

Modeling and Predictive Control Using Fuzzy Logic: Application for a Polymerization System

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In this study, a predictive control system based on type Takagi-Sugeno fuzzy models was developed for a polymerization process. Such processes typically have a highly nonlinear dynamic behavior causing the performance of controllers based on conventional internal models to be poor or to require considerable effort in controller tuning. The copolymerization of methyl methacrylate with vinyl acetate was considered for analysis of the performance of the proposed control system. A nonlinear mathematical model which describes the reaction plant was used for data generation and implementation of the controller. The modeling using the fuzzy approach showed an excellent capacity for output prediction as a function of dynamic data input. The performance of the projected control system and dynamic matrix control for regulatory and servo problems were compared and the obtained results showed that the control system design is robust, of simple implementation and provides a better response than conventional predictive control. © 2009 American Institute of Chemical Engineers AIChE J, 56: 965–978, 2010

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Introduction

A great diversity of products of high industrial interest can be produced with polymerization processes. They generate materials with a broad field of application, including plastics, rubber, furniture, inks, and drugs. However, the dynamic behavior of such processes is quite complex, char-

acterized by strong nonlinearity and intense system variable interactions. These factors make it very difficult to build a sufficiently detailed deterministic model able to take into account the main phenomena taking place in the system. The difficulties are primarily related to the large number of differential algebraic equations and the associated parameters needed to represent the reactants, the intermediates, and the product species. Additionally, for control and on-line optimization procedures, such models have to be solved in a relatively short period of time.

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A possible way to deal with the problem is to develop simplified models which may lead to restrictions in terms of process representation, especially when high specifications are required. The lack of accurate process representation is a severe limitation in designing reliable and robust control systems. In fact, failure in the process representation directly influences the success of the control strategies. Thus, a large number of works have been developed focusing on suitable process representation to be used as model for process control design. Basically, the most common approach is to use the concept of model predictive controllers with a linear model as an internal model. Furthermore, attention has been directed to the applications of techniques of artificial intelligence in the modeling of chemical processes, as for example the use of artificial neural networks (ANN). This entails either the use of ANN directly as a controller design tool or as an internal model in predictive controllers, resulting in nonlinear controllers. Bearing this last approach in mind, an alternative of great potential is the development and use of fuzzy models, which may be applied in the design of the control system as well as to model the process. Such models have quite an interesting ability to represent the process with different types of data, including operator information. This modeling approach is suitable for polymerization plants which have complex behavior, and are able to build models dealing with concepts of uncertainty, including definitions of probabilistic logic. Moreover, they allow the inclusion of information about the process in the generation of the mathematical model, which makes it an alternative of great interest from the operational point of view.

Alexandridis et al.¹ introduced a systematic methodology based on fuzzy systems to the problem of nonlinear system identification. The new methodology resulted in both a linguistic and an analytical model of the system. The method was successfully tested in the identification of certain operating regions in a Continuous Stirred Tank Reactor (CSTR) exhibiting various types of nonlinear behavior, such as limit cycles and multiple steady states. Habbi et al.² presented a nonlinear dynamic fuzzy model for a natural circulation drum-boiler-turbine. It was shown that the dynamic fuzzy model results in appropriate and accurate global nonlinear prediction and, at the same time, that their local models are close approximations to the local linearizations of the nonlinear dynamic system. Cerrada et al.³ proposed an approach for dynamical adaptive fuzzy modeling. The approach allows the incorporation of the temporal behavior of the system variables into the fuzzy membership functions. The illustrative examples of system identification showed that the performance of the proposed fuzzy models based on the identification error is adequate. These models followed the real output even if there were sudden changes in the input variables. This is an important characteristic of an adequate identification model in real time applications. The approach is oriented to applications needing an identification model such as process control, supervision, fault diagnosis, etc., of nonlinear and time-varying systems. As in Sala et al.,⁴ the current research on new methods of modeling and control is based on the application of fuzzy systems. It is important to highlight that the use of the fuzzy logic as a modeling and control methodology may significantly simplify the way in which algorithms for integration are executed. In fact, it is

quite attractive in terms of time, simplicity of implementation, relatively low cost and ability to rapidly model complex systems.

Analyzing the aspects related to the process control more specifically, it is worth emphasizing that many of the conventional control algorithms may be inadequate in dealing with very high specifications imposed in some industrial processes, especially when a high quality product is required. This may be the case of some polymerization processes in which specific properties such as molecular weight distribution and mean molecular weight with impact on plastic processability have to be met. In such cases, a model based predictive controller, known as MPC (Model Predictive Control), which uses a dynamic model of the process as an integral part of the control system, is a suitable approach. According to Campello et al.,⁵ the great acceptance of MPC algorithms for chemical process control is due to their ability to deal with restrictions involving input and output variables in procedures, and the fact that they are relatively easy to use. Schnelle and Rollins⁶ applied a model predictive control tool on a prototype continuous polymerization (CP) process. It was shown that MPC technology is a good alternative for solving CP control problems (minimizing settling time after transition, coping with multivariable interactions, and unusual process dynamics). Santos et al.⁷ implemented an on-line nonlinear model predictive control algorithm to control the liquid level and temperature in a CSTR pilot plant, where an irreversible exothermic chemical reaction was simulated experimentally by steam injection. Several sources of model mismatch and unmeasured disturbances that affect the quality of the model in representing the reactor dynamics were identified. Despite such mismatches and disturbances, it was observed that the closed loop system is able to track set-point changes and reject disturbances quite well. Park and Rhee⁸ applied an extended Kalman filter based nonlinear MPC to property control of a semibatch MMA/MA (Methyl MethAcrylate/MethAcrylate) copolymerization reactor. The experimental results demonstrated the good performance of the control strategy when compared with other previously used techniques. Ramaswamy et al.⁹ used MPC to control a nonlinear continuous stirred tank bioreactor in an unstable steady state, which was the desired set point. The effect of variations on the prediction horizon, an important MPC controller tuning parameter, was studied.

Among MPC control techniques, the dynamic matrix control (DMC) strategy is the one with most industrial applications due to the simplicity of its design and implementation, and its ability to work well with restrictions in the manipulated variable. According to Dougherty and Cooper,¹⁰ MPC has become the leading form of advanced multivariable control in the chemical process industry. In an alternative approach, they introduced a multiple model adaptive control strategy for multivariable DMC. The method combines the output of multiple linear DMC controllers and does not introduce additional computational complexity in relation to non-adaptive DMC. Guiamba and Mulholland¹¹ developed and implemented an Adaptive Linear DMC (ALDMC) algorithm in a two-input/two-output pump-tank system with an integrating behavior in the form of an off-line step response convolution model. ALDMC showed better performance than the non-adaptive Linear DMC (LDMC) in the case of

plant/model mismatch. Haeri and Beik¹² considered an extended approach to the nonlinear DMC algorithm, which can handle constrained and MIMO (Multi-Input/Multi-Output) systems under certain defined conditions. Simulation results to illustrate the effectiveness of the method were presented for the control of a nonlinear model of a stirred tank reactor with two inputs and two outputs and also for a power unit nonlinear model with three inputs and three outputs.

Using the potential of predictive strategies coupled with the ability to represent systems using fuzzy logic for designing controllers is an interesting approach. Roubos et al.¹³ described work focusing on the use of Takagi-Sugeno fuzzy models in combination with MPC algorithms. First, the fuzzy model-identification of MIMO processes was given and then the developed fuzzy model was used in combination with MPC. The studied methodology was tested and evaluated with a simulated laboratory setup for a MIMO liquid level process with two inputs and four outputs. Abonyi et al.¹⁴ explained the identification and control of nonlinear systems by means of Fuzzy Hammerstein (FH) models, which consists of a static fuzzy model connected in series with a linear dynamic model. The obtained FH model was incorporated in a model-based predictive control scheme and a new constraint-handling method was presented. A simulated water-heater process was used as an illustrative example. Simulation results showed that not only was good dynamic modeling performance achieved, but also the steady-state behavior of the system was well-captured by the proposed FH model. Sousa and Kaymak¹⁵ investigated the use of fuzzy decision making (FDM) in MPC, and compared the results to those obtained from conventional MPC. Experiments on a non-minimum phase, unstable linear system, and on an air-conditioning system with nonlinear dynamics were analyzed. It was shown that the performance of the model predictive controller can be improved by the use of fuzzy criteria in a fuzzy decision making framework. Mollov et al.¹⁶ proposed the synthesis of a predictive controller for a nonlinear process based on a fuzzy model of the Takagi-Sugeno type, resulting in a stable closed-loop control system. The effectiveness of the approach was demonstrated through a simulated example and in the real-time control of a laboratory cascaded-tanks process. Sarimveis and Bafas¹⁷ introduced a predictive control technique based on a Takagi-Sugeno dynamic fuzzy model, which was used for predicting the future behavior of the output variable in a SISO (Single-Input/Single-Output) control loop. The objective function of the controller was solved on line using a genetic algorithm. The proposed methodology was applied to a random process in a non-isothermal CSTR and can be used with any type of fuzzy model, being particularly useful when a direct fuzzy controller cannot be designed due to the complexity of the system. Mendonça et al.¹⁸ introduced a generalization of fuzzy predictive filters to multivariable processes to solve non-convex optimization problems resulting from the application of model predictive control to nonlinear processes. The proposed scheme was applied to the control of a gantry crane. Simulation results showed the advantages of the method. Karer et al.¹⁹ presented the Takagi-Sugeno fuzzy formulation for a hybrid fuzzy modeling approach. A MPC algorithm suitable for systems with discrete inputs was examined and the results demonstrated the benefits of the

MPC algorithm using the proposed hybrid fuzzy model on a batch-reactor simulation example. Causa et al.²⁰ described the design of a hybrid fuzzy predictive control based on a genetic algorithm. The temperature of a batch reactor was controlled by using two on/off input valves and a discrete-position mixing valve. The proposed strategy proved to be a suitable method for the control of hybrid systems, giving a similar performance to that of typical hybrid predictive controllers and significant savings in computation time. Sáez et al.²¹ developed solution algorithms based on computational intelligence for solving the dynamic multi-vehicle pick-up and presented a problem formulated under a hybrid predictive adaptive control scheme. Promising results in terms of computation time and accuracy were presented through a simulated numerical example.

Therefore, this study proposes a Fuzzy Model based Predictive Control system (FMPC), in which the internal models for the proposed system are developed using fuzzy logic, taking into account process restrictions and nonlinearities. The control strategy design is multivariable with four outputs to control by manipulating four inputs. The copolymerization of methyl methacrylate with vinyl acetate is considered as a case study.

Fuzzy Systems Applied to the Modeling of Complex Processes

Many engineering problems are characterized by having very little information and are said to be complex. These problems are imbued with a high degree of uncertainty. To deal with this, in 1965, Lotfi Zadeh introduced his seminal idea in a continuous-valued logic that he called fuzzy set theory.²² Zadeh's work had a profound influence on the thinking about uncertainty because it challenged not only probability theory as the sole representation for uncertainty, but also the very foundations upon which probability theory was based: classical binary (two-valued) logic.²³

A fuzzy set contains elements that have varying degrees of membership in the set. The elements of a fuzzy set, because their membership need not be complete, can also be members of other fuzzy sets in the same universe. All the information contained in a fuzzy set is described by its membership function. The algorithm developed in this study incorporates Gaussian membership functions $\mu(x)$ for the inputs x ,^{24,25} given by Eq. 1:

$$\mu(x_i) = \exp \left[-\frac{1}{2} \cdot \left(\frac{x_i - c_i}{\sigma_i} \right)^2 \right] \quad (1)$$

where x_i is the i th input variable, c_i is the i th center of the membership function, and σ_i is a constant related to spread of the i th membership function. Figure 1 illustrates a typical Gaussian membership function and its parameters.

Fuzzy set operations

The operations of union, intersection, and complement are the standard fuzzy operations. They are defined the same way as for crisp sets, when the range of membership values is limited to the unit interval. For each of the three standard operations, there is a broad class of functions whose members can be

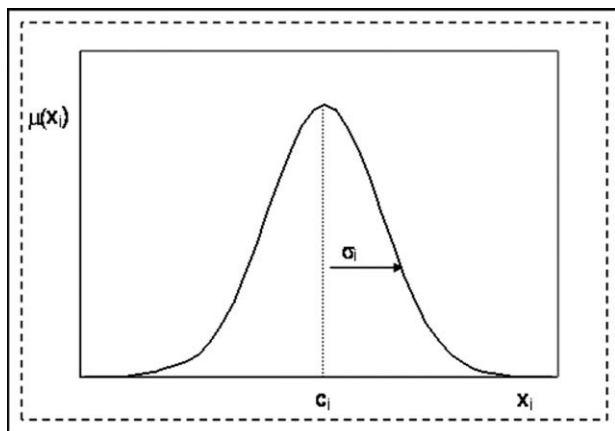


Figure 1. Typical Gaussian membership function.

considered fuzzy generalizations of the standard operations. In such a case, fuzzy intersections are usually referred to as t-norms and fuzzy unions are usually referred to as t-conorms (or s-norms). These t-norms and t-conorms are so named because they were first introduced as triangular norms and triangular conorms, respectively, in study of statistical metric spaces.²² The more widely used t-norms and t-conorms, relating two fuzzy sets \underline{X}_1 and \underline{X}_2 , with elements x_1 and x_2 , respectively, are shown in Table 1. The probabilistic t-norm and t-conorm will be applied in the calculation of the inferred output of the fuzzy rule-base for the process considered in this study.^{24,25}

Fuzzy modeling

The basis of the fuzzy model is a set of rules that represent the knowledge of the process. To achieve this, the fuzzification, inference, and defuzzification stages must be processed.

The process called fuzzification converts numeric inputs into fuzzy sets so that they can be used by the fuzzy system.²⁶ This transformation is possible through the use of membership functions.

The inference mechanism is carried out by an expression of the following type:

$$\text{IF premise (antecedent) THEN conclusion (consequent)} \quad (2)$$

This form is commonly referred to as the IF-THEN rule-based form; it is generally referred to as the deductive form. Each rule represents a cause and effect relationship. For a given operating condition, there is a corresponding action.

Defuzzification is used to convert the fuzzy results into crisp results. This procedure provides a means to choose a crisp single-valued quantity (or a crisp set) based on the implied fuzzy sets.

According to Lima et al.,²⁴ fuzzy modeling is interesting in that it enables the incorporation of qualitative information on the process behavior during model building. Possible changes in kinetic as well as heat and mass transfer parameters due to alterations in operating conditions may also be incorporated in the process model through the fuzzy approach.

Takagi-Sugeno Fuzzy Model

The Takagi-Sugeno fuzzy model is a special case among functional fuzzy models. Its structure was proposed by Takagi and Sugeno.²⁷ In this approach, the fuzzy model substitutes the consequent fuzzy sets in a fuzzy rule by a linear equation of the input variables. Thus, a fuzzy model can be regarded as a collection of several linear models applied locally in the fuzzy regions defined by the rule premises where the overall model of the system is represented as the interpolation of these linear models. Therefore, it has a conveniently dynamic structure so that well-established linear systems theory can be easily applied to the theoretical analysis and design of the overall closed-loop system.²⁸

The Takagi-Sugeno model for generation of fuzzy rules from a given input-output data set, which has two-inputs x_1 and x_2 , and output y , can be written in the following way:

$$\text{IF } x_1 \text{ is } X_1 \text{ and } x_2 \text{ is } X_2 \text{ THEN } y \text{ is } y = f(x_1, x_2) \quad (3)$$

where \underline{X}_1 and \underline{X}_2 are fuzzy sets (membership functions) of x_1 and x_2 , respectively, and $y = f(x_1, x_2)$ is a crisp consequent function. The generalization of expression (3) for a linear structure with an entrance number n leads to the Takagi-Sugeno model as follows:

$$\begin{aligned} &\text{IF}(x_i \text{ is } X_{i,1}) \text{ and } (x_2 \text{ is } X_{i,2}) \text{ and } \dots \text{ and } (x_j \text{ is } X_{i,j}) \\ &\text{and } \dots \text{ and } (x_n \text{ is } X_{i,n}) \\ &\text{THEN } y_i = a_{i1} \cdot x_1 + a_{i2} \cdot x_2 + \dots + a_{ij} \cdot x_j + \dots + a_{in} \cdot x_n \end{aligned} \quad (4)$$

where $i = 1, \dots, R$, being R the number of rules of the fuzzy model; $j = 1, \dots, n$; and a_{ij} are parameters of the consequent function of the fuzzy model.

For a given input, the output of the fuzzy model is inferred by the weighed average of referring output i to each rule, calculated by:

$$y = \frac{\sum_{i=1}^R f_i \cdot \mu_i(x)}{\sum_{i=1}^R \mu_i(x)} \quad (5)$$

where $\mu_i(x)$ are membership functions and f_i is a consequent function to each rule i .

This is the basic objective in this study; to develop a fuzzy model to be used in control system design.

Identification of Functional Fuzzy Models

To develop a FMPC controller using the concepts of fuzzy logic and DMC predictive control, it is necessary initially to

Table 1. Main t-norms and t-conorms

Type	Zadeh	Probabilistic	Lukasiewicz	Weber
t-norm	$\min(x_1, x_2)$	$x_1 \cdot x_2$	$\max(x_1 + x_2 - 1, 0)$	$\begin{cases} x_1, & \text{if } x_2 = 1 \\ x_2, & \text{if } x_1 = 1 \\ 0, & \text{if not} \end{cases}$
t-conorm	$\max(x_1, x_2)$	$x_1 + x_2 - x_1 \cdot x_2$	$\min(x_1 + x_2, 1)$	$\begin{cases} x_1, & \text{if } x_2 = 0 \\ x_2, & \text{if } x_1 = 0 \\ 1, & \text{if not} \end{cases}$

generate the functional fuzzy models. The fuzzy model will be used as an internal model of the DMC predictive controller in substitution of its respective convolution model (forecast model), thus modifying the basic structure of the DMC and generating a FMPC controller. An interesting characteristic of the proposed controller is its ability to deal with nonlinearities. This is due to the fact that the developed fuzzy models start to represent the process in a linear way for each one of the operational regions, however, since overlapping between the membership functions is possible, the combination of the models can generate nonlinear representations of the system.

Steps for the development of functional fuzzy models

Important decisions must be taken in the initial phases of the modeling procedure which will directly influence the quality of the obtained model.^{24,25}

First, the fuzzy model structure that composes the rule base of the system must be defined. The variables that will be used and the interconnection amongst them must be selected. The number and types of the chosen variables must be in accordance with the requirements of the problem. These models will possess a dynamic configuration in such a way as to represent the behavior of the process throughout a time horizon. A close look at the fuzzy model structure and the way in which it is built reveals its recursive properties.

To predict an output at time k , fuzzy models usually use not only inputs from time k but also inputs and output from time points previous to k (that is: $k-1, k-2, \dots, k-P$). The number of past time points to be used (i.e., P) is an important parameter for optimization because it has considerable influence on the final quality of the model.

The next stage is the data generation for the identification of the model. At this point, the maximum and minimum limits of variation of the variable must be defined so that the model operation range is determined. First, the training data are generated and are then applied to attain the parameters of the model. This model is validated later through the use of test data. The data generation is carried out through a random excitation of the input variables of the process. An input variable is changed instantly and, at the same time, the behavior of the output variables is collected. Then, the same procedure is performed for the other input variables and finally a data set for the training of the fuzzy model and a data set for its validation are obtained. It must be observed that the data generation of the training and test sets is done in different conditions of frequency and amplitude of excitation of the entrance variables.

Another important point to consider in dynamic fuzzy model development is the determination of the sampling rate. The time constant of the process has to be taken into account. Alternatively, when the model is used for control, as in this study, the sampling rate must be related with the controller action interval.

Generation of functional fuzzy models

As already described, the functional fuzzy models developed in this study will be of the Takagi-Sugeno type with the structure defined by Eq. 4.

The initial stage for the construction of these models is to complete the data identification process. A process representative data set including possible qualitative information should be made available and the next steps include the stages of fuzzification (membership functions), inference (through the use of t-norms and t-conorms), and calculation of the inferred numerical output by the weighed average of referring numerical outputs to each rule.

However, the dimension of the model is not known initially: the number of rules, the number and parameter values of the membership functions associated to each variable (centers and spread constant, since Gaussian membership functions will be used), and the parameters of the consequent functions of the rules. To obtain a minimum realization (model dimension) of the process the following methods can be used.

- Subtractive clustering method: which determines the number of rules and the parameters of the membership functions.

- Gradient Method: the quality of the fuzzy model can be improved by modifications in the entrance parameters. The gradient method acts by adjusting the entrance data, and thus improving model quality.

- Learning From Example (LFE): it only constructs the rules. The complete specification of the membership functions is left to the analyst.

- Least square algorithm: which requires the number of rules and the membership functions of the premises. It is used to calculate the parameters of the consequent functions.

- Modified Learning From Example (MLFE): in contrast with LFE, MLFE calculates the rules and the parameters of the membership functions.

As presented above, each of the methods is used for a specific objective. Thus, they can be combined for a specific need. For the system analyzed in this article, the functional fuzzy models will be generated through the combination of the subtractive clustering method with the least square algorithm. Details on subtractive clustering and least square methods are given by Chiu^{29,30} and Passino and Yurkovich,²⁶ respectively.

Validation of functional fuzzy models

In this study, the results of the model validation are illustrated through figures and quantified through the average quadratic error, given by Eq. 6:

$$\text{Error} = \sqrt{\frac{\sum_{k=1}^m (\bar{y}_k - y_k)^2}{m}} \quad (6)$$

where k is the time point, m is the number of considered discrete instants, \bar{y}_k is the predicted output by the fuzzy model in instant k , and y_k is the output of the process in instant k (phenomenological model).

Multivariable DMC

DMC was developed at Shell Oil Company in 1979. The basic idea is to use time-domain step-response models (called convolution models) of the process to calculate the

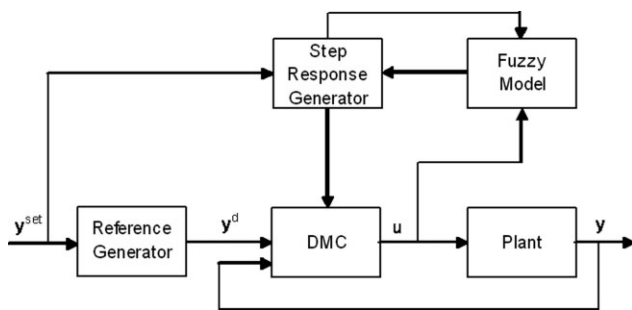


Figure 2. Structure of the predictive control using fuzzy model.

future changes in the manipulated variables that will minimize some performance index. In the DMC approach, it is desirable to have PH (prediction horizon) future outputs responses matching some “optimum” trajectory by finding the “best” values of CH (control horizon) future changes in the manipulated variables. This is exactly the concept of a least square problem of fitting PH data points with an equation with CH coefficients. This is a valid least square problem as long as PH is greater than CH.

The aim of a predictive control law is to drive future outputs close to the reference trajectories. The computation sequence calculates the reference trajectories and then estimates the outputs using the convolution models. Then, the errors between predicted and reference trajectories are calculated.³¹ The next step is to estimate the sequence of the future controls by minimizing an appropriate quadratic objective function J for each output. However, only the first element is implemented. At this point, the data vectors are shifted so that the calculations can be repeated at the next sample instant. This function J is defined by Eq. 7:

$$J = \sum_{i=1}^{PH} (y_i^d - y_{CL,i}^{pred})^2 + f^2 \cdot \sum_{k=1}^{CH} [(\Delta u_k)^{future}]^2 \quad (7)$$

where i and k are the time points; y is the output variable (controlled); u is the input variable (manipulated), with $\Delta u_k = u_k - u_{k-1}$; and f is the suppression factor for the movements of the manipulated variable.

In the original DMC strategy, the term y_i^d is the setpoint. In the present study, to prevent drastic control actions, a term is introduced based on the Model Algorithmic Control (MAC) strategy.³² The desired output is calculated through an optimal trajectory defined by a first-order filter:

$$y_i^d = \alpha \cdot y_{i-1}^{actual} + (1 - \alpha) \cdot y_{i-1}^{set} \quad (8)$$

where y_{i-1}^{actual} is the vector of current measured values of the controlled variable at sampling time $i-1$; y_{i-1}^{set} is the vector of setpoints of the controlled variable at sampling time $i-1$; and α is the reference trajectory parameter that must be precisely adjusted by optimization of the objective function J , with $0 \leq \alpha \leq 1$.

Predicted values $y_{CL,i}^{pred}$ in Eq. 7 can be obtained directly from a model of the process. However, when this model is not perfect (and this is generally the case), the controller will not be sufficiently robust. Therefore, the following

incremental model is applied to remove modeling inaccuracies:

$$y_{CL,i}^{pred} = y_{CL,i} + (y_{i-1}^{actual} - y_{CL,i-1}) \quad (9)$$

where $y_{CL,i}$ is defined by convolution model. In Eq. 9, it is considered that the difference between the predicted and actual values in the previous instant is valid for the current instant. Thus, the system reaches the desired value for successive corrections of the shunting line. Details on DMC and on obtaining the convolution model are given by Luyben.³³

Fuzzy Model Based Predictive Control System

For the FMPC control system, the convolution models of the original configuration of DMC will be substituted by the functional fuzzy models. The fuzzy models act as a predictor in the strategy of predictive control, and the control action for each output is given by the minimization of an objective function similar to Eq. 7. In this case, however, the term $y_{CL,i}^{pred}$ in Eq. 7 is calculated through Takagi-Sugeno fuzzy models. In general, the fuzzy model makes the predictions of the output variable as a function of the last and current signals of input and of the last signals of output. The FMPC control scheme is shown schematically in Figure 2.³⁴

The control system tuning is carried through the integral of the absolute value of the error (IAE), defined by Eq. 10, looking up the best combination of parameters (PH, CH, f , α) that minimizes this performance criterion. Therefore, the following optimization problem is solved during tuning procedures:

$$\min_{PH, CH, f, \alpha} \left[J(PH, CH, f, \alpha) = IAE = \int_{t_0}^{t_f} |y^{set}(t) - y^{actual}(t)| \cdot dt \right] \quad (10)$$

In Eq. 10, t_0 and t_f are the initial and final times of the evaluation period.

Case Study: Copolymerization of Methyl Methacrylate with Vinyl Acetate

The process considered in this study as case study is the solution copolymerization of methyl methacrylate with vinyl acetate in a continuous stirred tank reactor.³⁵ Figure 3 is a flow diagram of a copolymerization reactor with a recycle loop. Monomer A is methyl methacrylate, monomer B is vinyl acetate, the solvent is benzene, the initiator is azobisisobutyronitrile (AIBN), and the chain transfer agent is acet-aldehyde. 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 with the fresh feeds as an impurity. These feed streams are combined (stream 1) with the recycle stream (stream 2) and flow to the reactor (stream 3), which is assumed to be a jacketed, well-mixed tank. A coolant flows through the jacket to remove the polymerization heat. Polymer, solvent, unreacted monomers, initiator, and chain transfer agent flow out of the reactor to the separator (stream 4).

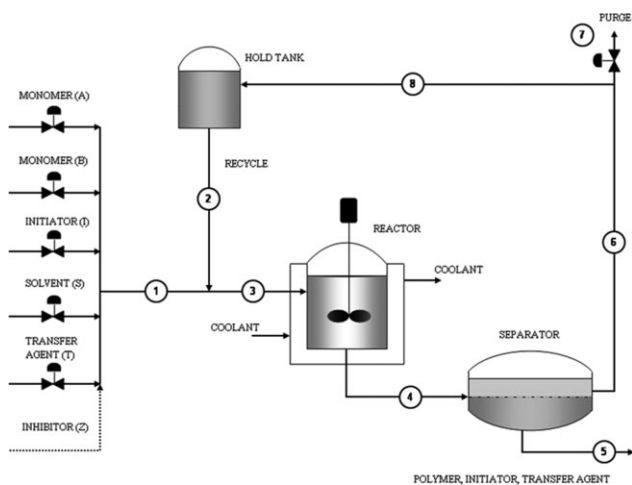


Figure 3. Basic process configuration.³⁵

Here, the polymer is removed from the stream (stream 5). Residual initiator and chain transfer agent are also removed in this step. In the real process, the separator often involves a series of steps, which may include dryers and distillation columns. Here, unreacted monomers and solvent (stream 6)

Table 2. Steady-State Operating Conditions

Inputs	
Monomer A (MMA) feed rate	$G_{af} = 18 \text{ kg/h}$
Monomer B (VAc) feed rate	$G_{bf} = 90 \text{ kg/h}$
Initiator (AIBN) feed rate	$G_{if} = 0.18 \text{ kg/h}$
Solvent (benzene) feed rate	$G_{sf} = 36 \text{ kg/h}$
Chain transfer (acetaldehyde) feed rate	$G_{zf} = 2.7 \text{ kg/h}$
Inhibitor (<i>m</i> -DNB) feed rate	$G_{zf} = 0$
Reactor jacket temperature	$T_j = 336.15 \text{ K}$
Reactor feed temperature	$T_{rf} = 353.15 \text{ K}$
Purge ratio	$\xi = 0.05$
Reactor parameters	
Reactor volume	$V_r = 1 \text{ m}^3$
Reactor heat transfer area	$S_r = 4.6 \text{ m}^2$
Outputs	
Polymer production rate	$G_{pi} = 23.4 \text{ kg/h}$
Mole fraction of A in polymer	$Y_{ap} = 0.5591$
Weight average molecular weight	$M_{pw} = 34994.7 \text{ kg/kmol}$
Reactor temperature	$T_r = 353.02 \text{ K}$

continue on to a purge point (stream 7), which represents venting and other losses. Purging is required to prevent the accumulation of inerts in the system. After the purge, the monomers and solvent (stream 8) are stored in the recycle hold tank, which acts as a surge capacity to smooth out variations in the recycle flow and composition. The effluent (stream 2) recycled is then added to the fresh feeds.

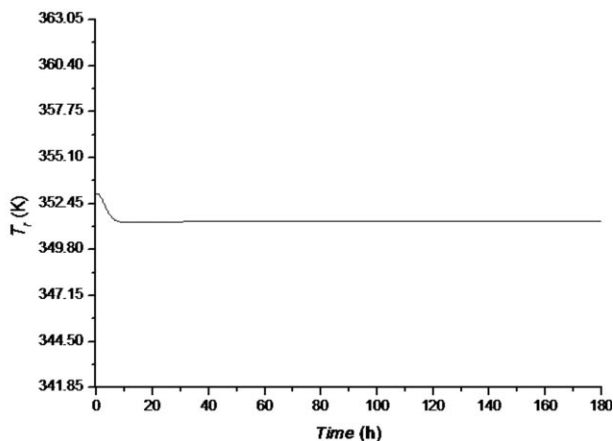
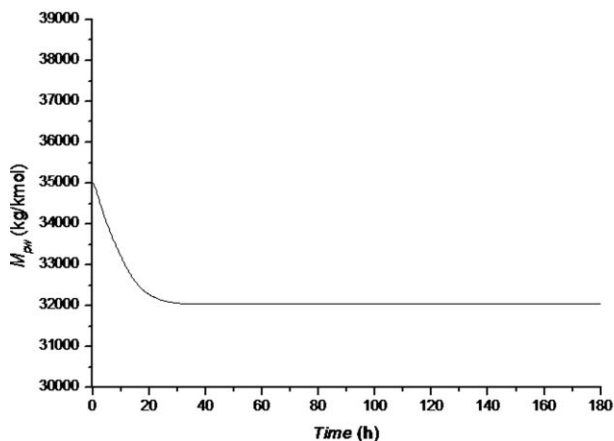
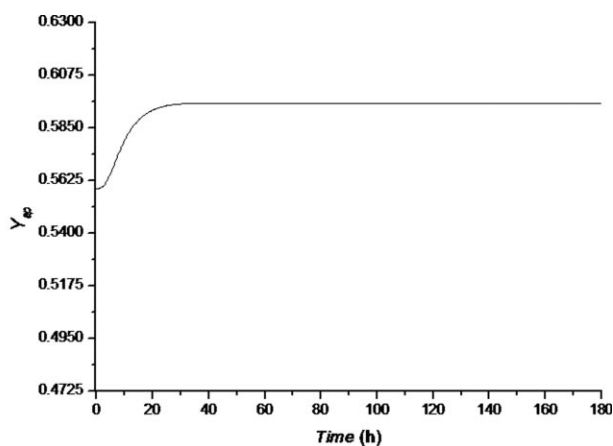
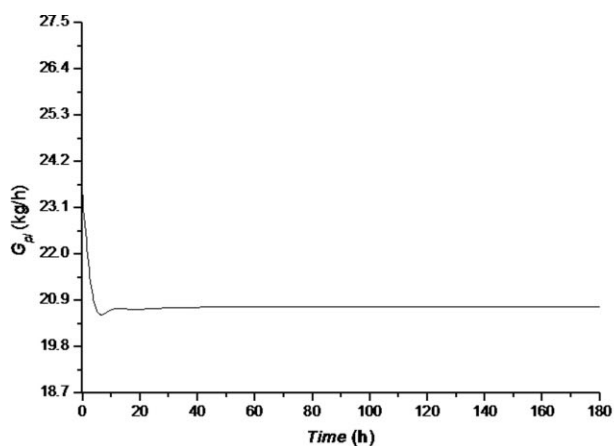


Figure 4. Open-loop output variables response to inhibitor disturbance.

Table 3. Selected Control Loops

Manipulated	Output
G_{bf}	G_{pi}
(G_{af}/G_{bf})	Y_{ap}
G_{if}	M_{pw}
T_j	T_r

The important reactor output variables for product quality control are the polymer production rate (G_{pi}), mole fraction of monomer A in the copolymer (Y_{ap}), weight average molecular weight (M_{pw}), and reactor temperature (T_r). The inputs are the reactor flows of monomer A (G_{af}), monomer B (G_{bf}), initiator (G_{if}), chain transfer agent (G_{ct}), solvent (G_{st}), inhibitor (G_{zt}), the temperature of the reactor jacket (T_j), and the temperature of the reactor feed (T_{rf}). The reactor, separator, and hold tank contain at startup pure solvent preheated to 353.15 K.

The steady-state operating point is summarized in Table 2. Under these conditions, the reactor residence time is $\theta_r = 6$ h and the overall reactor monomer conversion is 20%. These operating conditions ensure that the viscosity of the reaction medium remains moderate. Table 2 also indicates that the temperature of the reactor feed T_{rf} is practically equal to the reactor temperature T_r , because it was chosen to simulate re-

actor operation with a preheated feed where the single source of heat removal is through the jacket.

Feedforward control of recycle

The presence of the recycle stream introduces disturbances in the reactor feed which affect the polymer properties. To overcome this, Congalidis et al.³⁵ implemented a feedforward controller in the process to compensate for these disturbances by manipulating the fresh feeds to maintain constant feed composition and flow to the reactor. Feedforward control of the recycle stream enabled the designer to separate the control of the reactor from the rest of the process. Thus, the reactor can be analyzed separately. Details of the feedforward control of recycling are given in Congalidis et al.,³⁵ Maner and Doyle,³⁶ and Lima et al.²⁴

Deterministic model

This case study has previously been described in the literature by a nonlinear phenomenological mathematical model and kinetic parameters. This model, which is composed by a set of algebraic and ordinary differential equations, is considered as the real plant for data generation, identification of the fuzzy model, and implementation of the controllers. Details of the phenomenological model as well as the kinetic

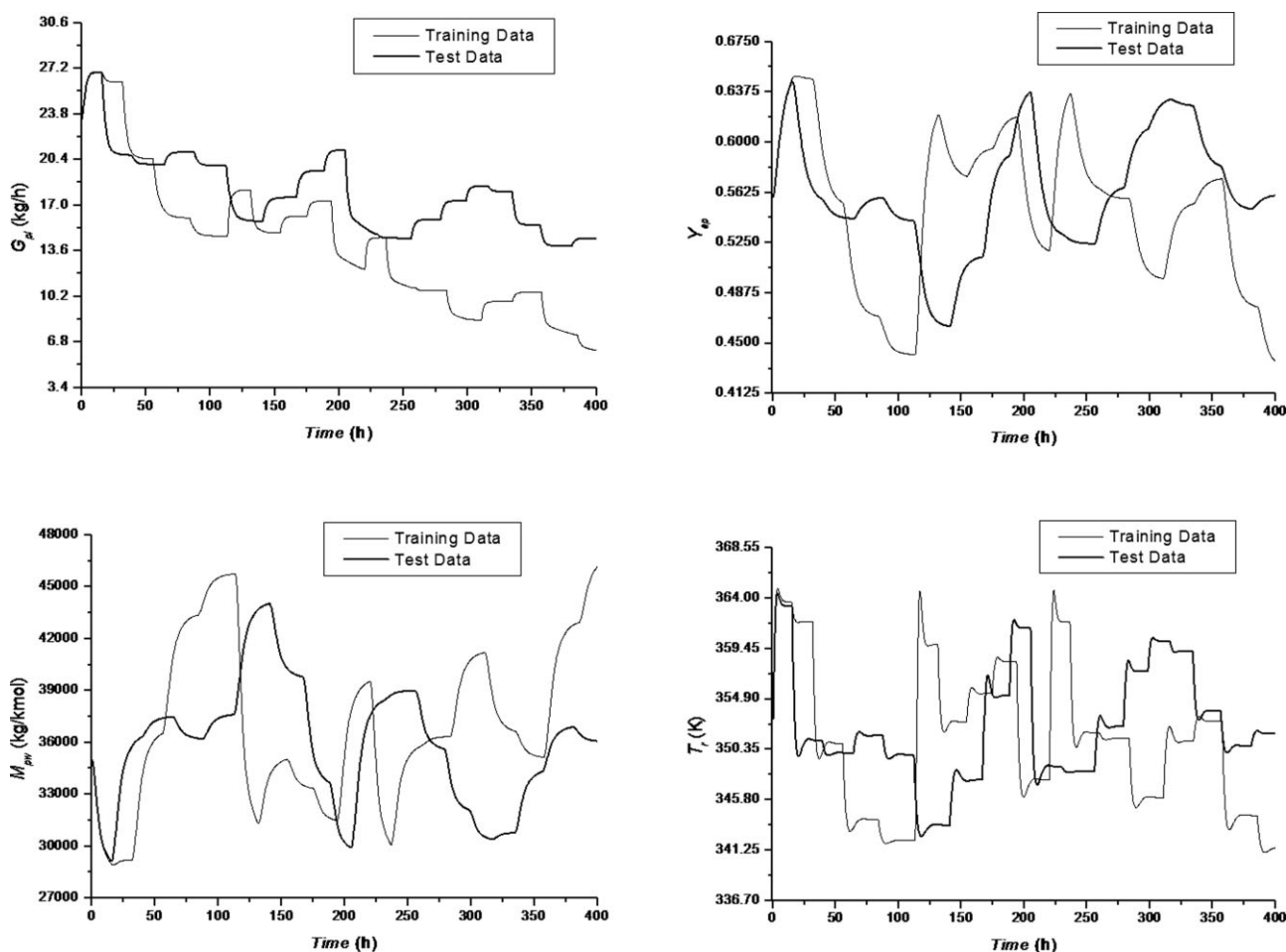


Figure 5. Identification data of the fuzzy models.

Table 4. Parameters of the Fuzzy Model for G_{pi}

Number of Rules = 1				
Antecedent part				
Rule i	$u(k), u(k-1)$		$w(k)$	
	$c_i \times 10^2$	$\sigma_i \times 10^2$	$c_i \times 10^2$	$\sigma_i \times 10^2$
$i = 1$	10.84	41.06	50.48	23.59
Consequent part				
Rule i	$a_{i1} \times 10^2$	$a_{i2} \times 10^2$	$b_{i1} \times 10^2$	
$i = 1$	1.80	-1.04	99.31	

mechanism and initial concentrations are given in Congalidis et al.³⁵ and Maner and Doyle.³⁶

Open-loop behavior and selection of the control loops

This system consists of six inputs (G_{af} , G_{bf} , G_{if} , G_{tf} , G_{sf} , and T_j) and four outputs. The temperature of the reactor feed (T_{rf}) is considered constant and purge ratio (ξ) is manipulated by the feedforward controller. Table 2 also indicates that the inhibitor feed rate is equal to zero. Given this, the deterministic model was solved by a Runge-Kutta type algorithm written in Fortran 90. Figure 4 presents the behavior of the four output variables in open-loop for an inhibitor disturbance of 4 parts per 1000 (mole basis) in the fresh feed. As observed, even with this low inhibitor molar concentration, the polymer properties are noticeably affected. This disturbance is the same as that considered by Congalidis et al.³⁵ and Maner and Doyle.³⁶ The fresh feed corresponds to the addition of the molar outflows of monomers, initiator, solvent, and chain transfer agent in the system entrance.

Lima et al.²⁴ developed a factorial planning using *Statistica Version 7.0 Software* to discriminate the variables which have a greater impact on the process performance. The selected control structure resulting from this analysis is shown in Table 3.

Dynamic fuzzy modeling

An algorithm for functional multivariable dynamic fuzzy modeling was developed using the subtractive clustering and least squared methods. This was further inserted in the simu-

Table 5. Parameters of the Fuzzy Model for Y_{ap}

Number of Rules = 4				
Antecedent part				
Rule i	$u(k), u(k-1)$		$w(k)$	
	$c_i \times 10^2$	$\sigma_i \times 10^2$	$c_i \times 10^2$	$\sigma_i \times 10^2$
$i = 1$	10.84	17.11	18.48	17.82
$i = 2$	91.50	17.11	103.59	17.82
$i = 3$	39.86	17.11	68.74	17.82
$i = 4$	100.00	17.11	64.23	17.82
Consequent part				
Rule i	$a_{i1} \times 10^2$	$a_{i2} \times 10^2$	$b_{i1} \times 10^2$	
$i = 1$	-1.11	4.08	97.41	
$i = 2$	0.00	1.24	98.76	
$i = 3$	-0.24	2.18	98.30	
$i = 4$	-1.84	0.56	103.53	

Table 6. Parameters of the Fuzzy Model for M_{pw}

Number of Rules = 5				
Antecedent part				
Rule i	$u(k), u(k-1)$		$w(k)$	
	$c_i \times 10^2$	$\sigma_i \times 10^2$	$c_i \times 10^2$	$\sigma_i \times 10^2$
$i = 1$	39.86	52.77	44.67	48.09
$i = 2$	12.34	52.77	72.18	48.09
$i = 3$	73.71	52.77	28.13	48.09
$i = 4$	39.86	52.77	6.38	48.09
$i = 5$	91.04	52.77	60.66	48.09
Consequent part				
Rule i	$a_{i1} \times 10^2$	$a_{i2} \times 10^2$	$b_{i1} \times 10^2$	
$i = 1$	28.00	-65.26	74.60	
$i = 2$	-16.97	21.95	101.30	
$i = 3$	12.95	-14.22	98.36	
$i = 4$	-23.52	52.16	134.86	
$i = 5$	-24.78	22.53	125.00	

lation program in open-loop. A sampling rate equal to 0.25 h and a simulation interval of 400 h were used. Three entrances for the four models were considered: manipulated variable on time instants k and $k-1$ ($nu = 2$); controlled variable on time instants $k-1$ ($ny = 1$). The generated models were later used for the regulatory and servo controls.

Figure 5 presents the training (model generation) and test (validation) data for the four output variables and Tables 4–7 present the parameters for the fuzzy models. A set of 1600 points was obtained both for training and testing. In Tables 4–7, k refers to time instant; u refers to manipulated variable; w and y_i refers to output, where $i = 1, \dots, R$; R being the number of rules of the fuzzy model; and a_{in} and b_{ih} the consequence function parameters of the fuzzy model for the input and output, respectively, where $n = 1, \dots, nu$ and $h = 1, \dots, ny$.

An i th specific rule is shown in Eq. 11, where X_{in} and W_{ih} are fuzzy sets (membership functions) of input and output, respectively.

$$\begin{aligned}
 & \text{IF}(u(k) \text{ is } X_{i,1}) \text{ and } (u(k-1) \text{ is } X_{i,2}) \text{ and } (w(k-1) \text{ is } W_{i,1}) \\
 & \text{THEN } y_i(k+1) = a_{i1} \cdot u(k) + a_{i2} \cdot u(k-1) + b_{i1} \cdot w(k-1)
 \end{aligned}
 \tag{11}$$

Table 7. Parameters of the Fuzzy Model for T_r

Number of Rules = 3				
Antecedent part				
Rule i	$u(k), u(k-1)$		$w(k)$	
	$c_i \times 10^2$	$\sigma_i \times 10^2$	$c_i \times 10^2$	$\sigma_i \times 10^2$
$i = 1$	10.84	17.11	17.27	15.65
$i = 2$	91.50	17.11	91.04	15.65
$i = 3$	39.86	17.11	45.59	15.65
Consequent part				
Rule i	$a_{i1} \times 10^2$	$a_{i2} \times 10^2$	$b_{i1} \times 10^2$	
$i = 1$	-6.72	17.19	93.59	
$i = 2$	9.42	8.45	81.47	
$i = 3$	11.53	7.78	82.65	

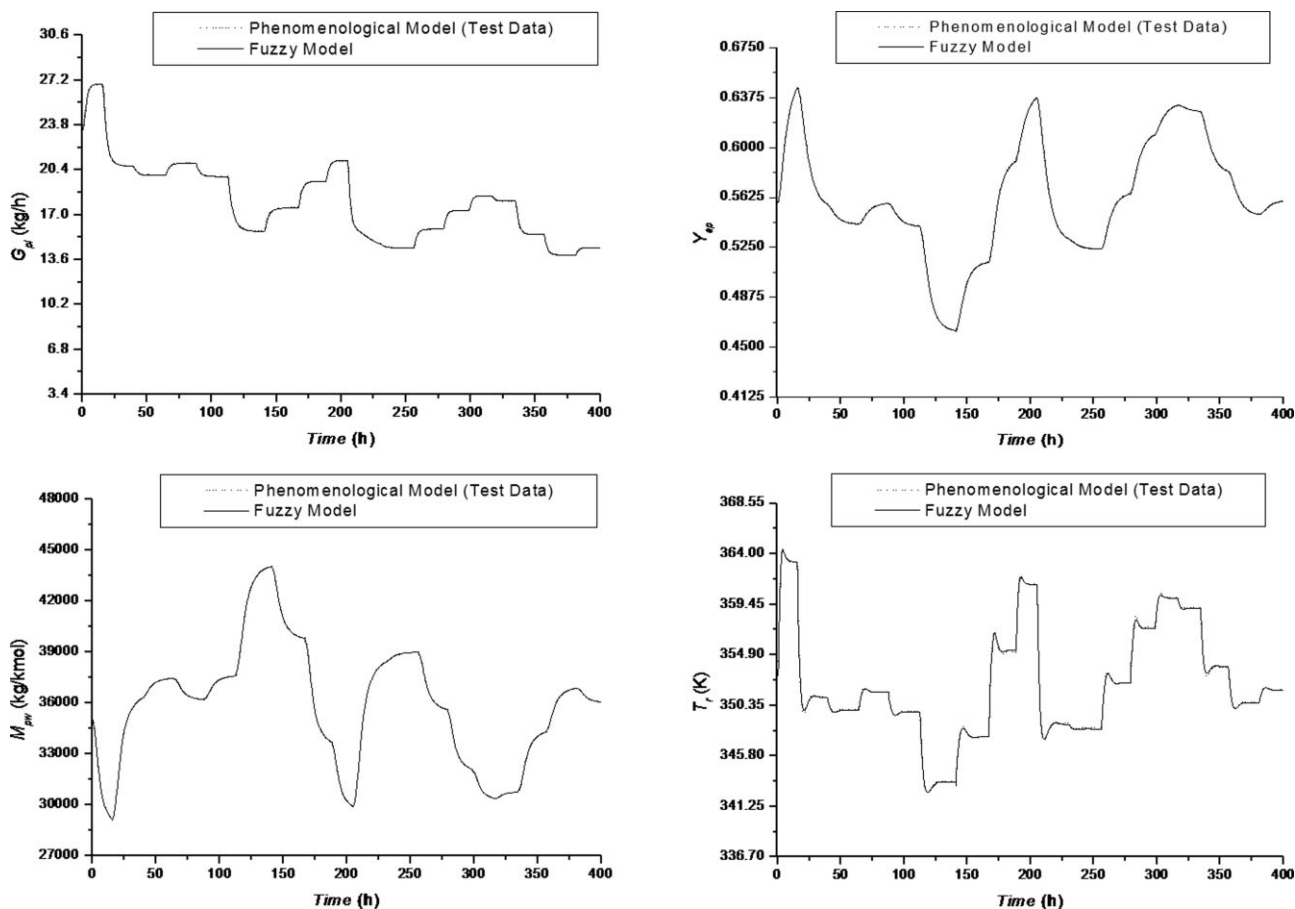


Figure 6. Validation of the fuzzy models.

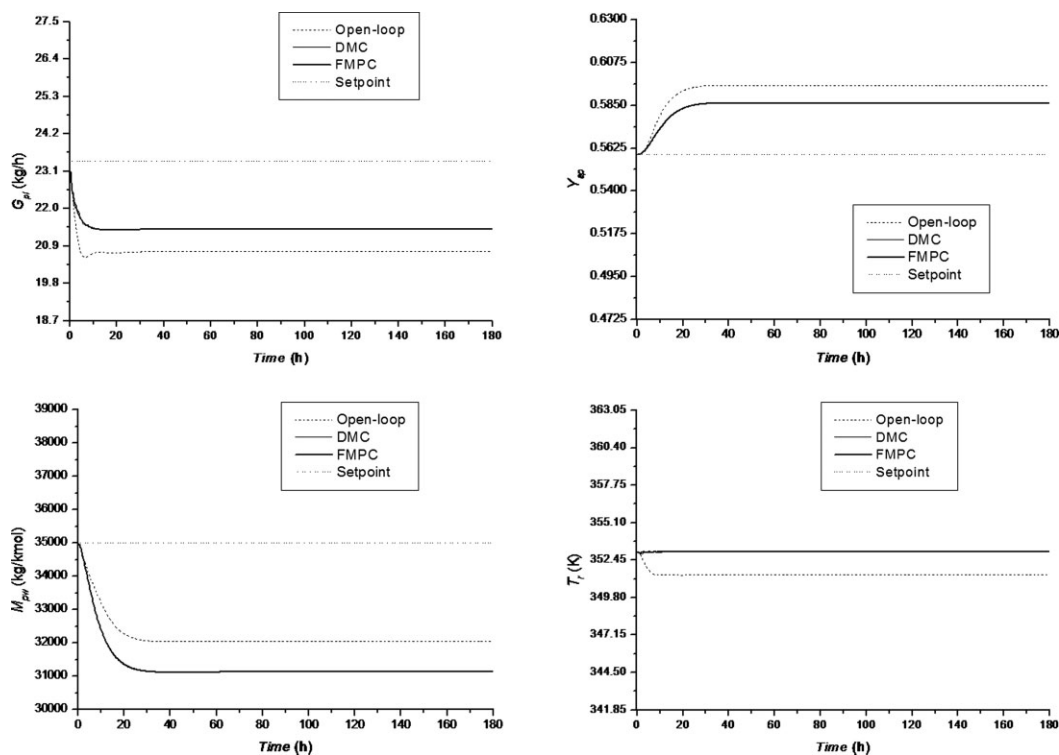


Figure 7. Response of output variables to inhibitor disturbance, with temperature control only.

Table 8. Tuning Parameters and Control Errors for the Regulatory Problem

Output	Parameters				IAE	
	PH	CH	f	α	DMC	FMPC
G_{pi}	2	1	0.003	0.80	54.9 kg/h	26.4 kg/h
Y_{ap}	5	2	0.023	0.95	0.6450	0.0425
M_{pw}	15	3	1.500	0.01	104735.7 kg/kmol	278715.2 kg/kmol
T_r	2	1	0.169	0.01	2.05 K	0.76 K

Figure 6 presents the validation results of the fuzzy models, which shows a very good prediction for the output variable. The average quadratic errors (calculated by Eq. 6) are equal to 0.0576 kg/h, 0.0004, 24.8106 kg/kmol, and 0.1284 K for the G_{pi} , Y_{ap} , M_{pw} , and T_r , respectively. As observed, very small errors were obtained.

Performance of the fuzzy model based predictive control system and discussion

An algorithm for the proposed control structure was developed in Fortran 90 and further inserted in the simulation program. To verify the performance of the FMPC strategy, a comparison with the DMC algorithm was made.

In the regulatory problem, an inhibitor disturbance of four parts per 1000 (mole basis) in the fresh feed was considered. Figure 7 indicates the futility of just controlling the reactor

temperature in response to this disturbance. The temperature is very well controlled by the two control schemes, but the polymer properties and production rate are still considerably influenced by the disturbance. For example, the molecular weight actually deviates more from its setpoint (34994.7 kg/kmol) with the temperature loop closed (31132.6 kg/kmol) than with the temperature loop open (32051.5 kg/kmol).

Table 8 shows the parameters used for DMC and FMPC multivariable control structures, and also presents the control errors for these configurations. Figure 8 presents a graphic analysis of the closed-loop performance of the four output variables, comparing the controllers with the open-loop system behavior. Computation times of 23 and 24 s were obtained for DMC and FMPC control, respectively.

As can be observed in Table 8 and Figure 8, the proposed control system performs better than the DMC, with a lower IAE value, a quicker answer and a smaller overshoot for the G_{pi} , Y_{ap} , and T_r . For the M_{pw} , the value of the IAE for the FMPC control system is larger than that for the DMC. However, the FMPC promotes a smoother and continuous behavior of the M_{pw} , while the DMC causes oscillations, which are not desired.

As regards the servo problem, the parameters used for the DMC and FMPC control structures are given in Table 9, as well as the control errors. Figure 9 presents the behavior of the four output variables for the reactor under control with setpoint changes. Computation times of 4 and 5 s were obtained for DMC and FMPC control, respectively. Such variable setpoint change policies seek to comply with the

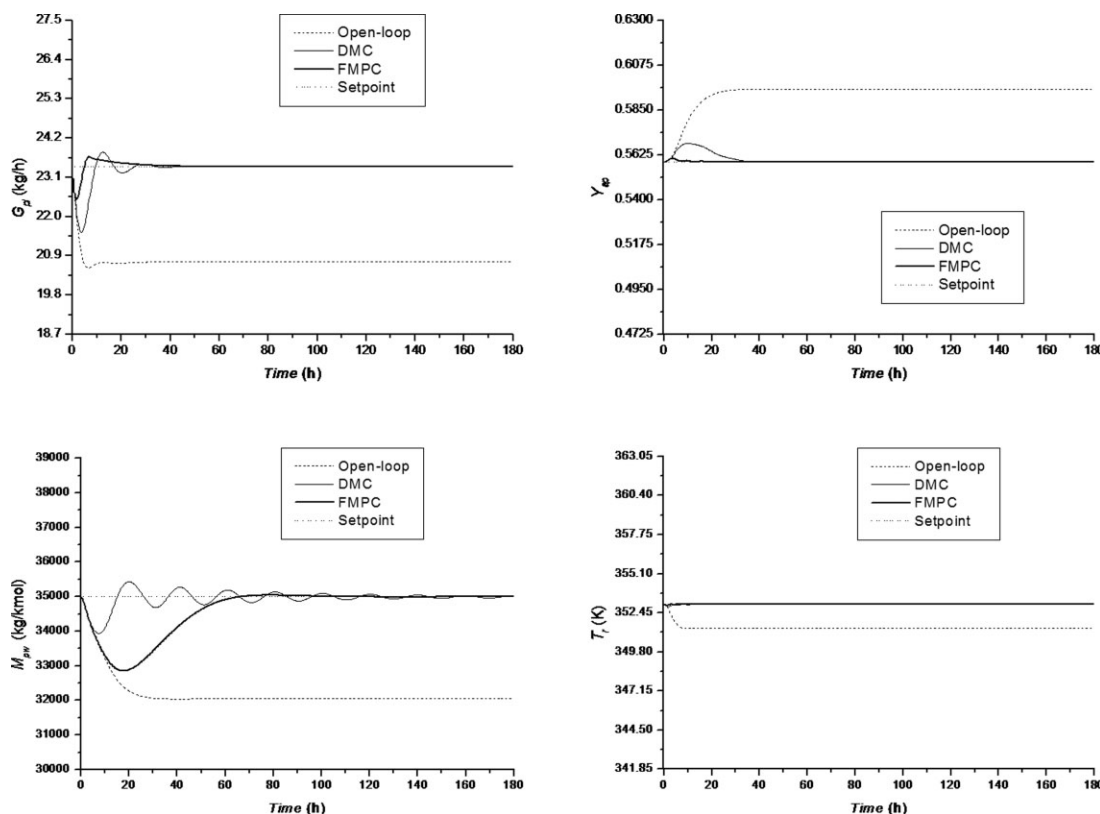


Figure 8. Closed-loop and open-loop simulations for inhibitor disturbance.

Table 9. Tuning Parameters and Control Errors for the Servo Problem

Output	Parameters				IAE	
	PH	CH	f	α	DMC	FMPC
G_{pi}	2	1	0.330	0.55	53.5 kg/h	159.7 kg/h
Y_{ap}	5	2	0.300	0.95	6.8010	10.6427
M_{pw}	9	1	0.040	0.98	331569.2	240357.0
					kg/kmol	kg/kmol
T_r	2	1	0.500	0.01	329.36 K	300.03 K

maximum and minimum limits allowed for variations on the output variables due to the dynamic nature of the process, taking into account the operational issues of product quality and safety.

Table 9 shows that the values of the control errors for the projected control system are greater for the G_{pi} and Y_{ap} , and lower for the M_{pw} and T_r . On the other hand, on analyzing Figure 9, it can be observed that the DMC promotes oscillations in the Y_{ap} and the FMPC control provides a slightly noisy behavior in the M_{pw} . However, in general, it can be concluded that the two controllers present similar responses for the four output variables. This can be explained by the fact that T_r depends linearly on T_j .

For the regulatory and servo controls, the selection of different values for the parameters for each output variable should be noted. This occurs because of the existence of dissimilar sensitivities between each controlled variable

and each manipulated variable, requiring the use of different tuning parameters. Also, it is important to emphasize that the regulatory and servo problems represent two different control directions and, thus, they require different control settings.

Conclusions

A fuzzy model based multivariable predictive control system was developed and applied to a copolymerization reaction because of its complexity. The polymer rate, composition, molecular weight, and reactor temperature were analyzed for regulatory and servo problems. The proposed control structure was compared with the DMC configuration, and presented the following main advantages.

1. Using a nonlinear model to represent a nonlinear process can often yield better results compared to a classic linear model.
2. Only input and output process data is required to represent the nonlinear model.
3. Equivalent computational effort achieves better results than those of linear predictive control. This indicates that the FMPC control system can certainly provide lower computational effort when compared to a conventional nonlinear predictive control.

As for disadvantages, it is important to mention that a sufficiently representative data set of the process is required to obtain a good model and consequently suitable control.

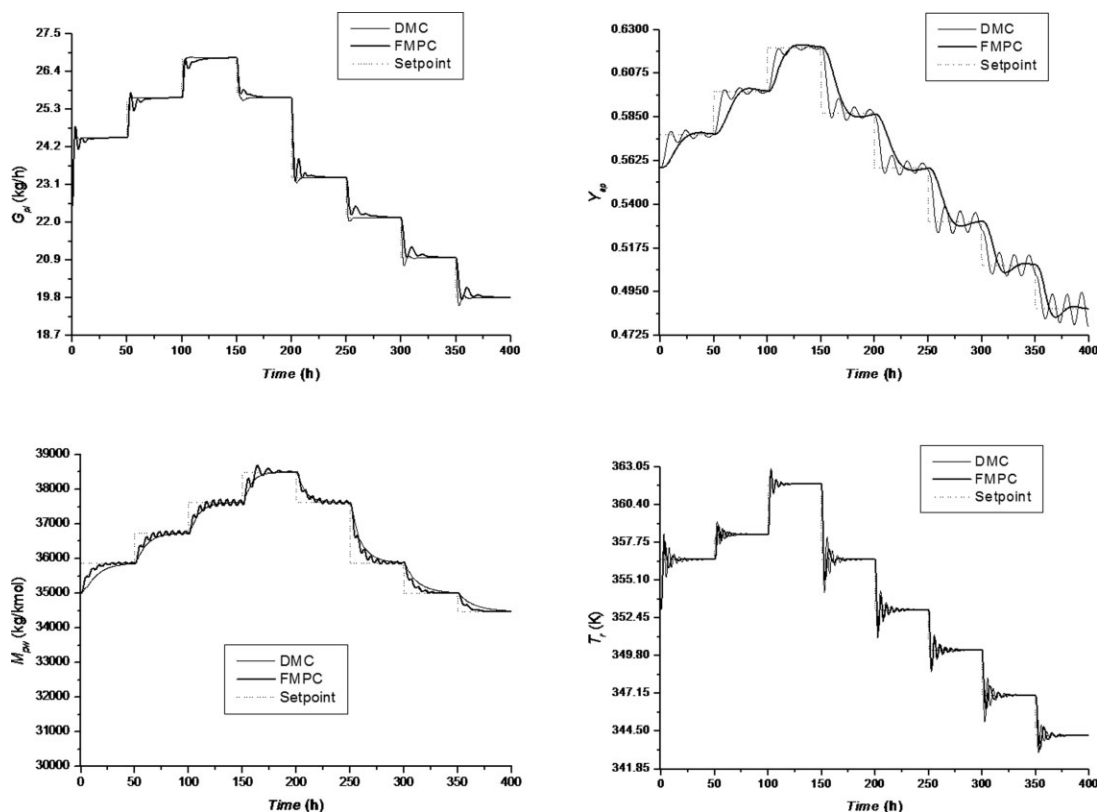


Figure 9. Closed-loop simulation for changes in setpoint.

In fact, the use of internal fuzzy dynamic models in the structure of predictive control has outstanding potential in the development of advanced control strategies and real-time optimization. This is because it is possible to take into account the operator information in the design of model. It has also been shown here that it is possible to find a set of parameters which leads to good control action without drastic changes in the controlled variables. It can, therefore, be concluded that the designed control strategy presented a sufficiently satisfactory performance, providing a better response than the DMC in most of the situations examined.

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Notation

a, b = parameter of the consequent function of the fuzzy model
 A = monomer A
 B = monomer B
 c = center of the Gaussian membership function
 CH = control horizon
 CP = continuous polymerization
 $CSTR$ = continuous stirred tank reactor
 DMC = dynamic matrix controller
 f = suppression factor
 $FMPC$ = fuzzy model based predictive control system
 G = mass flow rate, kg/h
 IAE = integral of the absolute value of the error
 k = time instant, h
 m = number of discrete instants
 M = molecular weight, kg/kmol
 MPC = model predictive control
 PH = prediction horizon
 R = number of rules of the fuzzy model
 T = temperature, K
 u = input variable of the process, input variable of the fuzzy model—manipulated variable
 w = input variable of the fuzzy model—controlled variable
 W = fuzzy sets of the output variable of the process
 x = input variable of the process
 X = fuzzy sets of the input variable of the process
 y = output variable of the process
 Y = mole fraction
 \bar{y} = predicted response

Greek letters

α = reference trajectory parameter
 μ = Gaussian membership function
 σ = constant spread of the Gaussian membership function
 ξ = molar purge fraction

Subscripts

a = monomer A
 b = monomer B
 CL = closed-loop
 f = feed to the reactor, final time of the evaluation period
 i = initiator, instantaneous, rule of the fuzzy model
 j = cooling jacket, entrance of the fuzzy model
 k = time instant
 p = polymer
 r = reactor
 s = solvent
 t = chain transfer agent
 w = weight average polymer property
 z = inhibitor
 0 = initial time of the evaluation period

Superscripts

actual = actual value
 d = desired output value
 future = future value
 pred = predicted value
 set = set-point

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