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Model-Based Control Strategies for a Chemical Batch Reactor with Exothermic Reactions

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Abstract–Batch reactor control provides a very challenging problem for the process control engineer. This is because a characteristic of its dynamic behavior shows a high nonlinearity. Since applicability of the batch reactor is quite limited to the effectiveness of an applied control strategy, the use of advanced control techniques is often beneficial. This work presents the implementation and comparison of two advanced nonlinear control strategies, model predictive control (MPC) and generic model control (GMC), for controlling the temperature of a batch reactor involving a complex exothermic reaction scheme. An extended Kalman filter is incorporated in both controllers as an on-line estimator. Simulation studies demonstrate that the performance of the MPC is slightly better than that of the GMC control in nominal case. For model mismatch cases, the MPC still gives better control performance than the GMC does in the presence of plant/model mismatch in reaction rate and heat transfer coefficient.

Key words: Process Control, Batch Reactor, Model Predictive Control, Generic Model Control, Kalman Filter

INTRODUCTION

A chemical reactor, which is one of the most important units in the chemical industry, can be broadly classified into two categories: a continuous and batch reactor. Although chemical reactors in large-scale operation have been operated in a continuous fashion, some reactors have been operated in a batch mode. This is because the batch reactor has the flexibility to be used for producing multi-products in small-scale processes.

It is commonly accepted that the control of batch reactors, especially when exothermic reactions are involved, is a difficult and challenging problem [Rotstein and Lewin, 1992]. Since it shows a high nonlinearity produced by heat generation term and its dynamic behavior can also strongly change with time. In addition, the batch reactors do not have a steady state condition; therefore, they are unstable under an open-loop operation.

A process for controlling the batch reactor generally consists of two steps: heating the reactor from ambient condition to desired temperature and then controlling it at this condition. Traditionally, these steps can be coped with by i) solving an open-loop optimal control problem (e.g. minimum time problem) to set the optimal temperature trajectory, ii) using a feedback control to keep the temperature at final desired value. However, the difficulty of this approach is that since there is no feedback information in the first step, it is not allowable for modeling errors; the heat released from the reaction in the heating period may increase until greater than the cooling capacity and make the reactor runaway [Jutan and Uppal, 1984].

In order to cope with such problems, many advanced control techniques have been applied for the control of a batch reactor, e.g. Nonlinear feedforward-feedback control [Jutan and Uppal, 1984; Kravaris et al., 1989], Adaptive control [Rotstein and Lewin, 1992], Generic model control [Cott and Macchietto, 1989; Kershenbaum and Kittisupakorn, 1994]. In addition to these control techniques, recently Park and Park [1999] applied a feedback linearization control technique to control a batch reaction system. It was found that this control strategy gave a better control performance than the PID controller in both set point tracking and disturbance rejection. Furthermore, Lee and Lee [1997] and Lee et al. [1999] proposed a novel model predictive control algorithm incorporating it with the iterative batch-to-batch learning control technique for nonlinear batch processes. The developed algorithm could eliminate persisting errors from unknown repeated disturbances as well as plant model mismatch and has been evaluated through simulation and experimental studies.

As can be seen from the literature on the control of batch reactors, many research works have stated the superior performance of advanced control techniques in comparison to a conventional control technique (PID). However, no such work has compared the control performance of a use of advanced control technique with other advanced control techniques. Thus this motivates us to the objective of this work that focuses on a designing and implementing of MPC and GMC which have been addressed extensively and compares their performance for controlling an exothermic batch reactor. Simulation studies of MPC and GMC in case of set point tracking under nominal and model mismatch cases are performed. In addition, since both MPC and GMC are model-based control techniques, they require the knowledge of process variables and/or some parameters in a control algorithm which are not all measured or known with sufficient accuracy for control purposes. For this purpose, it is necessary to use an online estimator to estimate unmeasurable process variables and unknown/uncertain process parameters. An extended Kalman filter, one of several estimation techniques applied to estimate states and parameters with great success [Valliere and Bonvin, 1989], is also used in this work to estimate the unmeasured heat released of reactions.

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BATCH REACTOR

In this section, the model equation of a batch reactor used in this simulation work is described. The batch reactor system studied by Cott and Macchietto [1989] and Kershenbaum and Kittisupakorn [1994] consists of a batch reactor and a jacket controlling system. For this reactor it is assumed that two parallel exothermic reactions occur in liquid phase and the rates of reaction depend on a reactant concentration as shown below:

$$A+B \xrightarrow{k_1} C \qquad R_1=k_1M_AM_B$$
$$A+C \xrightarrow{k_2} D \qquad R_1=k_1M_AM_C$$

where C and D are desirable product and undesirable by-product, respectively. The rate constants k_1 and k_2 are temperature dependence according to the Arrhenius equation. M_A, M_B and M_C represent the number of moles of components A, B and C in the reactor.

The operating objective of this reactor is to maximize the product C but minimize the production of D. This can be achieved by heating the reactor temperature from an initial condition to a desired set point rapidly and keeping it at this condition. The optimal temperature set point of 95 °C is chosen here.

In order to control the reactor temperature, the jacket inlet temperature is used as a manipulated input and can be regulated by a heat exchanger; the diagram of this system is shown in Fig. 1. The dynamics of the jacket temperature control can be reasonably assumed by a first order model with time constant [Liptak, 1986]. Moreover, since in a real situation the ability of jacket system is limited in a specific temperature range by the heat-exchanger capacity. Therefore, a lower temperature of 20 °C and an upper temperature of 120 °C are assumed in this work. In addition, a measurement noise is always present in a real application; thus, we also assume that both reactor and jacket temperature measurements have a Gaussian noise with zero mean and 1 °C standard deviation. The addition of both jacket temperature limitation and measurement error makes this simulation work reflect the actual process.

In the simulation work, the behavior of the batch reactor can be simulated by solving mass and energy balances [Eqs. (1)-(15)], which describe the dynamics of the reactor. The process parameters and initial condition are given in Table 1.

$$\frac{dM_A}{dt}=-R_1-R_2 \tag{1}$$

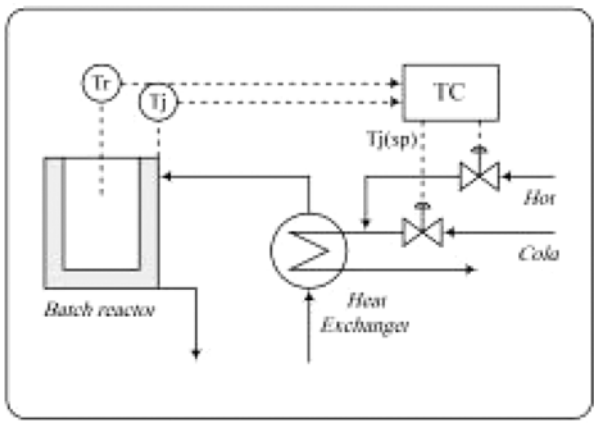

Fig. 1. Batch reactor system.

Table 1. The values of process parameters and initial condition

MW_A	=30	kg/kmol	Cp_A	=75.31	kJ/(kmol °C)
MW_B	=100	kg/kmol	Cp_B	=167.36	kJ/(kmol °C)
MW_C	=130	kg/kmol	Cp_C	=217.57	kJ/(kmol °C)
MW_D	=160	kg/kmol	Cp_D	=334.73	kJ/(kmol °C)
k_1^1	=20.9057		ΔH_1	=−41840	kJ/kmol
k_1^2	=10000		ΔH_2	=−25105	kJ/kmol
k_2^1	=38.9057		ρ	=1000	kg/m^3
k_2^2	=17000		ρ_j	=1000	kg/m^3
r	=0.5	m	Cp_j	=1.8828	kJ/(kg °C)
F_j	=0.348	m^3/min	V_j	=0.6912	m^3
τ_j	=1	min	U	=40.842	kJ/(min m^2 °C)
M_A (0)	=12	kmol	M_B(0)	=12	kmol
M_C (0)	=0	kmol	M_D(0)	=0	kmol
T_r (0)	=20	°C	T_j (0)	=20	°C

$$\frac{dM_B}{dt}=-R_1 \tag{2}$$

$$\frac{dM_C}{dt}=+R_1-R_2 \tag{3}$$

$$\frac{dM_D}{dt}=+R_2 \tag{4}$$

$$k_1=\exp\left(k_1^1-\frac{k_1^2}{T_r+273.15}\right) \tag{5}$$

$$k_2=\exp\left(k_2^1-\frac{k_2^2}{T_r+273.15}\right) \tag{6}$$

$$W=MW_AM_A+MW_BM_B+MW_CM_C+MW_DM_D \tag{7}$$

$$M_r=M_A+M_B+M_C+M_D \tag{8}$$

$$Cp_r=(Cp_AM_A+Cp_BM_B+Cp_CM_C+Cp_DM_D)/M_r \tag{9}$$

$$Q_r=-\Delta H_1R_1-\Delta H_2R_2 \tag{10}$$

$$Q_j=UA(T_j-T_r) \tag{11}$$

$$\frac{dT_r}{dt}=\frac{Q_r+Q_j}{M_rCp_r} \tag{12}$$

$$\frac{dT_j}{dt}=\frac{F_j\rho_jCp_j(T_{jsp}-T_j)-Q_j}{V_j\rho_jCp_j} \tag{13}$$

$$T_{rm}=T_r+a^{(k)} \tag{14}$$

$$T_{jm}=T_j+a^{(k)} \tag{15}$$

where A is given by 2w/ρr and $a^{(k)}$ is Gaussian noise with a standard deviation of 1 °C. The meanings of other variables and parameters are given in the Nomenclature.

MPC FORMULATION

Model predictive control (MPC) can be normally defined as a class of control strategy that computes a control trajectory by using a process model to predict future state outputs and optimize a cost function of a plant subject to state and/or input constraints [Kittisupakorn and Hussain, 2000]. Reviews regarding the MPC technique can be seen in many articles by, e.g. Biegler and Rawlings [1991],

Table 2. Comparison between MPC and GMC

Comparison	MPC	GMC
Control law	• Optimization problem	• Transformed control action with external PI
Tuning method	• Weighting parameters, prediction and control horizon	• Controller tuning curve
Advantages	• Capability to handle constraints and plant stabilization	• Direct use of system models in the control law
	• Nonlinear MIMO control	• Nonlinear SISO control
Limitation	• Reliable system's models	• Reliable systems model
		• Relative order one system

Henson [1998], and Morari and Lee [1999]. Although a nonlinear MPC is available, it may not be straightforwardly applicable to a real system due to two main difficulties. The first one involves optimization problem solving numerical techniques, computer hardware as well as computational time. The other one involves the complexity of the mathematical model of a system and, state and parameter estimation techniques to estimate unknown/unmeasurable states and parameters. As a result, a linear MPC is considered to apply to control the batch reactor in this work.

A formulation of the linear MPC technique for batch temperature control problem is shown below. It is clear that the process model of a system is the heart of the MPC technique. In general, the process model can be arranged in a discrete time model in state space form in which x, u, y are state, input, and output variables, respectively. From the previous section, although process models of the batch reactor are known, we assumed that only energy balances around the reactor and jacket are used in the MPC algorithm. The discrete state space form (T_r, T_j) is obtained from Eqs. (12) and (13) by local linearization around a current condition; this means that the process model in the control algorithm is updated at every time interval.

$$x(k+1)=A(k)x(k)+B(k)u(k) \tag{16}$$

$$y(k)=C(k)x(k) \tag{17}$$

The manipulated input profile (T_j) can be determined by solving a minimization problem based on an objective function which is the sum of squares of the deviation of set point and predicted value on outputs and inputs over the prediction horizon (P). The optimization decision variables are control inputs (U) M time steps.

$$\min_{U(k)\cdots U(k+M-1)} \sum_{i=k+1}^{k+P} [y_{sp}(i)-y_{pred}(i)]^2_{W1}+[u_{sp}(i)-u_{pred}(i)]^2_{W2} \tag{18}$$

subject to the system models [Eqs. (16) and (17)] and a constraint on the manipulated variables. W1 is a weighting matrix on outputs and W2 is a weighting matrix on inputs.

However, even though a set of inputs is computed, only the first control action is applied to the system and when feedback information becomes available after the control action is implemented, a computation is repeated again for the next sampling time.

GMC FORMULATION

Generic model control (GMC), developed by Lee and Sullivan [1988], refers to a control technique based on a process model. The basic concept is that it directly inserts nonlinear process models into the controller itself; the nonlinear process models do not need to be linearized. The control action is calculated based on a transformed control action with external PI control action. To have a clear view of the difference between MPC and GMC, the concepts, advantages and limitations of these control techniques are included in Table 2. GMC control technique can be given as follows:

$$\frac{dy}{dt}=K_1(y_{sp}-y)+K_2\int_0^t (y_{sp}-y)dt \tag{19}$$

where y represents the controlled variables. K_1 and K_2 are GMC tuning constants. The tuning parameters K_1 and K_2 can be determined by choosing a target profile of a controlled variable as suggested by Lee and Sullivan [1988].

To apply the GMC for controlling a temperature of a batch reactor, an energy balance around the reactor is needed; it gives the relation between a controlled variable (reactor temperature) and a manipulated variable (jacket temperature).

$$\frac{dT_{rm}}{dt}=\frac{Q+UA(T_j-T_{rm})}{WCp} \tag{20}$$

where T_{rm} and T_j are the measured reactor and jacket temperature. W is the mass of the reactor content and Cp is the mass heat capacity of the reactor content. Both values of W and Cp are assumed to be constant at this stage.

Then replacing T_{rm} for y in Eq. (19) and rearranging to obtain T_j yield:

$$T_j=T_{rm}+\frac{WCp}{UA}[K_1(T_{rsp}-T_{rm})+K_2\int_0^t (T_{rsp}-T_{rm})dt]-\frac{Q}{UA} \tag{21}$$

Eq. (21) gives the jacket temperature computed by the GMC controller in a continuous form. For the purpose of applying the GMC in a real system, the discrete form is required:

$$T_j(k)=T_{rm}(k)+\frac{WCp}{UA}\left(K_1[T_{rsp}-T_{rm}(k)]+K_2\sum_0^k[T_{rsp}-T_{rm}(k)]\Delta t\right)-\frac{Q(k)}{UA} \tag{22}$$

Since, the jacket temperature determined from Eq. (22) is an actual temperature which is not a set point value for the jacket temperature control system. In order to compensate the effect of a dynamic of the jacket control system, as stated in the system model section, a first order model with time constant is assumed. Consequently, the jacket temperature set point (T_{jsp}) is:

$$T_{jsp}(k)=T_j(k-1)+\tau_j\left(\frac{T_j(k)-T_j(k-1)}{\Delta t}\right) \tag{23}$$

With this temperature set point, a control valve (setting as a PI

controller) opens or closes, reflecting the ratio of hot water and cold water feeding into the jacket.

ESTIMATION OF HEAT RELEASED FROM REACTION

Since model based control techniques utilize a process model of a system to calculate the control action, all states and model parameters are needed. In most processes many of them cannot be measured or known exactly. Online estimation techniques are used to estimate unknown/uncertain states and parameters.

For temperature control of the batch reactor, the knowledge of heat released (Qr) is necessary to the control algorithm and affects the performance of the controller. Accordingly, in this work, an extended Kalman filter with simplified process models [Kershenbaum and Kittisupakorn, 1994] has been applied to estimate the heat evolution term. The reason for using the simplified model, not the exact model of the plant, is that it is well known that parameters are not all known exactly and states are not all measurable. Therefore, if the exact model is used, too many uncertain/unknown parameters as well as too many unmeasurable states would be involved. These would lead to poor performance of the Kalman filter. Hence, the simplified model with less uncertain/unknown parameters and unmeasurable states is used instead.

In order to develop the simplified models of a batch reactor, it is assumed that the total rate of reaction (R) is a function of reactor temperature (T_{rm}) and number of total mole of component in the reactor (M_r) as in the form:

$$\frac{dM_r}{dt} = -R = -cM_rT_{rm} \tag{24}$$

where c is a *pseudo* rate constant.

Additionally, we also assume that an *estimated* heat released (Q_{re}) from reaction can be written as a product of the total rate of reaction and the heat of reaction:

$$Q_{re}=(-\Delta H)(R)=-c\Delta HM_rT_{rm} \tag{25}$$

From Eq. (25), we obtain

$$\frac{dQ_{re}}{dt} = -c\Delta H\left(M_r\frac{dT_{rm}}{dt} + T_{rm}\frac{dM_r}{dt}\right) \tag{26}$$

Eqs. (24) and (26) incorporating with energy balances [Eqs. (12) and (13)] are used in the Kalman filter. Table 3 gives the parameters and initial condition used in the Kalman filter.

SIMULATION RESULTS

The application of MPC with the extended Kalman filter to control the batch reactor temperature is demonstrated in this section. The performance of the MPC technique for all tests is compared with that of the GMC.

In all simulations studied, the batch reactor is initially charged with 12 kmol of component A and 12 kmol of component B. Both the reactor and jacket temperatures are 20 °C at the initial condition. The tuning parameters of MPC and GMC controller are summarized in Table 4.

First, the performance of the controllers is tested in the nominal case; the model parameters used in the controllers are determined

Table 3. Parameters and initial condition for Kalman filter

T_{rm}	=20 °C	P	=diag[1 1 1 1]
T_{jm}	=20 °C	Q(1,1)	=4
Q_r	=0 kJ	Q(2,2)	=16
M_r	=0	Q(3,3)	=10^9
R(1,1)	=50	Q(4,4)	=10^4
R(2,2)	=30		

Table 4. Parameters in MPC and GMC algorithm

MPC controller			
M	=20	P	=50
$W_1(1,1)$	=2000	$W_1(2,2)$	=50
$W_2(1,1)$	=1.2		
GMC controller			
K1	=0.33	K2	=6.94×10^{-5}

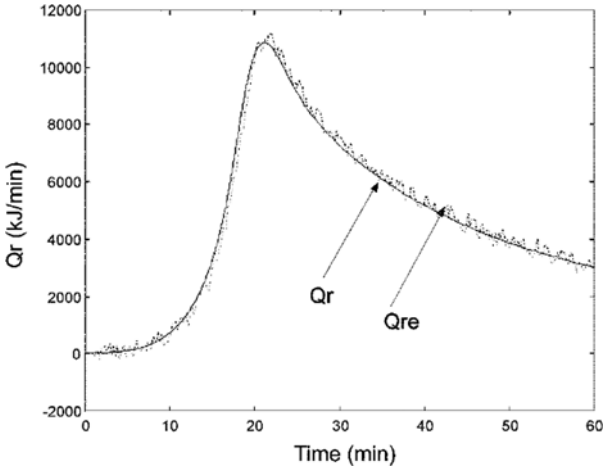

Fig. 2. Heat released curve in nominal case both from reactor and estimate.

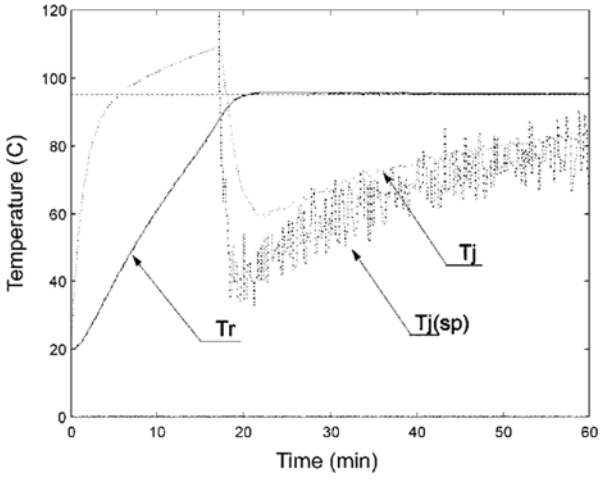

Fig. 3. Response of MPC in nominal case.

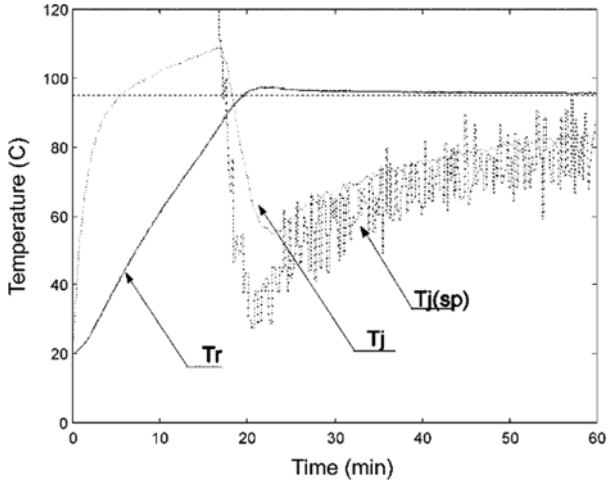

Fig. 4. Response of GMC in nominal case.

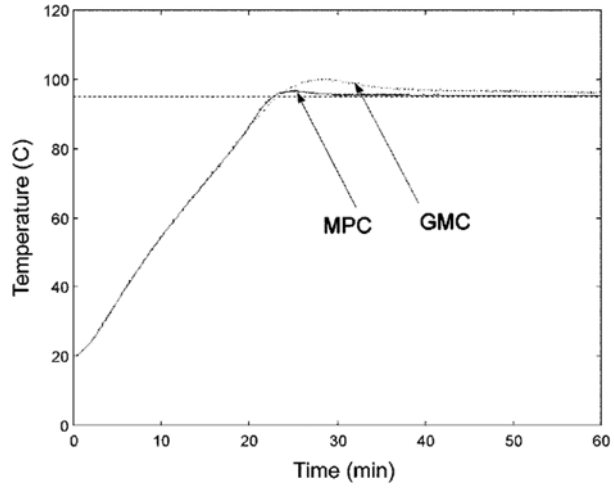

Fig. 5. Response of system for heat transfer coefficient change.

correctly as the same as process parameters. Fig. 2 shows the comparison of the actual and estimated heat released of reactions. It can be seen that the extended Kalman filter gives excellent estimation of the heat released. With this heat released, both MPC and GMC controllers can give reasonably good reactor temperature control although an overshoot occurs in the case of GMC controller as can seen from Figs. 3 and 4.

Since both MPC and GMC techniques use the process model of the system in the control algorithm, these controllers need to be tested for robustness with respect to plant/model mismatch. Fig. 5 illustrates the response of both MPC and GMC controller when the heat transfer coefficient decreases 25% from the nominal value. It can be seen that the MPC controller gives a better control response than the GMC does. In other words, MPC can control the reactor temperature at the desired set point whereas the GMC controls the reactor temperature with some overshoot and offsets.

Similarly, the kinetic data in rate equation may not be known exactly. Here it is assumed that the reaction rate of the first reaction increases 40% from the actual reaction rate (Fig. 6). Again, the MPC controller is still able to cope with this mismatch; it still gives good control response without any offset. On the other hand, the GMC

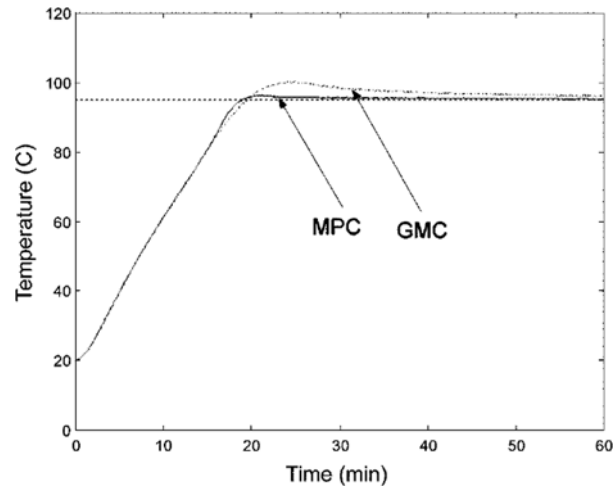

Fig. 6. Response of system for reaction rate change.

controller controls the reactor temperature at the set point with some offset. The simulation results show that in the presence of plant/model mismatch the MPC is more robust than the GMC. This is because the MPC has a plant stabilization property, whereas the GMC does not have the property. Therefore, in the presence of plant/model mismatch, the MPC is still able to control the system at a steady state condition. The GMC on the other hand cannot guarantee that it can control the system at a steady state condition.

CONCLUSIONS

Model predictive control has been applied to control an exothermic reactor. Its control performance is compared with that of Generic model control. Since both controllers are model-based control techniques, they need the measurement/estimation of states and parameters. Here the heat released of reactions cannot be measured. Therefore, an extended Kalman filter is used to estimate heat released of the reactions. Simulation results show that both MPC and GMC can give good control response in a nominal case. However, in the presence of plant/model mismatch in heat transfer coefficient and reaction rate, the MPC is more robust than the GMC; it still gives good control performance, whereas the GMC gives deteriorative control performance.

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NOMENCLATURE

Ar : heat transfer area [m^2]
Cp : mass heat capacity [kJ/(kg °C)]
Cpi : molar heat capacity of component i [kJ/(kmol °C)]
ΔHi : heat of reaction of reaction i [kJ/kmol]
Δt : sampling time [min]
F : flowrate [m^3/min]

K1, K2 : GMC controller constants
k_i : rate constant for reaction i [$kmol^{-1}s^{-1}$]
k_i^1 : rate constant 1 for reaction i
k_i^2 : rate constant 2 for reaction i
Mi : number of moles of component i [kmol]
Mwi : molecular weight of component i [kg/kmol]
Q : heat released from reactions [kJ/min]
ρ : density of reactor content [kg/m^3]
Ri : rate of reaction i [kmol/min]
t : time [min]
T : reactor temperature [°C]
U : heat transfer coefficient [$kJ/(min\,m^2\,°C$]
u : input variables
V : reactor volume [m^3]
W : reactor content [kg]
W1,W2 : MPC weighting parameters
x : state variables
y : output variables

Subscripts

f : filter
j : jacket
m : measured
r : reactor
sp : set point
pred : prediction

REFERENCES

Biegler, L. T. and Rawlings, J. B., "Optimization Approaches to Nonlinear Model Predictive Control," In Chemical Process Control CPCIV Proceedings (1991).

Cott, B. J. and Macchietto, S., "Temperature Control of Exothermic Batch Reactors Using Generic Model Control," *Ind. Eng. Chem. Res.*, **28**, 1177 (1989).

de Valliere and Bonvin, D., "Application of Estimation Techniques to Batch Reactors-II. Experimental Studies in State and Parameter Estimation," *Computers chem. Engng.*, **13**(1/2), 11 (1989).

Henson, M. A., "Nonlinear Model Predictive Control: Current Status and Future Directions," *Computers chem. Engng.*, **23**, 187 (1998).

Jutan, A. and Uppal, A., "Combined Feedforward-Feedback Servo Control Scheme for an Exothermic Batch Reactor," *Ind. Eng. Chem. Process Des. Dev.*, **23**, 597 (1984).

Kershenbaum, L. S. and Kittisupakorn, P., "The Use of a Partially Simulated Exothermic (PARSEX) Reactor for Experimental Testing of Control Algorithms," Trans IChemE., 72, Part A, 55-63, Jan. (1994).

Kittisupakorn, P. and Hussain, M. A., "Model Predictive Control for the Reactant Concentration Control of a Reactor," *Korean J. Chem. Eng.*, **17**, 368 (2000).

Kravaris, C., Wright, R. A. and Carrier, J. F., "Nonlinear Controllers for Trajectory Tracking in Batch Processes," *Computers chem. Engng.*, **13**(1/2), 73 (1989).

Lee, K. S., Chin, I. S., Lee, H. J. and Lee, J. H., "Model Predictive Control Technique Combined with Iterative Learning for Batch Processes," *AIChE J.*, **45**(10), 2175 (1999).

Lee, K. S. and Lee, J. H., "Model Predictive Control for Nonlinear Batch Processes with Asymptotically Perfect Tracking," *Computer chem. Engng.*, **21**, s873 (1997).

Lee, P. L. and Sullivan, G. R., "Generic Model Control (GMC)," *Computer chem. Engng.*, **12**(6), 573 (1988).

Liptak, B. G., "Controlling and Optimizing Chemical Reactors," *Chemical Engineering*, May 69-81 (1986).

Morari, M. and Lee, J. H., "Model Predictive Control: Past, Present and Future," *Computers chem. Engng.*, **23**, 667 (1999).

Park, S. Y. and Park, S., "Nonlinear Control of a Batch Ester-interchange Reactor," *Korean J. Chem. Eng.*, **16**, 745 (1999).

Rotstein, G. E. and Lewin D. R., "Control of an Unstable Batch Chemical Reactor," *Computers chem. Engng.*, **16**(1), 27 (1992).