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Multivariable Nonlinear Advanced Control of Copolymerization Processes

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Abstract

A reliable multivariable model of a process is a fundamental prerequisite for the design of an efficient control strategy. Though, such a model is often very hard to obtain via a first-principles approach. The development of two fuzzy model-based multivariable nonlinear predictive control schemes and their implementation on a copolymerization process are described in this paper. Multi-input/single-output models are developed using fuzzy logic and combined to form a parallel system model for simulation and on-line prediction. The behavior of the outlined controllers were compared to the dynamic matrix control (DMC) and to a typical nonlinear model-based predictive control (NMPC) for regulatory problem and the obtained results showed the effectiveness of the proposed structures.

Keywords: nonlinear model-based multivariable predictive control, nonlinear system identification, fuzzy dynamic model, copolymerization

1. Introduction

Control of copolymerization processes is characterized by the existence of operational constraints due to economic or safety concerns as well as restrictions related to equipment size/capacity/design. In addition, such systems present strong interactions among variables and they are intrinsically multivariable and nonlinear, by making the performance of conventional controllers to be poor or to require considerable efforts in controller tuning (Lima *et al.*, 2009a). To cope with this fact, model-based predictive control (MPC) has been the most successful advanced control technique applied to the chemical process industry. This formulation basically handles time-delays, multivariable interactions and constraints, where the dynamical model is directly implemented in the control structure (Manenti *et al.*, 2009; Manenti and Rovaglio, 2008).

However, it is very difficult to build up a sufficiently detailed physical model (white box model) able to take into account the main phenomena taking place within the process. Difficulties are related to the large amount of differential and algebraic equations and the solution of these models could take a relevant mathematical effort, sometimes requiring simplifications which create uncertainties about the solution accuracy obtained. Moreover, such models have to be integrated in a relatively short period of time (Lima *et al.*, 2009b) to ensure the on-line feasibility of control and optimization procedures. Thus, accurate nonlinear models based on input-output data (black box models) using soft computing techniques are increasingly being used in model-based control.

This work presents the development of two multivariable nonlinear predictive controllers based on linear and exponential fuzzy models (in the following, LFMPC and NFMPC, respectively) for a copolymerization process. So, internal models for the controllers are developed through the fuzzy logic, accounting for both process restrictions and nonlinearities. Such an approach takes the great benefit of not requiring a deep process acquaintance and understanding, which makes it widely applicable in the case of complex systems. The copolymer solution of methyl metacrylate and vinyl acetate was considered to check the performance of the proposed control structures. Specifically, the copolymerization process consists of a jacketed continuous stirred tank reactor, a separator, and a recycle loop. The behavior of the control strategies here proposed was compared to the well-established methodologies of optimal control (Dynamic Matrix Control, DMC, and Nonlinear Model Predictive Control, NMPC) for regulatory problems. The comparison highlighted the significant robustness as well as the easy implementation of both the proposed LFMPC and NFMPC approaches by enhancing their effectiveness in matching quality and production specifications of nonlinear systems such as polymer processes. The first-principles nonlinear system developed for the comparison consists of 53 differential and algebraic equations and it is implemented in Fortran 90/95 to simulate the plant and to setup the NMPC. The numerical solution is performed by using IMSL library.

2. Identification of Fuzzy Dynamical Models

A fuzzy implication is defined by expressions like: *IF premise (antecedent), THEN conclusion (consequent)*. This logical structure is commonly referred to as the IF-THEN rule-based form. Thus, according to Lima *et al.* (2007), the first point to be considered in the fuzzy modeling is the definition of the fuzzy model structure that composes the rules base of system. Many structures have been already proposed in the literature and, among them, Takagi and Sugeno (1985) proposed a design and analysis scheme for overall fuzzy systems, where the qualitative knowledge of a process was first represented by a set of local Takagi-Sugeno fuzzy model. This approach involves fuzzy sets for the premise portion and a linear equation of input variables for the conclusion. A complex, large-scale nonlinear modeling problem is decomposed into a set of simpler linear models valid within certain operating regimes defined by fuzzy boundaries. Fuzzy inference is hence used to interpolate the outputs of the local models in a smooth fashion to get a global model (Mahfouf *et al.*, 2000). Takagi-Sugeno structure is used for the linear fuzzy model and it is made exponential for the nonlinear fuzzy model of the system under study in this paper. The subtractive clustering method is employed for determination of the amount of rules and parameters of Gaussian membership functions (Chiu, 1996). Consequent function parameters are obtained by solving a least square optimization problem (Passino and Yurkovich, 1998). The next step is the data generation for the identification of the models. At first, the training data set is generated and the models parameters are evaluated. These models are then validated through the test data observing the average quadratic error between the predicted outputs and the real outputs (differential and algebraic mathematical model).

3. Fuzzy Model-Based Predictive Controllers

Predictive controls generate a set of manipulated variable profiles by means of the minimization of some performance indexes over the time. A feedback loop is incorporated in the control structure since the measurements are used to update the optimization problem for the next time step. The method is aimed at calculating a set of *CH* (Control Horizon) future input moves such that the sum of the squared deviations between the output projections, over a *PH* (Prediction Horizon) future time intervals, and the desired values is minimized, using a moving horizon methodology. Thus, future outputs are driven close to the reference trajectory. The basic idea of the multivariable predictive algorithm is to:

I. Calculate the reference trajectory for each output variable *Io* (y_{Io}^{d});

II. Estimate the closed-loop output predictions ($\hat{y}_{Io}^{CLpred}$) using the process prediction models. In this paper, these models are formulated in the form of linear and exponential functional fuzzy models for the linear and nonlinear model-based predictive controllers, respectively;

III. Compute the errors between predicted and reference trajectories;

IV. Estimate the sequence of future controls (movements) of each manipulated variable *Ii* (u) through the minimization of the objective function *J*, expressed by Eq. (1):

$$J=\sum_{Io=1}^{NOV}\sum_{n=1}^{PH} w_{Io}\cdot\left(y_{Io,n}^{d}-\hat{y}_{Io,n}^{CLpred}\right)^{2}+\sum_{Ii=1}^{NIV}\sum_{k=1}^{CH}\left[f_{Ii}\cdot\left(\Delta u_{Ii,k}\right)^{new}\right]^{2} \tag{1}$$

where *NOV* = number of output variables; *NIV* = number of input variables; $\Delta u_{k}=u_{k}-u_{k-1}$; *f* = suppression factor to the movements of the manipulated variables; and *w* = weight. In this study, the reference trajectory is calculated by a first order filter:

$$y_{Io,n}^{d}=\alpha\cdot y_{Io,n-1}^{actual}+\left(1-\alpha\right)\cdot y_{Io,n-1}^{SET} \tag{2}$$

where $y_{Io,n-1}^{actual}$ = vector of current measured value of the controlled variable *Io* at the sampling time *n*-1; $y_{Io,n-1}^{SET}$ = vector of setpoint of the controlled variable *Io* at the sampling time *n*–1; and α = reference trajectory parameter, with $0\le\alpha\le1$.

4. Case Study

Figure 1 reports a flow-sheet of the copolymerization reactor with a recycle loop (Congalidis *et al.*, 1989; Maner and Doyle III, 1997): monomer A is methyl methacrylate (MMA); monomer B is vinyl acetate (VAc); the solvent is benzene; the initiator is azobisisobutyronitrile (AIBN); and the chain transfer agent is acetaldehyde. The monomer stream may also contain inhibitors such as m-dinitrobenzene (m-DNB). Monomers A and B are continuously added with initiator, solvent, and chain transfer agent. In addition, an inhibitor may enter the fresh feeds as impurity. These feed streams (stream 1) are mixed to the recycle stream (stream 2) and fed to the reactor (stream 3), which is assumed to be a jacketed, perfectly-mixed tank. A coolant is fed to the jacket to remove the heat of reaction. Polymer, solvent, unreacted monomers, initiator, and chain transfer agent exit the reactor and reach the separator (stream 4) where polymer, residual initiator, and chain transfer agent are all removed (stream 5). Unreacted monomers and solvent (stream 6) are sent to a purge line for venting (stream 7). After the purge, monomers and solvent (stream 8) are both stored in the recycle hold tank operating as a surge capacity to smooth out variations in the recycle flow and composition. The effluent recycle (stream 2) is then added to the fresh feeds. The separator and the hold tank are both modeled as first-order lags with constant level and residence time equal to the reactor residence time. Relevant output variables to match the product quality are: copolymer production rate (G_{pi}), mole fraction of monomer A in the copolymer (Y_{ap}), weighted average molecular weight (M_{pw}), and reactor temperature (T_r). Steady-state operating conditions are summarized in Table 1.

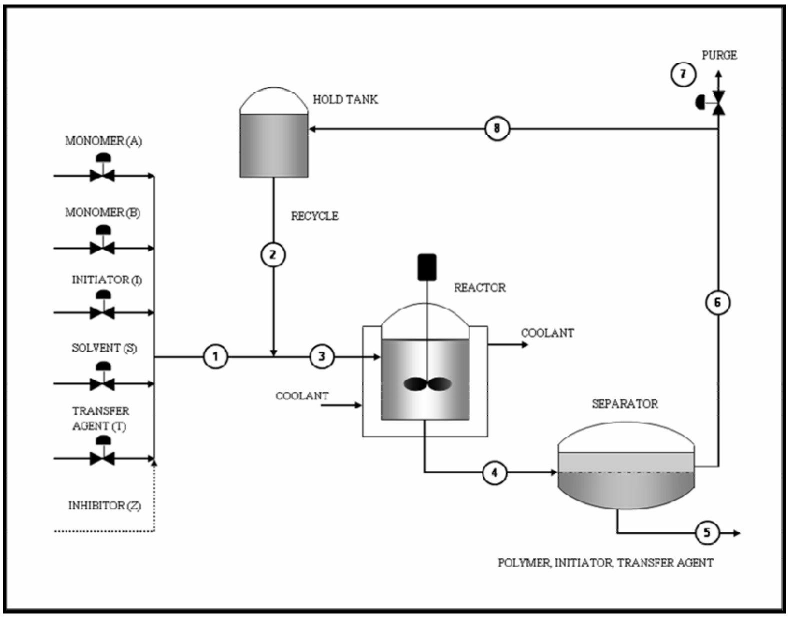

Figure 1. Process layout.

The presence of the recycle stream introduces disturbances in the reactor feed and a feedforward controller was implemented to compensate for them by manipulating fresh feeds in order to preserve feed composition and flowrate to the reactor. Feedforward control of the recycle stream allows the designer to separate reactor control from the rest of the process. Details on the feedforward control are given in Congalidis *et al.* (1989).

4.1. Selection of control loop

Lima *et al.* (2007) developed a factorial planning to discriminate the variables with higher impact on the process performance. The selected control loop resulting from this analysis is shown in Table 2.

Table 1. Steady-state operating conditions.

Inputs	***Outputs***
MMA feed rate (G_{af}) = 18 kg/h	G_{pi} = 23.4 kg/h
VAc feed rate (G_{bf}) = 90 kg/h	Y_{ap} = 0.558
AIBN feed rate (G_{if}) = 0.18 kg/h	M_{pw} = 34,900 kg/kmol
Benzene feed rate (G_{sf}) = 36 kg/h	T_r = 353.18 K
Acetaldehyde feed rate (G_{tf}) = 2.7 kg/h	
m-DNB feed rate (G_{zf}) = 0 kg/h	
Reactor jacket temperature (T_j) = 336.15 K	
Reactor feed temperature (T_{rf}) = 353.15 K	
Purge ratio (ξ) = 0.05	

Table 2. Control scheme.

Manipulated Variables	***Controlled Variables***
G_{bf}	G_{pi}
G_{if}	T_r
T_j	

4.2. Results

The closed-loop performance of fuzzy model-based multivariable nonlinear predictive controllers was analyzed for the rejection of unmeasured disturbances (regulatory problem). The disturbance considered was the presence of an inhibitor in the fresh feed. This disturbance inhibits polymerization reaction. Also, as the reaction is exothermic, less polymerization results in less heat being generated and the reactor temperature decreases as well. Here, an inhibitor disturbance of 4 parts per 1,000 (mole basis) in the fresh feed was applied. In order to assess the performance of fuzzy model-based controllers, a comparative study with NMPC and DMC was carried out. The NMPC algorithm utilizes in Eq. (1) a prediction model in the form of nonlinear differential equations and the DMC methodology uses a linear step response prediction model. The controllers were tuned by IAE (Integral of the Absolute value of the Error) criterion. Figure 2 illustrates the closed-loop performance comparison of the four control strategies about the two controlled variables subject to the selected disturbance. Control system parameters and IAE errors are summarized in Table 3. Computation times of 24, 25, 48, and 23 s were obtained for LFMPC, NFMPC, NMPC, and DMC, respectively.

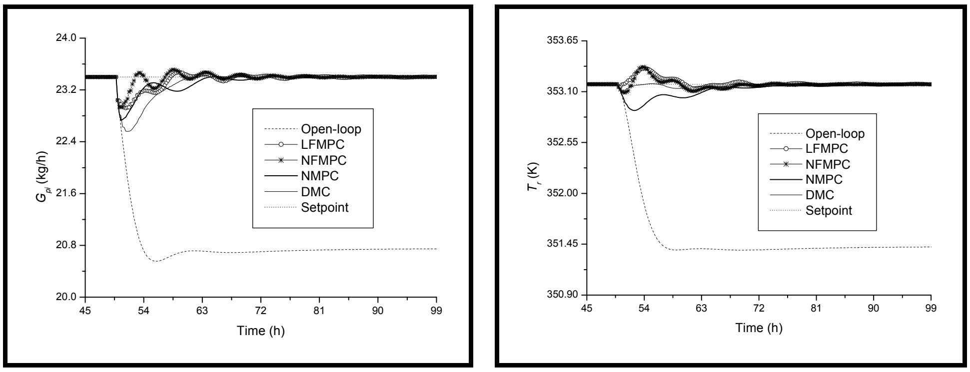

Figure 2. Closed-loop and open-loop simulations under inhibitor feed disturbance.

Table 3. Tuning parameters and IAE errors for predictive control structures.

Parameters	***LFMPC***	***NFMPC***	***NMPC***	***DMC***
PH	12	6	3	9
CH	1	1	2	2
$f\,(G_{bf}; G_{if}; T_j)$	(0.0; 0.3; 0.1)	(0.1; 0.3; 0.1)	(1.0; 0.1; 1.0)	(0.9; 0.9; 0.9)
$\alpha\,(G_{pi}; T_r)$	(0.6, 0.1)	(0.4, 0.1)	(0.0, 0.1)	(0.1, 0.1)
Weight $(G_{pi}; T_r)$	(2.0; 2.8)	(2.0; 2.8)	(2.5; 2.5)	(1.0; 1.0)
IAE (G_{pi} [kg/h]; T_r [K])	(12.0; 4.99)	(7.9; 4.89)	(14.0; 14.63)	(17.4; 1.58)

4.3. Discussion

As can be observed in Figure 2 and Table 3, NFMPC and LFMPC perform better than NMPC and DMC, with a lower IAE value and a smaller overshoot for G_{pi}. About T_r, the value of the IAE for DMC control is smallest, with similar outcomes for NFMPC and LFMPC, which can be explained by the fact that T_r linearly depends on T_j.

5. Conclusions

The problem of nonlinear model-based multivariable predictive control for complex processes was tackled. Specifically, two predictive controllers based on linear and exponential fuzzy models were developed for a copolymerization process. The copolymer rate and reactor temperature were analyzed for regulatory problem and compared for load effects against NMPC and DMC controllers. The simulation results showed good performance for the proposed structures and confirm potentialities and robustness of these techniques to reduce off-specifications due to disturbances in nonlinear systems.

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