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Batch control improvement by model predictive control based on multiple reduced-models

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ABSTRACT

In this research study, model predictive control (MPC) utilizing multiple reduced-models running in series is developed and studied to investigate an improved temperature-control performance of an exothermic batch reactor. Three steps of batch-model construction are presented, which involve (i) a reference-profile determination, (ii) an operating-condition selection and (iii) a model-reduction. Different pseudo steady-states conditions are properly selected along the closed-loop reference profiles with regards to overall closed-loop poles of the system. The models further individually determined their minimal-phases to attain only controllable and observable states. Consequently, different model-orders can be chosen corresponding to their controllability and observability. Simulation results have shown that, in a nominal case, the proposed controller provides control performances as good as a single-model based controller does. However, in presences of plant/model mismatches, the reduced-controller provides much better and more robust control performances.

1. Introduction

The temperature control of a batch reactor with exothermic reactions normally consists of (i) initial heating-up the reactor temperature from an ambient condition, and (ii) maintaining it at the desired value. Heating is initially required for driving the system to reach the desired operation as quickly as possible; this is to reduce overall cycle-time of a reaction process. Afterwards, cooling is used to keep the temperature at its set point. It can be seen that switching from heating to cooling always provide the difficulty of batch temperature control. As heat-released of reactions in a heating period may become very large very quickly, the reactions can become unstable, and cause the temperature to runaway if the heat-generated exceeds the cooling capacity of the reactor. Therefore, a careful control of change rate of the temperature and minimization of temperature overshoot are required.

Traditionally, a dual-mode control strategy has been employed to solve this type of problem. In industrial practices, an on–off type strategy is commonly implemented consisting of applying maximum heating (on) until the reactor temperature is within a specified range of set point (heating mode), and then switching to maximum cooling (off) to bring the change rate of the temperature to zero (cooling mode). Alternatively, a standard feedback-controller can be switched on in the second mode [16]. Nevertheless, as an optimal switching criterion from heating to cooling has been determined in off-line fashion, it is only valid for a specific range of operating conditions. Moreover, heating proceeds in an open-loop manner, no feedback from the reactor is used (switched-off controller), for that reason there is no allowance for modeling errors.

To overcome the problem of the open-loop strategy, many advanced-control techniques have been proposed and studied to control batch reactors, such as feedforward–feedback control [8], iterative learning control [4], etc. In addition to these, several works have focused on the development of effective estimators to provide the estimates of heat-released of reactions in a feedback-control framework, i.e. an extended Kalman filter [1,10,11], neural network [3] and dynamic data reconciliation [9].

In industrial applications, model predictive control (MPC), an optimization model-based controller, has achieved great successes [14]. Most of commercially available MPC products have utilized linear-model; this is because non-linear-MPC (using non-linear-model) performs computational complexity and convergence problem of an optimization [6]. The attempt to handle highly non-linear behavior of the linear-MPC has been addressed in many studies.

One of those, an idea of a global-model has been concentrated [2,7,12,15]. A set of models running in parallel has been weighted

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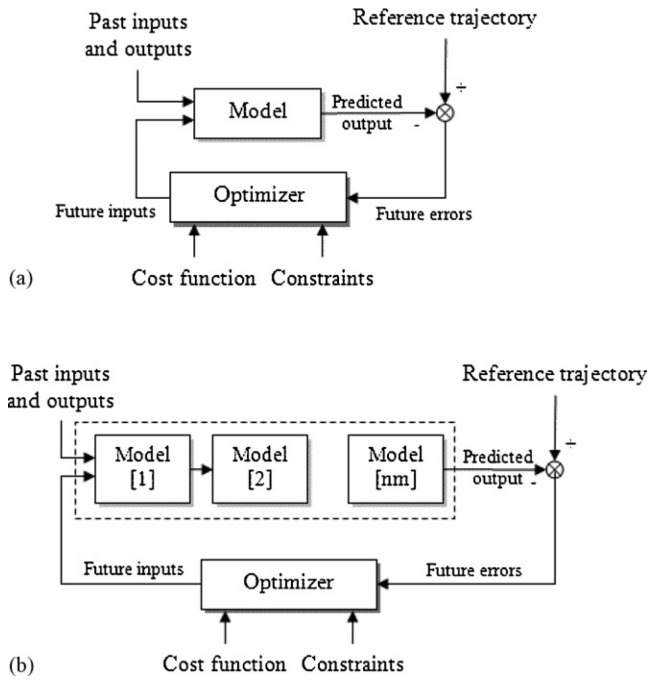

Fig. 1. (a) Conventional framework. (b) Proposed framework. Model predictive control (MPC) control frameworks.

via using a weighting function to provide the global-model, which is further used in a traditional MPC algorithm to calculate a set of control moves. It has been reported in literatures that the selection of proper number of models and weighting function have shown to be an important issue.

This work is mainly focused on the feedback-control design of a MPC controller for further improvement of a temperature-control performance over an entire batch operation. The controller has been developed by using multiple-models running in series to cope with whole batch-dynamic changes. The modeling strategy has been motivated by the fact that a batch reactor goes through a series of phases with substantially different characterizations. The models in a state-space form have been further determined their minimal phases individually [13,17,18] to eliminate uncontrollable and/or unobservable states, which may causes poor control performances. It is noted that the reduced state-space models can be developed directly through empirical data by a subspace state-space identification method, in which a model-reduction approach is readily built-in [5].

2. A proposed model predictive control

The basic idea of a MPC controller is to determine a set of control moves over a control-horizon by minimizing some criteria subject to a process-model and input/output constraints. The first value of the controls is then applied to the process. In a formulation of a conventional controller, a single model in a state-space form, as shown in Eq. (1), is used to provide an output prediction and to obtain process performance optimization (Fig. 1a).

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y^m &= C^m x \end{aligned} \tag{1}$$

where u, y^m are vectors of process inputs and measurable outputs, respectively.

Nevertheless, in high non-linearity and non-stationary applications such a batch process, the controller with a single model has proven in literatures to give poor control performance. This is because it is rarely possible to describe entire batch-dynamics with only one local-model due to time-varying behavior by nature. The capabilities of the conventional controller will degrade as an operating level moves away from an original design level of operation.

2.1. Multiple reduced-models development

Multiple reduced-models are developed around different pseudo-steady-states operating conditions, and utilized sequentially in the proposed control strategy to cope with the entire batch dynamics. Here, the batch process is divided into a certain period (*nm*), in which the model *j* is employed to describe the system dynamics within a particular duration $t_{j-1} < t \leq t_j$.

As state-controllability and -observability is commonly varied along a batch operation, the models should reduce their orders individually to avoid uncontrollable and/or unobservable states, which may cause poor control performances. In this study, a set of the reduced-models are obtained by applying the following two steps: system diagonalization and determination of minimum realization. Similar diagonal systems are firstly determined for simply identifying truncated-states. Subsequently, pole-zero cancellation is applied to provide minimum phases of the models.

By applying those steps, the reduced-model can be formulated as

$$\begin{aligned} \dot{x}_j^{\mathrm{r}} &= A_j^{\mathrm{r}} x_j^{\mathrm{r}} + B_j^{\mathrm{r}} u \\ y^m &= C_j^{\mathrm{mr}} x_j^{\mathrm{r}} \end{aligned} \tag{2}$$

where $A_j^{\mathrm{r}} = \vartheta_j \left(\varsigma_j^{-1} A_j \varsigma_j \right)_{\mathrm{nr}\times\mathrm{nr}} \vartheta_j^{-1}$, $B_j^{\mathrm{r}} = \vartheta_j \left(\varsigma_j^{-1} B_j^{\mathrm{r}} \right)_{\mathrm{nr}\times\mathrm{nu}}$, $C_j^{\mathrm{mr}} = \left(C_j^m \varsigma_j \right)_{\mathrm{ny}\times\mathrm{nr}} \vartheta_j^{-1}$, in which (nu) and (ny) are numbers of process inputs and outputs, respectively. The symbol $(\cdot)_{\mathrm{nr}\times\mathrm{nr}}$ denotes the matrix that only first (nr) rows and columns are considered, in other words, the last (nx − nr) states are truncated. The matrices ς and ϑ are transform matrices in diagonalization, and minimum-realization steps, respectively. Noted that the matrix $\left(\varsigma_j^{-1} A_j \varsigma_j \right)$ is diagonal, in which its elements are eigenvalues of the matrix A_j.

2.2. A control framework

A control framework of the proposed control-scheme is shown in Fig. 1b. The MPC formulation is established in which multiple reduced-models are employed sequentially for predicting future behavior of the process-outputs. Afterward the optimization problem is solved using a quadratic programming (QP). Noted that the QP method can be implemented directly when original full-states models are used.

As the models further reduce their orders individually, this provides multiple reduced-models with different orders (according to their controllability and observability) and state-domains. State transformation is required to give prediction consistency and continuity. It is also noted that although all reduced-models have same orders, the transformation is still needed because of different state-coordinates.

The transform matrix, K_j can be determined with the assumption that, at a model switching time (k), two considered models give same predicted values of both original full-states and measurable outputs. This is to preserve the primary direction of the states

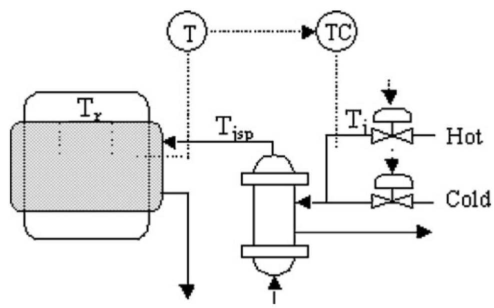

Fig. 2. Schematic diagram of a batch reactor.

estimates of the current model j.

$$\begin{bmatrix} C_j^x \\ C_j^{\mathrm{mr}} \end{bmatrix} x_{j,k}^{\mathrm{r}} \cong \begin{bmatrix} C_{j+1}^x \\ C_{j+1}^{\mathrm{mr}} \end{bmatrix} x_{j+1,k}^{\mathrm{r}} \tag{3}$$

From Eq. (3), the matrix K_j is,

$$K_j = \left(C_{j+1}^{\mathrm{T}} C_{j+1}\right)^{-1} C_{j+1}^{\mathrm{T}} C_j \tag{4}$$

where $C_j = \begin{bmatrix} C_j^x \\ C_j^{\mathrm{mr}} \end{bmatrix}$. The obtained transform matrix is solely dependent on a system matrix C of the two adjacent models, in other words, it is independent of the instant time.

To formulate a quadratic optimization problem, the reduced-states of the other models used in the controller are replaced with the correlation equation of those reduced-states and x_j^{r} (current model j); for example, $x_{j+1}^{\mathrm{r}} = (K_j)x_j^{\mathrm{r}}$, $x_{j+2}^{\mathrm{r}} = (K_{j+1}K_j)x_j^{\mathrm{r}}$, and so on. Comparing to the conventional MPC scheme, two additional steps are required which involves models specification, and states transformation. Now a whole batch behavior can be described using a set of local-models sequentially, even the models are developed in different state coordinates.

3. An exothermic batch reactor

3.1. Process description

A batch system consists of a batch reactor and a jacket heating/cooling system as shown in Fig. 2, in which two parallel exothermic reactions occur in liquid phase as below:

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} \quad \text{and} \quad \mathrm{A} + \mathrm{C} \rightarrow \mathrm{D}$$

where A, B are raw materials, and C, D are desirable and undesirable products, respectively. Further details of the system are given in Appendix A.

For this system, the reaction rates must be controlled to limit a production of D by heating reactor temperature (T_{r}) from its initial value to a desired set point rapidly and maintaining it at this condition. The optimal T_{r} of 95 °C is chosen in this case. A jacket inlet temperature (T_{jsp}) is used as a manipulated input, and can be regulated by a heat exchanger. To reflect the actual process, it is assumed that the ability of the jacket system is limited in a temperature range between 20 and 120 °C by heat-exchanger capacity.

3.2. Model-construction

As discussed above, a batch control problem involves time-varying and high non-linear behavior, non-stationary operating conditions, and uncontrollable and/or unobservable states. Therefore, three steps of linear time-invariant model construction have been proposed in order to manage the problems as shown in Fig. 3.

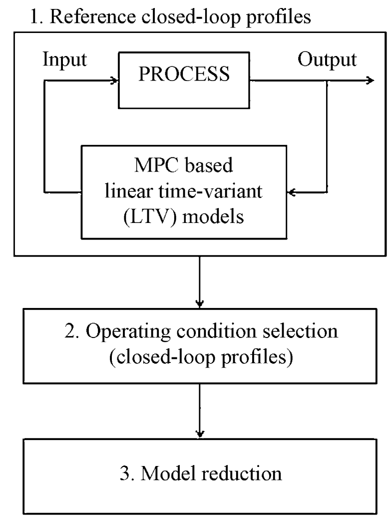

Fig. 3. Linear time-invariant (local) model construction steps.

Since dynamic behavior of the batch process is non-stationary, there is no steady-state operating condition needed for local linearization. So as to deal with this limit, reference closed-loop profiles have been firstly determined. After that, a set of models is obtained by linearizing an original non-linear fundamental-model around different pseudo steady-state operating conditions chosen in different parts along the reference profiles. To meet their controllability and observability, the models have been further reduced their orders individually.

4. Simulation results

In this study, reference closed-loop profiles have been obtained as shown in Fig. 4a by applying an adaptive MPC controller. Its tuning parameters including input weighting, a prediction horizon, and a control horizon, are 0.5, 30, and 20, respectively. Heating period is approximately between $0 \leq t \leq 17.1$ min, to provide maximum heating resulting in raising-up T_{r} as quickly as possible from initially 20 to 95 °C. After that at $t \geq 17.1$ min (cooling period), the controller starts cooling the temperature down to bring its change rate to zero, and to limit the production of the by-product.

After 20.5 min, the temperature control is performed subsequently for maintaining the temperature change rate near zero. This brings two unstable poles to left-half-plane (LHP) as seen in Fig. 4b. In other words, the process dynamics regarding the reactor temperature gradually move from unstable to stable responses. It is found that the system behavior becomes more stable at $t > 61.3$ min (all negative poles, $Re\{\lambda\} < 0$).

4.1. Conventional MPC controller

It is noted that heating-up is inevitable, so therefore a switching time from heating to cooling is a critical point of any designed controllers. An effectively designed control of the temperature change rate is then expected within this range. For developing the conventional controller, the pseudo steady-state operating condition is chosen only in a stable part, $61.3 < t \leq 120$ min, to provide stable controller. Three operating conditions are chosen here to represent the dynamics of the system for the whole operating range: (i) at time $t = 80$ min, (ii) at time $t = 100$ min, and (iii) at the final batch time $t = 120$ min.

The studied batch system has two zero-, two positive- and two negative-value poles (six full states); hence, it is analytically

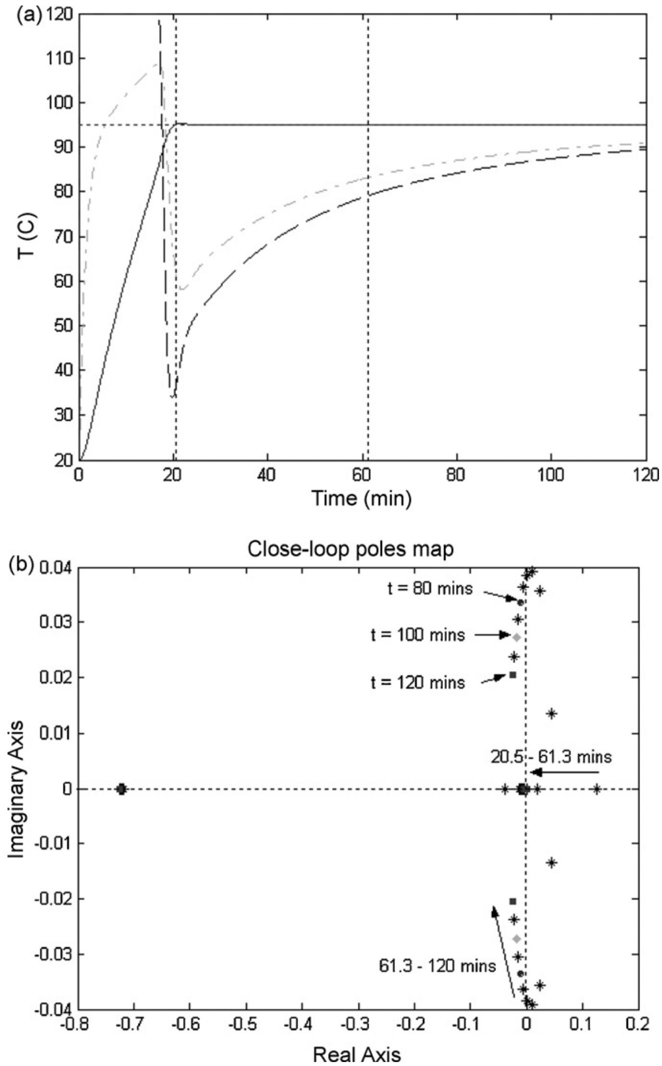

Fig. 4. (a) Control performances of an adaptive MPC controller: reference profiles. (b) Control performances of an adaptive MPC controller: poles of the batch system.

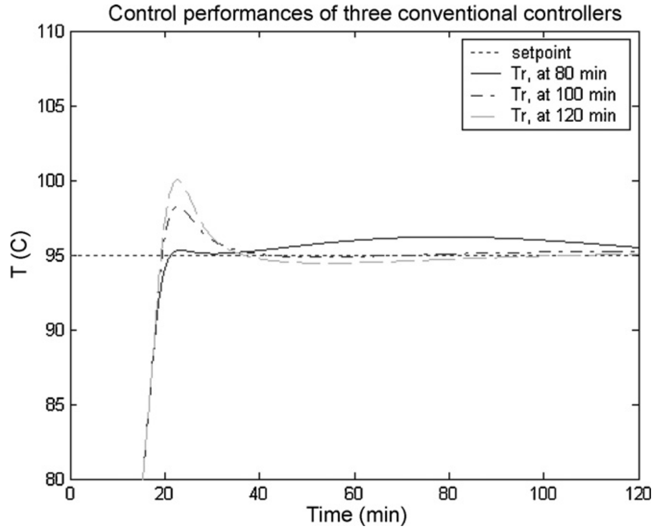

Fig. 5. Control performances of three conventional controllers.

unstable. The two zero-value poles can be cancelled by a pole-zero cancellation, this results in a minimal phase of the model with four reduced-states. The cancellation can be obviously seen by using process transfer-function. As controllability and observability matrices of the batch have four ranks, a further model-reduction is not needed in this case.

Fig. 5 shows a comparison of control performances of three conventional controllers using different minimal-order models. It has been found that, one with the model derived at time 100 min provides the smallest IAE (integral absolute error: IAE = 760). For one with the model derived at time 120 min, the largest overshoot is remarkably observed (IAE = 784). Furthermore, one with the model derived at time 80 min provides the slowest control response (IAE = 803). It should be noted that the controller with the model derived at $t < 80$ min provides sluggish response, and is rather sensitive to mismatches.

4.2. Proposed MPC controller

As seen in Fig. 5, the conventional controller with the model developed at time 80 min provides good control response at the beginning without overshoot, approximately 0–30 min. After that, the control response slightly deviates out of the set point, but is

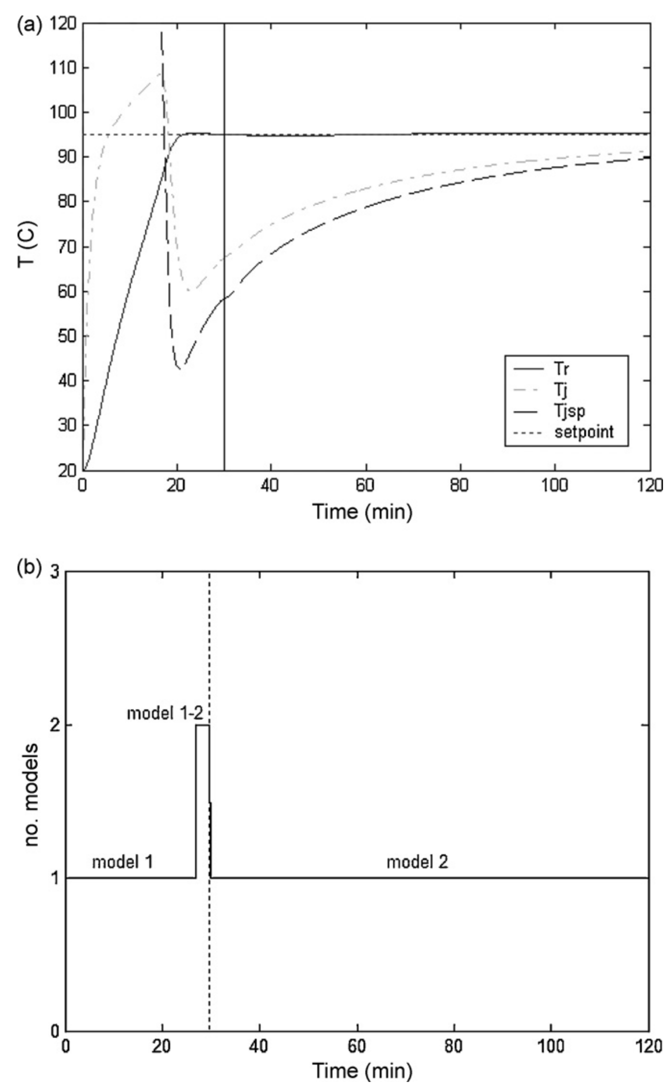

Fig. 6. (a) Controller with two reduced-models in series: control performance. (b) Controller with two reduced-models in series: a sequence of using two models.

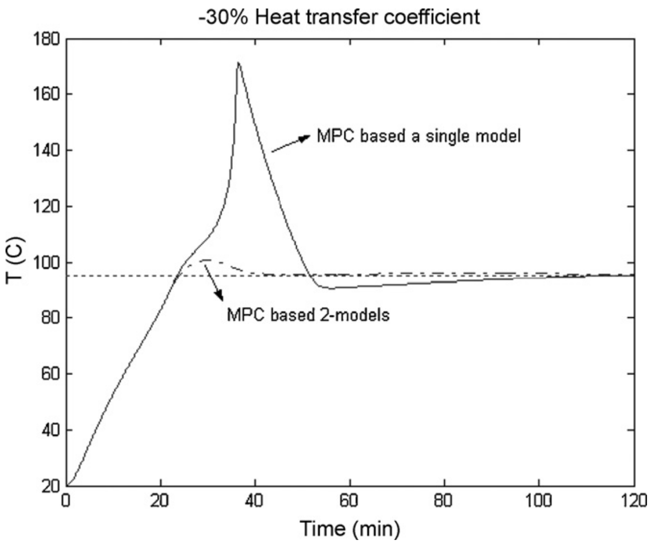

Fig. 7. Closed-loop profiles with heat transfer coefficient change.

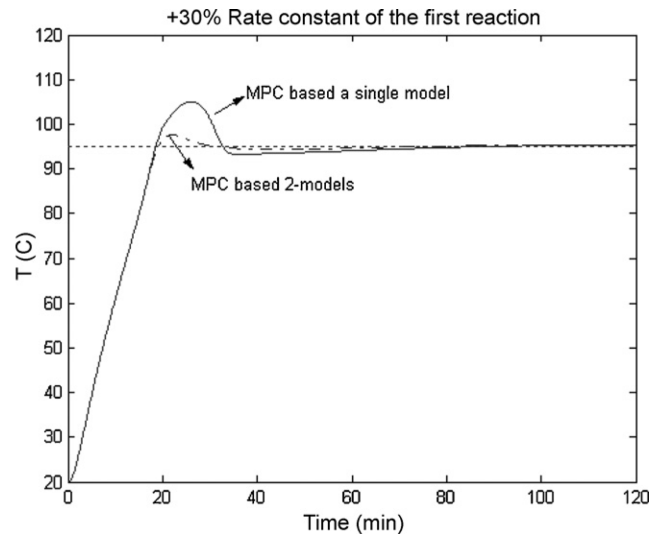

Fig. 8. Closed-loop profiles with rate constant change.

finally driven back to the set point. In order to improve the performance, two reduced-models running in series are then employed in the controller algorithm.

The control performance of the controller with a sequence of two reduced-models, which are derived at time 80 and 120 min, is shown in Fig. 6a. It can be seen that the control response after 30 min is significantly improved via using the second model. As sampling time is of 0.1 min, the output prediction is achieved 3 min ahead for each MPC calculation. A sequence of using the models is plotted with time as shown in Fig. 6b. For $t < 27$ min, the first model is used in the proposed controller. After that both models are employed in time range 27–30 min, because the prediction horizon covers both models. This is followed by using only the second model, $t \geq 30$ min.

The proposed MPC have also been examined by increasing the number of the reduced-models, however, it has been found that the control performance is rarely improved. This is because the stable period is limited in the range of 61.3–120 min, and the stable poles change negligibly. Accordingly, the temperature-control performance can be significantly improved by using only two minimal-models sequentially.

4.3. *Effect of plant/model mismatch*

As the controller is a model-based controller, it needs to be tested for robustness with respect to plant/model mismatches. Fig. 7 shows the responses of both conventional and proposed controllers, when heat transfer coefficient decreases 30% from its nominal value. The results show that the controller using two minimal-models sequentially still provides reasonable control response, whereas the conventional one cannot handle this mismatch. The IAE values of both controllers in the presence of the mismatch are summarized in Table 1.

Table 1
IAE values of both controllers in the presence of model mismatches

−30% Heat transfer coefficient		+30% Rate constant	
No. of models	Integral absolute error (IAE)	No. of models	Integral absolute error (IAE)
1	Unstable	1	865.0
2	1018	2	760.0

Similarly, kinetic data in rate equations may not be known exactly. Here, it is assumed that the rate constant of the first reaction increases 30% from its actual value. The proposed controller is still able to cope with this mismatch. The reactor temperature is maintained at the desired value (95 °C) with smaller overshoot comparing to the conventional one as shown in Fig. 8.

5. Conclusion

It has been well known that model predictive control (MPC) technology has been widely used in an industrial application. However, a conventional controller is rarely applicable to batch processes. This is because of non-stationary operating condition, which is needed for a local-model development. To manage the problem, three steps of a model construction have been proposed involving, a reference-profile determination, an operating-condition selection, and a model-reduction. Simulation results have shown that the conventional MPC controller with a reduced-model, developed by follows the steps, gives reasonable temperature-control performance. However, it is rather sensitive to plant/model mismatches.

To improve the control performance, a sequence of two reduced-models has been employed in a MPC framework to cope with time-varying behavior of the process. Full-models have been constructed around different pseudo-steady-state conditions along reference profile. Afterward they reduced their orders individually corresponding to their controllability and observability. Simulation results have demonstrated that MPC with two reduced-models running in series provides much better and more robust control performances than the conventional one.

Acknowledgement

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Appendix A

Table A.1.

Reaction 1: $A + B \rightarrow C$

Table A.1
Physical properties and initial conditions

M_{wa} = 30 kg/kmol	M_{wb} = 100 kg/kmol
M_{wc} = 130 kg/kmol	M_{wd} = 160 kg/kmol
C_{pa} = 75.31 kg/(kmol °C)	C_{pb} = 167.36 kg/(kmol °C)
C_{pc} = 75.31 kg/(kmol °C)	C_{pd} = 334.73 kg/(kmol °C)
$k_1^1 = 20.9057$	$k_1^2 = 10,000$
$k_2^1 = 38.9057$	$k_2^2 = 17000$
ΔH_1 = −41,840 kJ/kmol	ΔH_2 = −25,105 kJ/kmol
ρ_r = 1000 kg/m^3	r = 0.5 m
U_r = 40.842 kJ/(min m^2 °C)	ρ_j = 1000 kg/m^3
C_{pj} = 1.8828 kJ/(kg °C)	F_j = 0.348 m^3/min
V_j = 0.6812 m^3	Mb(0) = 12 kmol
Ma(0) = 12 kmol	Md(0) = 0 kmol
Mc(0) = 0 kmol	$T_j(0)$ = 20 °C
$T_r(0)$ = 20 °C	

Reaction 2: A + C → D

$$\frac{\mathrm{dMa}}{\mathrm{d}t} = -R_1 - R_2$$

$$\frac{\mathrm{dMb}}{\mathrm{d}t} = -R_1$$

$$\frac{\mathrm{dMc}}{\mathrm{d}t} = R_1 - R_2$$

$$\frac{\mathrm{dMd}}{\mathrm{d}t} = R_2$$

$$\frac{\mathrm{d}T_r}{\mathrm{d}t} = \frac{Q_r + Q_j}{M_r C_{pr}}$$

$$\frac{\mathrm{d}T_j}{\mathrm{d}t} = \frac{F_j \rho_j C_{pj}(T_j^{sp} - T_j) - Q_j}{V_j \rho_j C_{pj}}$$

where $R_1 = k_1\mathrm{MaMb}$, $R_2 = k_2\mathrm{MaMc}$, $k_1 = \exp\left[k_1^1 - k_1^2/(T_r + 273.15)\right]$, $k_2 = \exp\left[k_2^1 - k_2^2/(T_r + 273.15)\right]$, $W_r = M_{wa}\mathrm{Ma} + M_{wb}\mathrm{Mb} + M_{wc}\mathrm{Mc} + M_{wd}\mathrm{Md}$; $C_{pr} = [C_{pa}\mathrm{Ma} + C_{pb}\mathrm{Mb} + C_{pc}\mathrm{Mc} + C_{pd}\mathrm{Md}]/M_r$; $M_r = \mathrm{Ma} + \mathrm{Mb} + \mathrm{Mc} + \mathrm{Md}$; $V_r = W_r/\rho_r$; $A_r = 2V_r/r$; $Q_j = U_r A_r (T_j - T_r)$; $Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2$.

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