BILINEAR VERSUS LINEAR MPC: APPLICATION TO A POLYMERIZATION PROCESS

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Abstract: In this paper a comparison between a linear-model-based and a bilinear-modelbased identification and predictive control methodology is presented. Input-output data from a nonlinear first-principles simulation model of the free-radical polymerization of methylmethacrylate are used for black-box identification of a linear and a bilinear model. These black-box models are used within a model-based predictive controller that controls the nonlinear white-box simulation model. The results demonstrate a better performance of the bilinear-model-based methodology compared to the linear-model-based methodology.

Keywords: Bilinear systems, Predictive control, Subspace methods, Polymerization

1. INTRODUCTION

For many processes linear models can approximate accurately the process behavior about a single setpoint, i.e. in a narrow operating region. However, an increasing demand for flexibility of many processes requires that these processes are operated over larger operating regions. Due to the intrinsic nonlinearity of almost all processes, often linear models cannot approximate accurately the process behavior over these larger operating regions. In such cases nonlinear models are required for accurate approximate modeling.

In this paper the potential of a bilinear-model-based approach is demonstrated. The "real" process considered in this paper is a continuous-time white-box simulation model of the free-radical polymerization of methylmethacrylate (Schmidt and Ray, 1981), and is presented in detail in section 2. Note that this is a "general" nonlinear model (neither linear nor bilinear). From data obtained from an identification experiment both a linear and a bilinear model are computed. The identification algorithms are briefly described in section 3. These models are used within a model-based predictive control (MPC) framework based on the quasi-infinite horizon paradigm (Chen and Allgöwer, 1998). The details of the MPC algorithms are presented in section 4. In section 5 the identification and control results are presented both for the linear model and the bilinear model. Finally, a discussion is presented in section 6.

2. THE PROCESS

The process under consideration is a nonlinear whitebox simulation model of the free-radical polymerization of methylmethacrylate in a constant volume continuous stirred tank reactor. The model equations of this simulation model are given by (Schmidt and Ray, 1981):

$$\frac{\partial I}{\partial t} = \frac{q_f}{V} I_f - \frac{q}{V} I - k_d \cdot I \tag{1}$$

$$\frac{\partial M}{\partial t} = \frac{q_f}{V} M_f - \frac{q}{V} M - k_p \cdot M \cdot P \tag{2}$$

$$\frac{\partial S}{\partial t} = \frac{q_f}{V} S_f - \frac{q}{V} S \tag{3}$$

$$\frac{\partial T}{\partial t} = \frac{q_f}{V} T_f - \frac{q}{V} T + \frac{-\Delta H_p}{\rho \cdot C_p} k_p \cdot M \cdot P$$
$$-\frac{h \cdot A_c}{V \cdot \rho \cdot C_n} (T - T_c), \tag{4}$$

where q_f and q are the inlet and outlet flow rate respectively, V is the reactor volume; I_f , M_f and S_f denote the initiator, monomer and solvent concentrations in the feed, respectively; I, M and S denote the initiator, monomer and solvent concentrations in the reactor, respectively; T_f , T and T_c denote the temperature of the feed, the reactor and the cooling jacket, respectively; ΔH_p is the reaction enthalpy; ρ and C_p are the density and heat capacity of the reactor contents, respectively; h is the heat transfer coefficient to the reactor; A_c is the heat transfer area of the reactor; P is the total concentration of growing free radicals in the reactor, given by:

$$P = \left(\frac{2f \cdot k_d \cdot I}{k_t}\right)^{\frac{1}{2}},\tag{5}$$

where f is the initiator efficiency. Due to the increase in density as a result from the conversion of monomer to polymer, the outlet flow rate differs from the inlet flow rate and is given by:

$$q = q_f (1 + \epsilon_p x_p), \tag{6}$$

where

$$\epsilon_p = M \cdot W_m \left(\frac{1}{\rho_p} - \frac{1}{\rho_m}\right) \tag{7}$$

$$x_p = \frac{\phi_p \rho_p}{\phi_p \rho_p + W_m \cdot M}.$$
(8)

 W_m is the molecular weight of monomer, ρ_p and ρ_m are the densities of polymer and monomer, respectively; ϕ_p is the volume fraction of polymer. For the reaction rates the following holds:

$$k_d = 1.69 \cdot 10^{14} \exp\left(\frac{-30000}{R \cdot T}\right)$$
 (9)

$$k_p = k_{p0} \cdot g_p \tag{10}$$

$$k_t = k_{t0} \cdot g_t \tag{11}$$

where R is the gas constant,

$$k_{p0} = 4.92 \cdot 10^5 \exp\left(\frac{-4353}{R \cdot T}\right)$$
 (12)

$$k_{t0} = 9.8 \cdot 10^7 \exp\left(\frac{-701}{R \cdot T}\right),$$
 (13)

and the functions g_p and g_t , which are due to the "gel effect", are given by:

$$g_p = \begin{cases} 1, & V_f > 0.05 \\ 7.1 \cdot 10^{-5} \exp(171.53 \cdot V_f), & V_f \le 0.05 \\ g_t = \\ 10.10575 \cdot \exp(17.15 \cdot V_f - 0.01715(T - 273.2)) \\ & V_f > (0.1856 - 2.965 \cdot 10^{-4}(T - 273.2)) \\ 2.3 \cdot 10^{-6} \cdot \exp(75V_f) \\ & V_f \le (0.1856 - 2.965 \cdot 10^{-4}(T - 273.2)) \end{cases}$$

where the total free volume V_f is given by (Kurtz *et al.*, 2000):

$$V_f = \max[V_{fp}\phi_p + V_{fm}\phi_m + V_{fs}\phi_s , 0], (14)$$

where ϕ_p , ϕ_m , ϕ_s are the volume fractions of polymer, monomer and solvent in the mixture, calculated from:

$$\phi_m = \frac{W_m \cdot M}{\rho_m} \tag{15}$$

$$\phi_s = \frac{W_s \cdot S}{\rho_s} \tag{16}$$

$$\phi_p = \frac{\rho - \phi_m \rho_m - \phi_s \rho_s}{\rho_p},\tag{17}$$

under the assumption that the volume fraction of initiator is approximately zero. W_s and ρ_s are the molecular weight and the density of the solvent respectively. V_{fp} , V_{fm} and V_{fs} are given by:

$$V_{fm} = 0.025 + 0.001(T - 167) \tag{18}$$

$$V_{fn} = 0.025 + 0.00048(T - 387) \tag{19}$$

$$V_{fs} = 0.025 + 0.001(T - 181).$$
 (20)

In this paper the manipulable input is chosen to be the monomer concentration in the feed (which affects the solvent concentration in the feed), and the output is chosen to be the monomer concentration in the reactor. The values of the remaining model parameters are listed in table 1.

3. IDENTIFICATION

The bilinear model that is to be identified has the structure:

$$x(k+1) = Ax(k) + (B + [F_1x(k), \dots, F_mx(k)]) u(k) (21)$$
$$y(k) = Cx(k),$$
(22)

where $x \in \mathbb{R}^n$ is the state, $u \in \mathbb{R}^m$ is the input, and $y \in \mathbb{R}^p$ is the output. The matrices

parameter	value	unit	source
R	1.987	$cal/(K \cdot mole)$	
f	0.5		1,2,3
C_p	0.4	$cal/(g \cdot K)$	1,2
ρ	1038	g/L	1,2
$ ho_s$	901	g/L	2
$ ho_m$	939	g/L	2
$ ho_p$	1200	g/L	2
h	135.6	$cal/(m^2 \cdot s \cdot K)$	1
A_c	2.8	m^2	1
$-\Delta H_p$	$13.8\cdot10^3$	cal/mole	1
W_s	88.10	g/mole	2
W_m	100.11	g/mole	2,3
q_f	0.2813	L/s	2
Ň	900	L	2
I_f	0.02	mole/L	
T_{f}	298	K	3
T_c	350	Κ	
1. (Adebekun and Schork, 1989)			
2. (Kurtz et al., 2000)			
3. (Schmidt and Ray, 1981)			

 Table 1. Parameter values of the white-box polymerization model

 $A, B, C, F_1, \ldots, F_m$ are state-space matrices of conformal dimensions. For the process under consideration m = p = 1. The linear model has a structure similar to that of (21)–(22), but then F_1, \ldots, F_m are equal to zero.

The linear model is identified with the PO-MOESP subspace method (Verhaegen, 1994).

The bilinear model is obtained by a two step procedure. First, a bilinear subspace identification method is used to obtain an initial estimate of the system. Second, a nonlinear optimization-based approach is used to improve this initial estimate.

The key point in subspace identification for bilinear systems is the reconstruction of the state sequence. Once an estimate of the state sequence is available the system matrices follow by solving two least squares problems based on (21)–(22); the system matrices are estimated as

$$[\widehat{A}, \widehat{B}, \widehat{F}_{1}, \dots, \widehat{F}_{m}] = \widehat{X}_{2,N+1} \Phi_{1,N}^{T} \left(\Phi_{1,N} \Phi_{1,N}^{T} \right)^{-1} \\ \widehat{C} = Y_{1,N} \Phi_{1,N}^{T} \left(\Phi_{1,N} \Phi_{1,N}^{T} \right)^{-1},$$

where

$$\widehat{X}_{1,N} = \left[\ \widehat{x}(1) \ \widehat{x}(2) \ \cdots \ \widehat{x}(N) \ \right],$$

is the state estimate obtained from the bilinear subspace method, and

$$\Phi_{1,N} := \begin{bmatrix} X_{1,N} \\ U_{1,N} \\ U_{1,N} \odot \widehat{X}_{1,N} \end{bmatrix},$$
(23)

with $U_{1,N}$ and $Y_{1,N}$ defined similar to $\widehat{X}_{1,N}$. The symbol \odot is used to denote the Khatri-Rao product, which is a column-wise Kronecker product for two matrices with an equal number of columns. Let $M \in \mathbb{R}^{p \times q}$ and $N \in \mathbb{R}^{r \times q}$ be two arbitrary matrices, then the Khatri-Rao product of these matrices equals:

$$M \odot N = \left[m_1 \otimes n_1 \ m_2 \otimes n_2 \ \dots \ m_q \otimes n_q \right],$$

where \otimes denotes the Kronecker product, and m_i and n_i (i = 1, 2, ..., q) denote the columns of the matrices M and N, respectively.

The bilinear subspace identification method that is used in this paper, was described in detail by (Favoreel, 1999). It can also be obtained as a special case of the subspace identification method for linear parametervarying (LPV) systems presented by (Verdult and Verhaegen, 2000). The bilinear system can be viewed as an LPV system with an 'A' matrix that depends in an affine way on a time-varying parameter, which equals the input.

First, the available measurements of u_k and y_k are stored in some structured matrices, which are defined as

$$U_{k} := [u(k), u(k+1), \dots, u(k+N-1)]$$

$$Y_{k} := [y(k), y(k+1), \dots, y(k+N-1)]$$

$$Y_{j|j} := \begin{bmatrix} Y_{j} \\ P_{j} \odot Y_{j} \end{bmatrix}, \quad Y_{k+j|j} := \begin{bmatrix} Y_{k+j} \\ Y_{k+j-1|j} \\ U_{k+j} \odot Y_{k+j-1|j} \end{bmatrix}$$

$$\mathcal{Y}_{j|j} := Y_{j}, \quad \mathcal{Y}_{k+j|j} := \begin{bmatrix} Y_{k+j} \\ \mathcal{Y}_{k+j-1|j} \end{bmatrix}$$

The matrix $U_{k+j|j}$ similar to $Y_{k+j|j}$.

The next step is to perform the following QR factorization:

$$\begin{bmatrix} W_{j,0} \\ Z_{s,j,0} \\ \mathcal{Y}_{k+j|j} \end{bmatrix} = \begin{bmatrix} R_{11} & 0 & 0 \\ R_{21} & R_{22} & 0 \\ R_{31} & R_{32} & R_{33} \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix}, \quad (24)$$

with

$$W_{j,0} := \begin{bmatrix} U_{j-1|0} \\ Y_{j-1|0} \end{bmatrix}, \ Z_{s,j,0} := \begin{bmatrix} U_{s+j} \\ U_{s+j-1|j} \\ U_{s+j-1|j} \odot W_{j,0} \end{bmatrix}$$

It can be shown that

$$\Gamma_s X_j \approx \overline{R}(:, 1: n_w) W_{j,0}, \qquad (25)$$

where

$$\Gamma_s := \begin{bmatrix} CA_0^s \\ \vdots \\ CA_0 \\ C \end{bmatrix}, \quad \overline{R} := \begin{bmatrix} R_{31}, R_{32} \end{bmatrix} \begin{bmatrix} R_{11} & 0 \\ R_{21} & R_{22} \end{bmatrix}^{-1},$$

and n_w is the total number of rows in $W_{j,0}$.

The final step is to recover the state sequence. Based on equation (25) the state sequence can be recovered up to an unknown similarity transformation from a singular value decomposition (SVD) of the matrix $\overline{R}(:, 1: n_w)W_{j,0}$. Let this SVD be given by

$$\overline{R}(:,1:n_w)W_{j,0} = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix},$$

with $\Sigma_1 \in \mathbb{R}^{n \times n}$, then the state sequence can be estimated as $\widehat{X}_j = \Sigma_1^{1/2} V_1^T$, provided that $s \ge n-1$

and $j \ge n$. If the noise is not excessive, the singular values contained in Σ_1 will be much larger than the ones in Σ_2 ; and the order n of the system can be determined from this singular value decomposition.

A major problem with the subspace method described above is the fact that the number of rows in the data matrices $W_{j,0}$ and $Z_{s,j,0}$ grows exponentially with the block sizes j and s. Since the block sizes have to satisfy $s \ge n-1$ and $j \ge n$, already for relatively low order systems (small values for n) the number of rows in the data matrices can be too large to be handled on the average computer. To solve this problem, (Verdult and Verhaegen, 2000) described a method to reduce the dimensions of the data matrices. This method is basically a subset selection method based on a OR factorization that selects only the most dominant rows from the matrices $W_{j,0}$ and $Z_{s,j,0}$, and uses only these rows to compute the QR factorization (24). Since only the most dominant rows are used, an approximation error is introduced.

The bilinear model obtained from the subspace identification step is improved by using a nonlinear optimization-based method that minimizes the output error. Since the bilinear system can be regarded as a special case of an LPV system, the iterative LPV identification method proposed by (Lee and Poolla, 1999) can be used. This method uses a full parameterization of the system matrices. The resulting non-uniqueness of the state-space representation is dealt with by determining at each iteration the directions that do change the value of the cost function and only updating the parameters along these directions. This leads to numerical advantages: no special parameterization of the bilinear system is needed, the active parameters are determined from the data.

4. PREDICTIVE CONTROL

Suppose that the desired setpoint is the origin. Then the performance index to be minimized is given by (notation: $||b||_{\Psi}^2 = b^T \Psi b$):

$$J(k) = \sum_{i=1}^{H_s} \{ ||y(k+i)||_{Q_y}^2 + ||u(k+i-1)||_{R_u}^2 \} + ||x(k+H_s)||_{P_x}^2,$$
(26)

where Q_y and R_u are positive-definite weighting matrices, and P_x is a positive-definite weighting matrix such that $||x(k + H_s)||_{P_x}^2$ is an upper bound for the summation of the first two terms in (26) for $i = H_s +$ $1, \ldots, \infty$, under the restriction that $x(k + H_s)$ belongs to a target set (defined by an end-point inequality constraint) which is invariant under the model in closed loop with a feedback law. This corresponds to the so-called quasi-infinite-horizon paradigm (Chen and Allgöwer, 1998). For linear and bilinear models of which A has eigenvalues strictly within the unit disc, and in the presence of only input constraints, the above-mentioned feedback law is trivially given by u = 0 and the target set corresponds to the entire state space. Then P_x is given by the solution to the following Lyapunov equation:

$$P_x - A^T P_x A = A^T C^T Q_y C A.$$
⁽²⁷⁾

Since in this paper the models (linear and bilinear) are obtained via an open-loop identification experiment, the plant can only be operated in a stable operating region. Therefore it is plausible that the identified models have A matrices of which the eigenvalues are strictly within the unit disc.

If the desired setpoint does not correspond to the origin, the model can be shifted such that the origin of the shifted model corresponds to the desired setpoint of the original model, and one may proceed as above for the shifted model. If the model is linear, then the dynamics of the shifted model are equivalent to that of the original model (i.e. then shifting only affects an off-set term in the input, state and output). If the model is nonlinear the model equations are affected as well. Suppose the desired setpoint for a bilinear model is specified by $u = u_{ss}, x = x_{ss}, y = y_{ss}$. This corresponds to the origin of the shifted model in deviation variables $\bar{u} = u - u_{ss}, \bar{x} = x - x_{ss}, \bar{y} = y - y_{ss}$, where the shifted model is given by:

$$\bar{x}(k+1) = \bar{A}\bar{x}(k) + \left(\bar{B} + [F_1\bar{x}(k), \dots, F_m\bar{x}(k)]\right)\bar{u}(k)$$
(28)
$$\bar{y}(k) = C\bar{x}(k),$$
(29)

where

$$\bar{A} = A + \sum_{j=1}^{m} F_j u_{ss,j} \tag{30}$$

$$\bar{B} = B + [F_1 x_{ss}, \dots, F_m x_{ss}];$$
 (31)

i.e. shifting of the bilinear model affects the matrices A and B of the shifted model.

The minimization of (26) may be subject to input, state and output constraints. In this paper the input (provided by the controller) is constrained to lie within the range that is used for the identification experiment, in order to operate the process in the region in which it has been identified. Thus the minimization of (26) is subject to the constraints:

$$u_{min} \le u(k+i-1) \le u_{max} \tag{32}$$
$$\forall i = 1, \dots, H_s,$$

where for a feasible setpoint u = 0 must be feasible. For the derivation of P_x , equation (27), the inputs beyond time instant $k + H_s$ are assumed to be zero. In this way the input constraints are satisfied over the quasi-infinite horizon if (32) is satisfied over the finite horizon from k till $k + H_s - 1$. For linear models the problem of minimizing (26) subject to (32) is convex and can be solved by quadratic programming; for bilinear models this minimization problem is nonconvex. Algorithms for solving these bilinear MPC problems can be found in (Bloemen *et al.*, 2001).

In order to obtain a good controller performance the identified model, which is used within the controller, should be able to approximate accurately the behavior of the process (in this paper the white-box simulation model). However, in practice some degree of model mismatch is unavoidable (this could also arise on account of disturbances for example). In this paper the controller copes with model mismatch by adding the modeling error

$$e(k) = y_p(k) - y(k),$$
 (33)

to the predictions of the model

$$y(k+i) = Cx(k+i) + e(k), \ i \ge 1,$$
 (34)

where in (33) y_p is the output of the controlled process (Henson, 1998). Given a desired setpoint y_{ss} , a certain e(k) will affect the setpoints u_{ss} and x_{ss} . Again, the shifted model for this setpoint can be represented as (28)–(29). The feedback path (33)–(34) enables one to eliminate steady state off-set.

5. RESULTS

For the identification experiment, the volume fraction of monomer in the feed was varied between 0.5 and 0.9. The input signal was specified by a pseudorandom multi-level signal with a minimum switching time of 5 samples, a maximum switching time of 40 samples, an average switching time of 15 samples, and a sampling time of two minutes. The continuous-time white-box polymerization model was simulated with this input signal. No measurement noise was added in order to focus on the differences between the linearand the bilinear-model-based approach caused by the nonlinearity of the white-box simulation model (the modeling error can be regarded as process noise and is handled through (33)–(34) by the controller). Output data were collected over a period of 1500 samples with a sampling time of two minutes. The first 1000 data points were used for identification, the last 500 data points were used for validation, both for a linear model and for a bilinear model. The block size used in the linear subspace method was 5. The block sizes used in the bilinear subspace method were s = j - j1 = 4. With this choice, the matrix $W_{j,0}$ contains 60 rows, and the matrix $Z_{k,j,0}$ contains 436 rows. Subset regression was used to select the 12 most dominant rows from $W_{i,0}$ and the 33 most dominant rows from the $Z_{k,i,0}$.

Based on the singular values of the subspace identification algorithms for the linear and the bilinear models, the orders of both the linear model and the bilinear model were selected to be 3.

To measure the performance of the estimated models the variance accounted for (VAF) was used, The VAF is defined as

$$\text{VAF} = \max\left\{1 - \frac{\operatorname{var}(y_p(k) - y(k))}{\operatorname{var}(y_p(k))}, 0\right\} \times 100\%,$$

where $y_p(k)$ denotes the real output (polymerization process), and y(k) denotes the output of the blackbox model, and var(·) denotes the variance of a quasistationary signal. The VAF indices for the linear model were 94% and 92% for the identification data and validation data, respectively. The VAF indices for the bilinear model were 99% and 96% for the identification data and validation data, respectively. This indicates that the approximating ability of the bilinear model is better than that of the linear model for this example.

The tuning parameters of both the linear-model-based predictive controller (LMPC) and the bilinear-modelbased predictive controller (BMPC) were set to: $H_s =$ 3, $Q_y = 100$, $R_u = 1$. The input M_f was restricted such that the volume fraction of monomer in the feed remained between 0.5 and 0.9. The setpoint for the output M was changed every 50 samples, as indicated in figures 1 and 2, where the control results for LMPC and BMPC, respectively, are plotted. Due to space restrictions the input signals are not shown.

During the first 150 samples of figures 1 and 2 the performances of LMPC and BMPC were similar. During the first 150 samples the MPC algorithms operate approximately at the center of the operating region used for identification. In this region the behavior of the process is modeled well both by the linear model and by the bilinear model, resulting in a similar performance for both LMPC and BMPC. However, for larger values of M the approximation of the behavior of the process by the linear model deteriorates, which results in an oscillatory response of LMPC between samples 150 and 200, and, even more pronounced, between samples 350 and 400, see figure 1. The approximating properties of the bilinear model, indicated by the higher VAF values, are better than those of the linear model. Consequently, the performance of BMPC is better than that of LMPC for operating points that lie further from the center of the operating region used for identification. Between samples 150 and 200 and between samples 350 and 400 BMPC performs well, whereas LMPC does not, compare figures 1 and 2. The oscillatory behavior of the plant in closed loop with LMPC can be prevented by tuning down the controller. For this example this requires Q_y to be reduced to 1 for LMPC (data not shown). However, this re-tuning makes the controller very conservative which leads to a very slow response over the entire operating region, in which case the performance of LMPC using $Q_y = 1$ is (still) inferior to that of BMPC using $Q_y = 100$.



Fig. 1. Control results for LMPC; solid is the output M, dashed is the setpoint for M.

6. DISCUSSION

In this paper the performances of a linear-model-based and bilinear-model-based predictive control framework have been compared. Both MPC algorithms have been used to control a white-box simulation model of the free-radical polymerization of methylmethacrylate. Due to the intrinsic nonlinear nature of this model, a linear model cannot approximate accurately the behavior of the process over a large operating region. Bilinear models, which can be regarded as an extension of linear models by incorporating a product term between the current input and the current state into the state equation, possess more degrees of freedom and therefore should, from a theoretical point of view, be able to approximate the behavior of a nonlinear process more accurately than linear models. This has been demonstrated for the case study in this paper, where the higher VAF indices for the bilinear model than that for the linear model indicate a better approximation of the behavior of the nonlinear process by the bilinear model than by the linear model.

For MPC algorithms it is obvious that the quality of the controller depends on the quality of the model, see also figures 1 and 2. The performance of LMPC and BMPC is comparable when the process is operated at the center of the operating region which is used for identification. This is due to the fact that both for the linear and the bilinear model some "average" model is identified over the entire operating region, which will be most valid at the center of the operating region (under the assumption that the nonlinearity of the model over the entire operating region is averaged at the center). Further away from this center the performance of LMPC is worse than that of BMPC since the approximation of the nonlinear behavior by the linear model is worse than that by the bilinear model.

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Fig. 2. Control results for BMPC; solid is the output M, dashed is the setpoint for M.

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