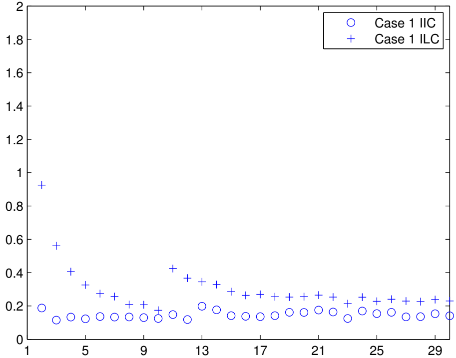
- ILC: convergence still despite mismatch

Simulation Results

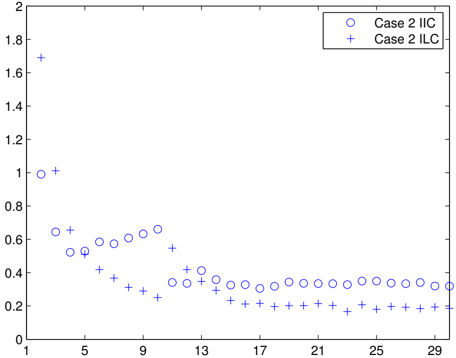
Overall results

Root Mean Square of the tracking Error $\frac{1}{\sqrt{N}}\|\bar{\mathbf{S}}_k - \tilde{\mathbf{S}}_k\|$

Case 1



Case 2



Outline

Control of Batch Cooling Crystallization

ILC vc IIC

Iterative Learning

- Tracking in presence of structure mismatch
- Close-form algorithm
- Slower convergence of the algorithm
- Learning of a trajectory: convergence lost if we change the set-point

Iterative Identification

- Fast convergence for the nominal case
- Learning of the full dynamics: easy to follow different setpoint
- Performance degradation with mismatches
- Numerical optimization required

- Combinig the strategies
- Consider system varying from batch to batch

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Thank you.
Questions?