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Nonlinear Model Predictive Control Using a Wiener model in a Continuous Polymerization Reactor

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Abstract

A subspace-based identification method of the Wiener model, consisting of a state-space linear block and a polynomial static nonlinearity at the output, is used to retrieve from discrete sample data the accurate information about the nonlinear dynamics. Wiener model may be incorporated into model predictive control (MPC) schemes in a unique way which effectively removes the nonlinearity from the control problem, preserving many of the favorable properties of linear MPC. The control performance is evaluated with simulation studies where the original first-principles model for a continuous MMA polymerization reactor is used as the true process while the identified Wiener model is used for the control purpose. On the basis of the simulation results, it is demonstrated that, despite the existence of unmeasured disturbance, the controller performed quite satisfactorily for the control of polymer qualities with constraints.

1. Introduction

In general, the modeling and control of polymerization reactors are difficult tasks for several reasons. These reactors often exhibit highly interactive nonlinear dynamic behavior and the first-principles model for a polymerization reactor may contain a large number of system parameters. Therefore, it may be advantageous to use a model structure whose parameters may be identified from input-output data. A Wiener system is given by the cascade interconnection of a linear time-invariant system with a static nonlinearity and is particularly useful in representing nonlinearities of a process without introducing the complications associated with general nonlinear operators. In the literature, the problem of Wiener model identification has been mostly analyzed in the prediction error framework. More recently, however, Westwick and Verhaegen proposed subspace based approach making use of the PI MOESP (Past Input MIMO Output-Error State-Space) method for the estimation of the system matrices of the linear part[1].

Introducing a nonlinear model into model predictive control(MPC) obviously increases the complexcity of the control algorithm. To reach a reasonable level of computational complexity, compromise can be made. The orthodox idea of nonlinear MPC is to use the nonlinear model for each prediction. According to the simplified option, the nonlinear model is linearized in each sampling interval, and the linearized model is used for prediction within the predictive horizon. This strategy cannot produce optimal results when a large set-point change occurs within the predictive horizon, but it reduces the computational effort significantly, so it is often used in real-life applications.

The structure of certain nonlinear models, such as Wiener and Hammerstein models, allows us to design a control structure which compensates for the nonlinearity of the model, so the process can be controlled with a linear model based MPC method. Such a scheme for a Wiener model was presented by Norquay *et al.*[2].

2. Continuous Polymerization Reactor Model

Here, we consider a continuous solution polymerization reactor system of methlymethacrylate (MMA) using benzoyl-peroxide (BPO) as the initiator and ethlyacetate (EA) as the solvent. The reaction kinetics are assumed to follow the free-radical polymerization mechanism including chain-transfer reactions to both solvent and monomer. The kinetic parameters are determined using the parameter estimation techniques and the gel effect is taken into account by the empirical correlations for the gel and glass effects proposed by Schmidt and Ray. The detailed correlations and other physical properties are presented in Ahn *et al.* [3].

One can derive the differential equations from the mass balances of various species in a polymerization reactor [3].

$$\frac{d(IV)}{dt} = q_f I_f - qI - k_d IV \tag{1}$$

$$\frac{d(MV)}{dt} = q_f M_f - qM - 2fk_d IV - (k_p + k_{trm})MG_0V \tag{2}$$

$$\frac{d(SV)}{dt} = q_f S_f - qS - k_{trs} SG_0V \tag{3}$$

$$\frac{d(G_0V)}{dt} = -qG_0 + 2fk_d IV - k_t {G_0}^2 V \tag{4}$$

$$\frac{d(G_1V)}{dt} = -qG_1 + 2fk_d IV + k_p MG_0V - k_t G_0G_1V + (k_{trm}M + k_{trs}S)(G_0 - G_1)V \tag{5}$$

$$\frac{d(G_2V)}{dt} = -qG_2 + 2fk_d IV + k_p M(G_0 + 2G_1)V - k_t G_0G_2V + (k_{trm}M + k_{trs}S)(G_0 - G_2) \tag{6}$$

$$\frac{d(F_0V)}{dt} = -qF_0 + \frac{1}{2}(k_t + k_{td}){G_0}^2V + k_{trm}MG_0V + k_{trs}SG_0V \tag{7}$$

$$\frac{d(F_1V)}{dt} = -qF_1 + k_t G_0G_1V + (k_{trm}M + k_{trs}S)G_1V \tag{8}$$

$$\frac{d(F_2V)}{dt} = -qF_2 + k_{tc}(G_0G_2 + {G_1}^2)V + k_{td}G_0G_2V + (k_{trm}M + k_{trs}S)G_2 \tag{9}$$

Here I, M, and S represent the concentrations of initiator, monomer and solvent, respectively, and subscript f denotes the feed condition. Also, q_f is the feed flow rate and q is the overflow rate that makes the reactor level fixed. The symbol f indicates the initiator efficiency. In addition, G_k and F_k denote the k-th moments of living and dead polymer concentrations, respectively. We also consider the energy balances for reactor and jacket, and use the equation for the volume change of the reaction mixture to calculate q [3].

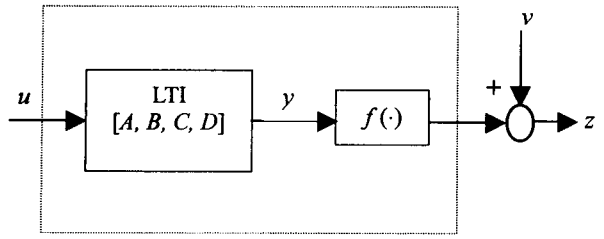

Figure 1. A schematic representation of the Wiener model.

3. Wiener System

We shall assume that the system to be identified may be described by the following Linear Time-Invariant (LTI) state space model :

$$x_{k+1} = Ax_k + Bu_{k-d}$$
$$y_{k+1} = Cx_k + Du_{k-d} \quad (10)$$

where $x_k \in R^n$ is the state vector, $u_k \in R^m$ the input vector, $y_k \in R^l$ the output vector and d the dead-time.

The measurement equation of the output is given by the expression :

$$z_k = f(y_k) + v_k \quad (11)$$

where $z_k \in R^l$ is the observed output, $f(\cdot): R^l \rightarrow R^l$ a non-linear vector function and v_k a zero-mean stochastic process of arbitrary color[4].

4. Procedure of Identifying Wiener System

For the identification of a continuous polymerization rector, we use the input-output data obtained from identification experiment for the continuous polymerization reactor. In this study, we use the inlet temperature of the reactor jacket T_{jin} (from 55°C to 85°C) and the feed flow rate q_f (from 5 *ml/min* to 25 *ml/min*) as the input signals. We use the pseudo random multi-level input signals because these are closer to white autocorrelation function, and excite adequately nonlinear modes of multiple-input/multiple-output system[5, 6].

For the purpose of evaluating the model accuracy measure, we use the Variance Accounted For (VAF) index, which is defined as follows :

$$\mathrm{VAF} = 100\left(1 - \frac{\sqrt{\sum_{i=1}^{N}(z_i - \hat{z}_i)^2}}{\sqrt{\sum_{i=1}^{N} z_i^2}}\right)$$

where N, z, and $\hat{z}$ denote the number of data points, the plant output and the identified model output, respectively. The VAF index is used as a measure of the relative accuracy of the model and its range is between $-\infty$ and 100%.

Identification is executed with reference to the systematic procedure to identify Wiener system proposed by Verheagen [4]. We first identify the LTI part of the Wiener system, using the PI(Past Input) subspace identification scheme as if the nonlinearities were not present and determine the order of the LTI system and the dead-time.

A MIMO static nonlinear function between the LTI outputs and the measured outputs is estimated on the basis of Tchebychev polynomials. Since the input used for identification is not Gaussian, the method used may give

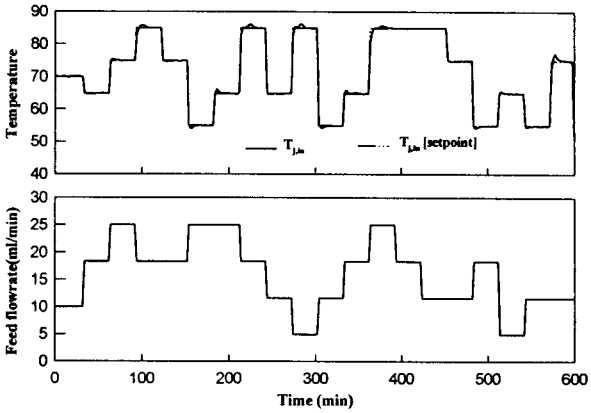

Figure 2. Identification input signals : (a) jacket inlet temperature (55 - 85°C), (b) feed flow rate (5 - 25 *ml*/min).

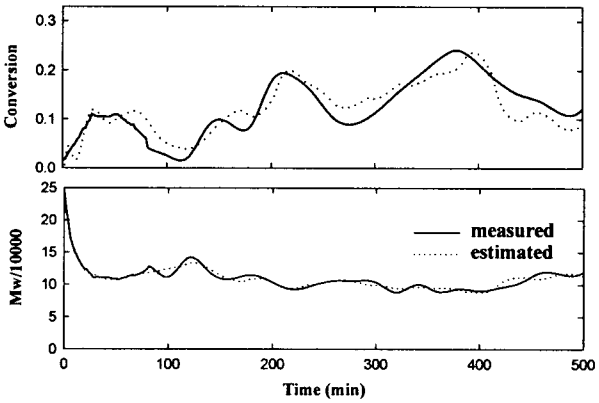

Figure 3. Comparison between the experimental ouputs (solid lines) and the outputs of the identified model (dotted lines) in the identification experiment.

biased estimate of the linear part. Therefore, we now need to use a nonlinear optimization technique to find the right model. Figure 2 presents the pseudo random multi-level input signals and Figure 3 shows a comparison between the experimental data and the response of the identified model to the same input. The VAF indices are 78.66 % and 93.78 % for conversion and *Mw*, respectively.

5. Wiener Model Predictive Control

The predictive control algorithm is based on a state-space MPC. The process is described by

$$x_{k+1} = Ax_k + Bu_k + B_d d_k + w_k$$
$$y_k = Cx_k \quad (12)$$
$$z_k = f(y_k) \quad (13)$$

where x_k, u_k, d_k, and w_k denote the state vector, the manipulated input vector, the measured disturbance vector, and the unmeasured disturbance, respectively. Also, y_k is the output vector of LTI state space model and z_k is the observed output vector. The state-space triplet $\{A, B, C\}$ of the linear block and the static nonlinear function $f(\cdot)$ in the Wiener model are identified in the previous identification step.

The inverse of the static nonlinear function is used in such a way that a linear model based MPC algorithm can be used to

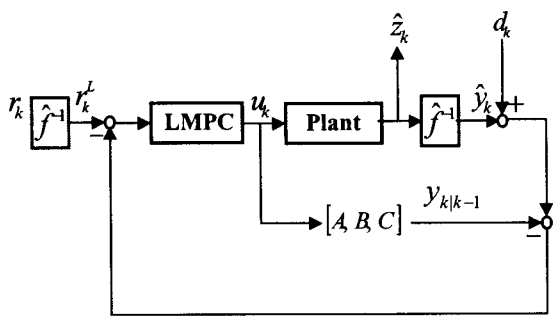

Figure 4. Block Diagram of the Wiener model predictive control concept.

control the nonlinear process. Of course, the static nonlineartiy must be invertible. The same inverse nonlinear function estimate is used for mapping the process output $\hat{z}_k$ to the controlled signal $\hat{y}_k$ and the reference signal r_k to the linearized reference r_k^L, so an inaccurate static nonlinearity estimate does not cause steady-state offset[7].

Differencing and rearranging the equation (12), we obtain the following augmented model:

$$\begin{bmatrix}\Delta x_{k+1}\\ y_{k+1}\end{bmatrix}=\begin{bmatrix}A & 0\\ CA & I\end{bmatrix}\begin{bmatrix}\Delta x_k\\ y_k\end{bmatrix}+\begin{bmatrix}B\\ CB\end{bmatrix}\Delta u_k+\begin{bmatrix}B_d\\ CB_d\end{bmatrix}\Delta d_k+\begin{bmatrix}I\\ CI\end{bmatrix}\Delta w_k$$
$$\hat{y}_k=\begin{bmatrix}0 & I\end{bmatrix}\begin{bmatrix}\Delta x_k\\ y_k\end{bmatrix}+v_k \tag{14}$$

Here Δ is the differencing operator and v_k is the measurement noise. Let Δw_k be white noise vector e_k so that w_k becomes the integrated white noise. In order to keep the notation simple, we express equation (14) as

$$\begin{aligned}X_{k+1}&=\Phi X_k+\Gamma\Delta u_k+\Gamma_d\Delta d_k+\Gamma_e e_k\\ \hat{y}_k&=\Xi X_k+v_k\end{aligned} \tag{15}$$

Then, state estimation is done by using a recursive Kalman filter as follows :

$$\begin{aligned}X_{k|k-1}&=\Phi X_{k-1|k-1}+\Gamma\Delta u_{k-1}+\Gamma_d\Delta d_{k-1}\\ X_{k|k}&=X_{k|k-1}+K(\hat{y}_k-y_{k|k-1})\end{aligned} \tag{16}$$

where $y_k=f^{-1}(\hat{z}_k)$ and $y_{k|k-1}=\Xi X_{k|k-1}$.

The prediction equation for p sampling intervals into the future can be written as equation (17), where m denotes the control horizon (that is, $\Delta u_{k+m|k}=\cdots=\Delta u_{k+p-1|k}=0$).

$$\begin{bmatrix}y_{k+1|k}\\ y_{k+1|k}\\ \vdots\\ y_{k+1|k}\end{bmatrix}=\begin{bmatrix}\Xi\Phi\\ \Xi\Phi^2\\ \vdots\\ \Xi\Phi^p\end{bmatrix}X_{k|k}+\begin{bmatrix}\Xi\Gamma_d\\ \Xi\Phi\Gamma_d\\ \vdots\\ \Xi\Phi^{p-1}\Gamma_d\end{bmatrix}\Delta d_k+\begin{bmatrix}\Xi\Gamma_d & 0 & \cdots & 0\\ \Xi\Phi\Gamma_d & \Xi\Gamma & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ \Xi\Phi^{p-1}\Gamma & \Xi\Phi^{p-2}\Gamma & \cdots & \Xi\Phi^{p-m}\Gamma\end{bmatrix}\Delta U_k \tag{17}$$

The above prediction equation can be simplified as follows :

$$Y_{k+1|k}=S^X X_{k|k}+S^d\Delta d_k+S^u\Delta U_k \tag{18}$$

On the basis of the prediction equation (18), a sequence of optimal control moves can be computed, which minimizes the following objective function with the input magnitude, rate and output magnitude constraints;

$$\min_{\Delta U_k}\left(Y_{k+1|k}-R^L{}_{k+1|k}\right)^T\overline{Q}\left(Y_{k+1|k}-R^L{}_{k+1|k}\right)+\Delta U_k{}^T\overline{R}\Delta U_k \tag{19}$$

where $R^L{}_{k+1|k}=[f^{-1}(r_{k+1|k})^T,\cdots,f^{-1}(r_{k+p|k})^T]^T$ is the linearized reference vector available at time k. $\overline{Q}$ and $\overline{R}$ are weighting matrices both of which are diagonal;

$$\overline{Q}=\begin{bmatrix}\ddots & & \\ & (\Lambda^y)^T\Lambda^y & \\ & & \ddots\end{bmatrix},\quad \overline{R}=\begin{bmatrix}\ddots & & \\ & (\Lambda^u)^T\Lambda^u & \\ & & \ddots\end{bmatrix} \tag{20}$$

where Λ^y and Λ^u are weighting factors of output and input, respectively. The optimization is solved via quadratic programming (QP) and only the first computed control move Δu_k is implemented. Also the whole optimization procedure is repeated at the next sampling time.

5. Simulation Results

The first-principles model of the MMA continuous polymerization reactor played the role of the real process while the predictive controller uses its discrete-time Wiener model. The set of reference conditions for the simulation is given in Table 1.

Table 1. Reference conditions for the continuous MMA polymerization reactor

	Initial charge	Feed concentration
Monomer	0.45 *l*	4.65 *mol/l*
Solvent	0.45 *l*	5.04 *mol/l*
Initiator	4.50g	0.02 *mol/l*

The sampling time of the discrete-time control algorithm is 2 min. In this case, the manipulated variable is the jacket inlet temperature and the controlled variables are the weight-average molecular weight and the monomer conversion. The maximum and minimum constraints of the jacket inlet temperature are 90 and 50 °C, respectively and the feed flow rate is maintained at 10 ml/min. It is assumed that the 1 % white noises are added for the measurements. Other parameters for two cases are shown in Table 2.

Table 2. Control tuning parameters used

Case	p	M	Λ^y	Λ^u	Setpoint
1	15	7	50	1	0.15→0.25→0.2
2	15	10	1	1	16.96→13→8→10

Control variable : Case 1 - Conversion
Case 2 – *Mw*/10,000

The simulation results for set point tracking control are shown in Figures 5 and 6. For stability of estimator, the initial states are taken as the steady state values which were calculated previously. In Figure 5, the controller quickly drives the conversion to its set point when the setpoints are raised to 0.15 and 0.25, respectively. When the setpoint falls from 0.25 to 0.20, however, the response is slow and the undershoot in

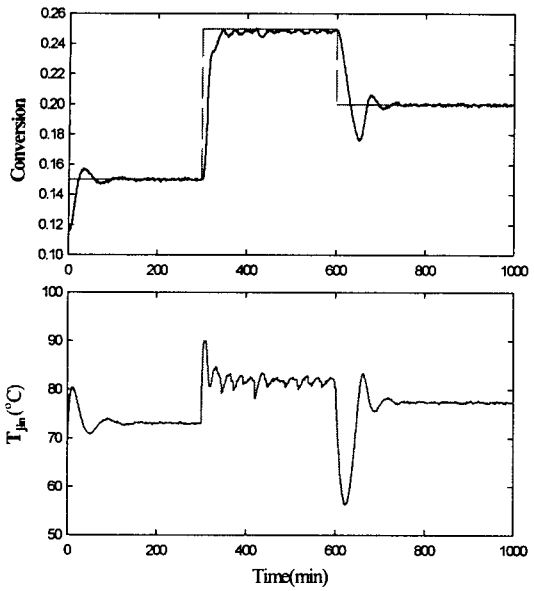

Figure 5. (Case 1) Servo and regulatory performances of Wiener model predictive control (the manipulated variable : $T_{j,in}$, the controlled variable : conversion).

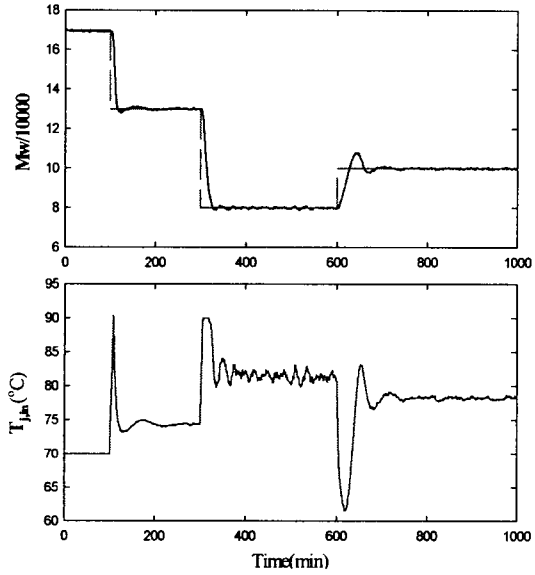

Figure 6. (Case 2) Servo and regulatory performances of Wiener model predictive control (the manipulated variable : $T_{j,in}$, the controlled variable : *Mw*).

the conversion is observed.

Figure 6 presents the performance of Wiener MPC for step changes in the setpoint for *Mw*. Within the first 100 min, the jacket inlet temperature is maintained at 70 °C. For the decrease in the *Mw* setpoint to 130,000 *g/mol*, the controller output (the setpoint of jacket inlet temperature) reaches a peak of its upper bound at 90 °C and subsequently varies around its steady-state value. For the second decrease in the *Mw* setpoint to 80,000 *g/mol*, the controller output fluctuates around its steady-state value. When there is an increase in the *Mw* setpoint to 100,000 *g/mol*, the control output touches bottom and shows the overshoot. Also, the response of *Mw* is slow and the overshoot is observed. From Figures 5 and 6, when the dramatic decrease of the jacket inlet temperature are needed, the control variable responds slowly and shows the overshoot or the undershoot.

5. Concluding Remarks

In this work, a case study evaluation of a Wiener model based model predictive control is conducted. At first, a Wiener model is developed by using subspace identification to describe the relationship between the manipulated variables (*e.g.* jacket inlet temperature and feed flow rate) and the important qualities (*e.g.* conversion and weight average molecular weight (*Mw*)) in a continuous polymerization reactor. As a result, we can obtain the accurate MIMO Wiener model without the exhaustive "trial-and-error" search procedure.

With an invertible static nonlinearity, the performance index of Wiener model predictive control has no local minima, which may cause problems with the common nonlinear model predictive control algorithms. The simulation results show that the controller performed quite satisfactorily for the control of polymer qualities in a continuous polymerization reactor under the presence of unmeasured disturbance.

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