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Dynamic Optimization of a MMA with VAc Copolymerization Reactor

Nádson Murilo Nascimento Lima[a,*], Lamia Zuñiga Liñan[a], Rubens Maciel Filho[a], Flavio Manenti[b], Davide Manca[b], Marcelo Embiruçu[c]
[a] School of Chemical Engineering, State University of Campinas – UNICAMP, P.O. Box 6066, 13083-970, Campinas-SP, Brazil
[b] CMIC Dept. "Giulio Natta" – Politecnico di Milano, Piazza Leonardo da Vinci, I-20133, Milano, Italy
[c] Polytechnique Institute, Federal University of Bahia – UFBA, 40210-630, Salvador-BA, Brazil
[*] Corresponding author. E-mail: nadson@feq.unicamp.br

Increasing worldwide market competitiveness and reduced profit margins are pressing chemical and process industries to move towards a predictive control approach, based on first-principles mathematical models, as well as plant dynamic optimization. In this perspective, the paper focuses on the development of a nonlinear model predictive control (NMPC) to manage the copolymerization process of methyl methacrylate (MMA) with vinyl acetate (VAc), consisting of a jacketed continuous stirred tank reactor, a separator, and a recycle loop. This system presents a highly complex behavior, thus making difficult the success of controllers based on linear models. A detailed differential and algebraic mathematical model consists of 53 equations and is implemented in Fortran 90/95 to simulate the plant and setup the NMPC. The numerical solution is performed by using IMSL library. NMPC is proved to be superior to a linear model predictive control approach and appears to hold a considerable promise for such a reactor system.

Keywords: Nonlinear Model Predictive Control; Dynamic Optimization Problems; Grade Change Transition; Copolymerization.

1. Introduction

A typical feature of chemical process control is the existence of various operative constraints due to economic, environmental, and safety concerns as well as restrictions related to valve sizes and actuator dynamics. As a result, all these issues limit the expected performance of the controlled system. The problems increase in the control of polymerization processes, which exhibit highly interactive nonlinear, time-varying and difficult mathematical modeling of their dynamic behavior. This means that such reactions must occur to severely strict conditions to match the product quality and the market demand.

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To cope with this fact and for the inadequate performances offered by the conventional feedback control scheme, there is a good deal of literature focusing on the importance of advanced control techniques applied in the polymerization reactors (Soroush and Kravaris, 1992; Maner and Doyle III, 1997; Özkan et al., 2006; among others). Model predictive control (MPC) methodologies have become very popular in the chemical process industry. This fact is basically due to flexible constraint-handling capabilities on the input and output variables of MPC and to its robustness properties as well (Bemporad and Morari, 1999). However, the most of MPC algorithms are based on linear models and they are not able to control effectively and precisely the nonlinear systems within a wide range with steady-state multiplicity or desired operating regions with distinctly different input-output behavior. These features basically comprise all the polymerization processes. Therefore, in recent years, many researches have been accomplished looking for extending linear MPC approach to obtain a nonlinear model based predictive control (NMPC) (Haeri and Beik, 2005; Manenti and Rovaglio, 2008).
The present research activity deals with the development and the implementation of a NMPC controller to manage the temperature of a jacketed CSTR (Continuous Stirred Tank Reactor), where the copolymerization of methyl methacrylate with vinyl acetate takes place. This kind of reactors are known to be an interesting challenge to application of advanced control techniques, presenting operational problems due to complex open-loop behavior such as input and output multiplicities and nonlinear oscillations as well. The reactor jacket temperature is selected as manipulated variable. A deterministic model and process operating conditions are both obtained from the literature. This model is assumed to be an adequate representation of the system and it is implemented in Fortran 90/95 to simulate the plant and setup the NMPC. The proposed control scheme has shown to overcome a linear MPC (i.e. DMC – Dynamic Matrix Control) to the regulatory response of a SISO loop (Single-Input / Single-Output). NMPC search both satisfy the manipulated variable constraints and to provide the desired output value, even in the presence of unmeasured disturbances.

2. Nonlinear Model-Predictive Controller

The predictive control generates a manipulated variable profile by means of the minimization of some performance indexes over the time. The feedback loop is incorporated in the control structure because the measurements are used to update the optimization problem for the next time step. The objective of the NMPC method is to calculate 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, the future outputs are driven close to the reference trajectory. The basic idea of the SISO predictive algorithm is to: I. Calculate the reference trajectory (y^d); II. Estimate the closed-loop output predictions ($y^{CL,pred}$) using the process prediction model. In NMPC this model is formulated in the form of nonlinear differential equations; III. Compute the errors between predicted and reference trajectories; and IV. Estimate the sequence of the future controls to the movements of the manipulated variable (u) through the minimization of the objective function *J*, expressed by the Eq. (1):

$$J = \sum_{i=1}^{PH} w_1 \left(y_i^d - y_i^{CL,pred} \right)^2 + \sum_{j=1}^{CH} w_2 \left(u_j - u_j^{SST} \right)^2 + f^2 \sum_{k=1}^{CH} \left(\Delta u_k \right)^2 \quad (1)$$

where: $\Delta u_k = u_k - u_{k-1}$; u_j^{SST} = vector of steady-state target of the manipulated variable at the sampling time *j*; *f* = suppression factor to the movements of the manipulated variable; and w_1, w_2 = weights. In this study, the reference trajectory is calculated by a first order filter: $y_i^d = \alpha . y_{i-1}^{actual} + (1-\alpha) . y_{i-1}^{SET}$, where y_{i-1}^{actual} = vector of current measured value of the controlled variable at the sampling time *i*-1; y_{i-1}^{SET} = vector of setpoint of the controlled variable at the sampling time *i*–1; and α = reference trajectory parameter, with $0 \leq \alpha \leq 1$. The predicted values $y^{CL,pred}$ in Eq. (1) can be obtained directly from a nonlinear model of the process with $y^{CL,pred} = y_i^{CL,nonlinear}$. However, when this model is not perfect (and this is generally true), the control strategy will be not sufficiently robust. Thus, the following correction is applied: $y_i^{CL,pred} = y_i^{CL,nonlinear} + \left(y_{i-1}^{actual} - y_{i-1}^{CL,nonlinear} \right)$. In Eq. (1), only the first element of the vector Δu_k is implemented. At this point, the data vectors are shifted at the time so that the calculations can be repeated at the next sample instant.

3. Case Study

The process considered in this paper is the solution copolymerization of methyl methacrylate with vinyl acetate in a CSTR (Congalidis et al., 1989; Maner and Doyle III, 1997; Lima et al., 2007). Figure 1 is a flow diagram of a copolymerization reactor with a recycle loop. 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 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 heat of polymerization. Polymer, solvent, unreacted monomers, initiator and chain transfer agent flow out of the reactor to the separator (stream 4). Here, polymer, residual initiator and chain transfer agent are removed (stream 5). Unreacted monomers and solvent (stream 6) continue on to a purge point (stream 7) that represents venting and other losses. Purging is requested to prevent accumulation of inerts in the system. After the purge, the 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 hold tank are modeled as first-order lags with constant level and residence time equal to the reactor residence time. The important reactor output variables to match the product quality are: the copolymer 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 steady-state operating conditions are summarized in Table 1.

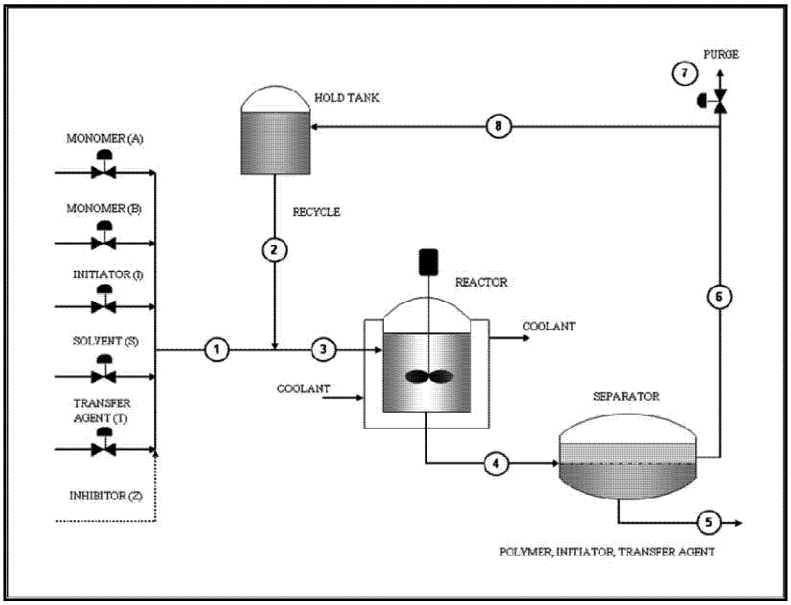

Figure 1. Process Layout (Congalidis et al., 1989).

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

3.1 Mathematical model

The analyzed process has a nonlinear deterministic mathematical model and kinetic parameters described in the literature. This model has been selected to simulate the plant and setup the NMPC, especially because it has been already validate in the range of our interest in the literature. Details on the deterministic model as well as system operating point are given in Congalidis et al. (1989) and Maner and Doyle III (1997).

Table 1. Steady-state Operating Conditions.

Inputs	***Outputs***
MMA feed rate (G_{af}) = 18 kg/h	G_{pi} = 23.3 kg/h
VAc feed rate (G_{bf}) = 90 kg/h	Y_{ap} = 0.56
AIBN feed rate (G_{if}) = 0.18 kg/h	M_{pw} = 35,000 kg/kmol
Benzene feed rate (G_{sf}) = 36 kg/h	T_r = 353.01 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	

3.2 Selection of the control loop

The analyzed system consists of seven inputs (G_{af}, G_{bf}, G_{if}, G_{sf}, G_{tf}, G_{zf}, T_j) and four outputs. T_{rf} is considered constant and ξ is under action of the feedforward controller. Thus, Lima et al. (2007) developed a factorial planning to discriminate the variables with higher impact on the process performance. Through this analysis, the selected control loop to this paper is: controlled variable = T_r, and manipulated variable = T_j.

3.3 Control results

The deterministic mathematical model was solved by a Runge–Kutta algorithm type in a software written in Fortran 90 language. Thus, the NMPC controller was developed and implemented in the process. The closed-loop performance of NMPC was analyzed for the rejection of unmeasured disturbances (regulatory problem). The disturbance considered by Congalidis et al. (1989) was the presence of an inhibitor in the fresh feed. This disturbance inhibits polymerization reaction. Since the polymerization 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 NMPC, a comparative study between NMPC and DMC was carried out. The DMC algorithm utilizes in Eq. (1) a linear prediction model adjusted by a step perturbation. The NMPC and DMC controllers were tuned by calculating the IAE (Integral of the Absolute value of the Error) criterion, and observing the output response. Figure 2 illustrates the closed-loop performance comparison of the two control strategies on the controlled and manipulated variables to the evaluated disturbance. The parameters of nonlinear and linear control systems as well as the IAE errors are summarized in Table 2.

3.4 Discussion

As it is shown in Figure 2, the reactor temperature remains very close to its desired trajectory under the action of NMPC controller. On the other hand, the DMC control causes some oscillations at the beginning of the disturbance. The DMC scheme brings the reactor temperature to its specification after 10.88 h, while NMPC strategy needs only 3.88 h. Also, the behavior of reactor jacket temperature with time is given in Figure 2. As observed, the NMPC and DMC responses are both satisfactory. However, it should be noted that DMC structure provides some fluctuations.

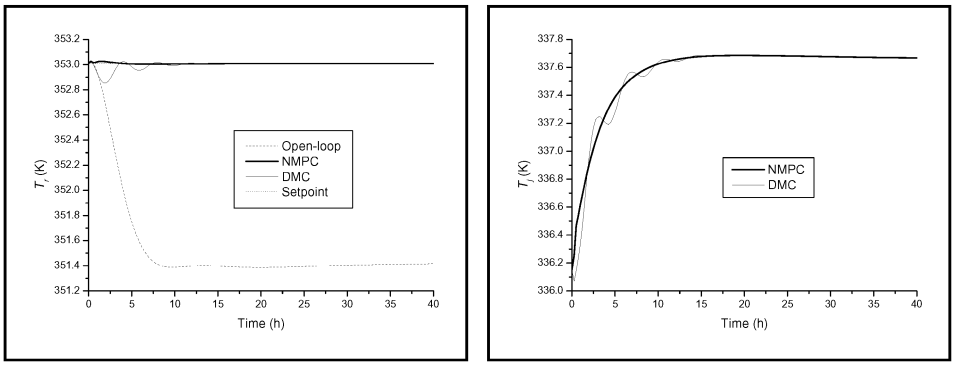

Figure 2 – Closed-loop and open-loop simulations to inhibitor disturbance.

Table 2. Tuning parameters and IAE errors for predictive control structures.

Parameters	***NMPC***	***DMC***
Prediction horizon - *PH*	4	2
Control horizon - *CH*	1	1
Suppression factor - f	0.001	0.001
Reference trajectory parameter - α	0.0001	0.0001
Weights - w_1, w_2	0.00064, 0.00010	1.00000, 0.00010
Sampling time (h)	0.25	0.25
IAE (K)	0.38658	1.80454

4. Conclusions

In the present paper the problem of nonlinear model predictive control for complex processes has been tackled. In particular, a solution copolymerization process has been considered for analysis. A NMPC control algorithm was developed and applied to a jacketed CSTR for tracking the reactor temperature. The regulatory behavior of NMPC strategy has been presented and compared for load effects against DMC controller. The simulation results show excellent performance for NMPC scheme and confirm the potential and robustness of this technique to reduce off-specifications during disturbances in nonlinear systems.

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