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A model predictive formulation for control of open-loop unstable cascade systems

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Abstract

Cascade control is commonly used in the operation of chemical processes to reject disturbances that have a rapid effect on a secondary measured state, before the primary measured variable is affected. In this paper, we develop a state estimation-based model predictive control approach that has the same general philosophy of cascade control (taking advantage of secondary measurements to aid disturbance rejection), with the additional advantage of the constraint handling capability of model predictive control (MPC). State estimation is achieved by using a Kalman filter and appending modeled disturbances as augmented states to the original system model. The example application is an open-loop unstable jacketed exothermic chemical reactor, where the jacket temperature is used as a secondary measurement in order to infer disturbances in jacket feed temperature and/or reactor feed flow rate. The MPC-based cascade strategy yields significantly better performance than classical cascade control when operating close to constraints on the jacket flow rate.

Keywords: Process control; Systems engineering; Optimization; Dynamic simulation; Model predictive control; Unstable cascade systems

1. Motivation

Chemical processes often have multiple time-scale dynamic behavior. Consider the control instrumentation diagram for a jacketed chemical reactor shown in Fig. 1. In this cascade control strategy, there is one manipulated variable (jacket flow rate) and several measured variables (reactor temperature and jacket temperature). The output of the primary controller is the setpoint (jacket temperature) to the secondary controller. The output of the secondary controller is the setpoint (jacket flow rate) to the tertiary controller. The tertiary controller rejects disturbances that directly affect the jacket flow rate (typically coolant pressure header disturbances), while the secondary controller rejects disturbances that directly affect the jacket temperature (typically jacket feed temperature disturbances). The primary controller provides long-term integral control of the reactor temperature. This control configuration also holds for the case with recirculating jacket flow. Note that the example control strategy is that of a double cascade controller. In the sequel, we neglect the dynamics associated with the flow control loop and assume that the jacket flow rate is directly manipulated.

A sequential procedure is normally suggested for cascade control system design. A proportional inner-loop controller with a high gain is often used to assure rapid rejection of inner-loop disturbances. Once the inner-loop controller is tuned, the outer-loop controller is tuned for setpoint changes and outer-loop disturbances. It should be noted that this procedure cannot be used for chemical reactors that are open-loop unstable, because closing the secondary loop alone does not stabilize the process. For these systems, both loops must be closed simultaneously. The objective of this paper is to develop a model predictive control (MPC) formulation for control of open-loop unstable cascade systems. We show how to combine state estimation with MPC to reject primary and secondary disturbances while satisfying manipulated variable constraints. The MPC structure explicitly handles constraints and state estimation provides offset removal and the ability to reject disturbances. We compare MPC with traditional cascade control on the nonlinear CSTR operating at an open-loop unstable steady state. State estimation is performed using a discrete dynamic Kalman filter using reactor and jacket temperature measurements.

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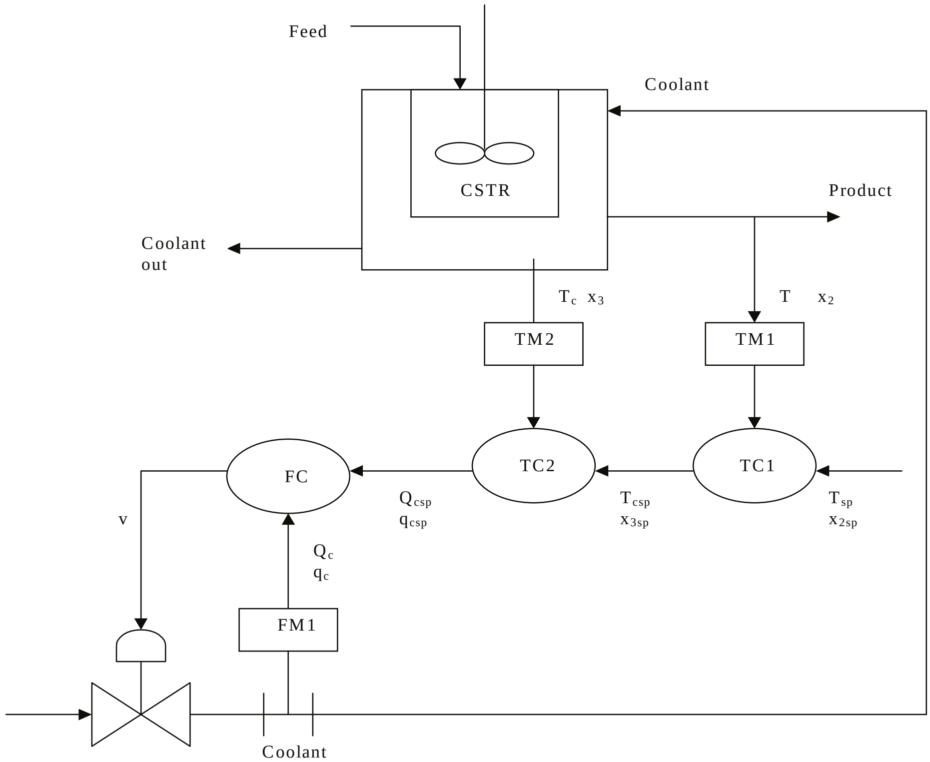

Fig. 1. Process flow diagram for cascade control of reactor temperature in a CSTR.

The structure of the paper is as follows: Section 2 provides a description of the process, Section 3 describes the controller design (for MPC and "classical" cascade control), Section 4 presents simulation results and Section 5 presents conclusions and suggestions for future work.

2. Process description

2.1. CSTR modeling equations

An exothermic diabatic irreversible first order reaction ($A \rightarrow B$) is described by a set of differential equations obtained from material and energy balances (with assumptions of constant volume, perfect mixing and constant physical parameters) as shown below:

$$\frac{dx_1}{d\tau} = q(x_{1f} - x_1) - \phi x_1 \kappa(x_2), \tag{1}$$

$$\frac{dx_2}{d\tau} = q(x_{2f} - x_2) - \delta(x_2 - x_3) + \beta\phi x_1 \kappa(x_2), \tag{2}$$

$$\frac{dx_3}{d\tau} = \delta_1[q_c(x_{3f} - x_3) + \delta\delta_2(x_2 - x_3)]. \tag{3}$$

Here, x_1 is the dimensionless concentration of reactant A, x_2 is the dimensionless reactor temperature, and x_3 is the dimensionless jacket temperature. The representative values of dimensionless variables and parameters are from Russo and Bequette (1997). Model parameter values are specified in Table 1.

Table 1
Three-state CSTR model parameter values

ϕ	0.072	δ_1	10
β	8.0	δ_2	1.0
δ	0.3	x_{1f}	1.0
γ	20	x_{2f}	0.0
q	1.0	x_{3f}	−1.0

This is a nonlinear system, since the reaction rate constant depends nonlinearly on the temperature as dictated by the Arrhenius rate expression. As mentioned by Russo and Bequette (1995), CSTRs present challenging operational and control problems due to complex open-loop behavior such as input and output multiplicities, ignition/extinction behavior, parametric sensitivity, nonlinear oscillations, and chaos. The parameters chosen are shown by Russo and Bequette (1997) to exhibit open-loop unstable behavior for a range of reactor temperatures bounded by the limit points ($x_2 \approx 1.5$ and 3.0). An important feature of this system with the parameter values given in Table 1 is that closing the secondary loop (jacket temperature control) alone does not stabilize the process, since the instability resides in the primary loop (reactor temperature control). The CSTR has multiplicity behavior with respect to the jacket temperature and jacket flow rate as shown in Fig. 2.

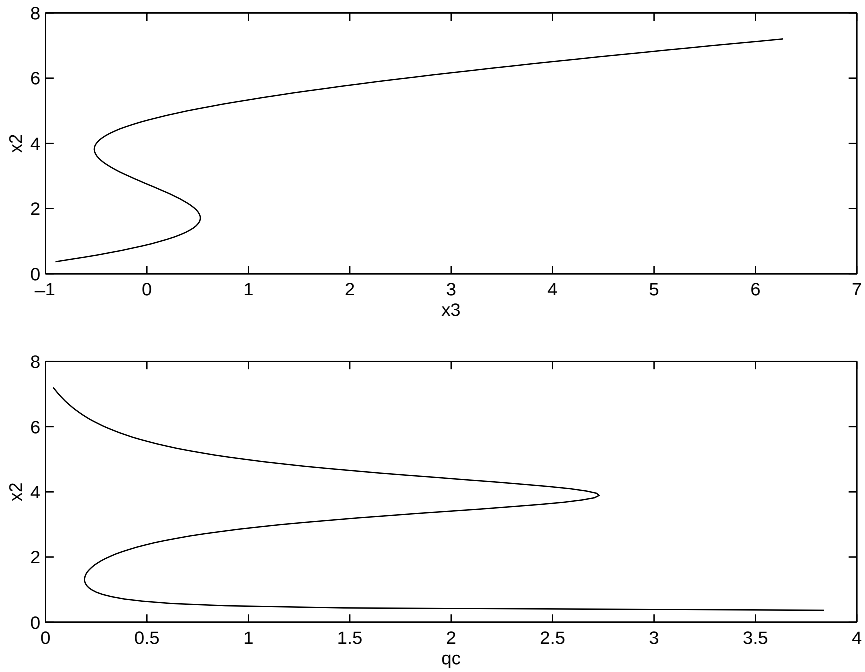

Fig. 2. Steady state dimensionless reactor temperature versus cooling jacket temperature (x_3) and flow rate (q_c) for the jacketed exothermic CSTR.

3. Controller design

The control objective is to keep the dimensionless temperature of the reacting mixture (x_2) constant at a desired value. Possible disturbances to the reactor include the feed temperature (x_{2f}) and the jacket feed temperature (x_{3f}). The only manipulated variable is the jacket flow rate (q_c). The reactor temperature responds much faster to changes in reactor feed temperature (x_{2f}) than to changes in jacket feed temperature (x_{3f}). Therefore, feedback control will be more effective in controlling variations in the reactor temperature, and less effective in controlling variations in jacket feed temperature. The response of feedback control to changes in the jacket temperature can be improved by measuring x_3 (outlet jacket temperature) and taking control action before its effect is felt by the reacting mixture. If the outlet jacket temperature increases, the jacket flow rate can be increased to remove the equivalent heat. The idea is to have two controlled loops using two different measurement $x_2$and x_3, but sharing a common manipulated variable q_c.

Cascade control design has been dealt with extensively in the literature. Russo and Bequette (1997) developed a state space-based representation for cascade control design. They have dealt with the case of linear control structures where an inner loop controller gain is pre-specified. Their result shows that an input–output representation of a cascade control system may not capture the true behavior of closed-loop system if primary and secondary processes are coupled in state-space. Semino and Brambilla (1996) have proposed an efficient structure for parallel cascade control which avoids interactions between the two loops, but their control structure is strictly based on the internal model control (IMC) being carefully designed. Semino, Porcari, and Brambilla (1998) suggest the use of predictive control in cascade systems, which are advantageous for the cases where constraints play an important role and also if process dynamics are complex. They do not, however, actually implement a predictive controller.

Dumur, Boucher, and Kolb (1996) have implemented a cascade predictive structure using a constrained receding horizon predictive control algorithm with multiple reference models (CRHPC/MRM) in the inner loop and generalized predictive control (GPC) in the outer loop. Their formulation restricts the use of CRHPC/MRM to the inner loop when setpoint tracking has to be followed. Linear model predictive control uses a linear process model to specify manipulated variable action to optimize an objective function over a future time horizon. The types of linear time invariant models used in MPC are state space, transfer-function matrix, and finite step or impulse response models. Convolution models can represent a variety of dynamic responses, but they lack the ability to represent unstable plants. Ricker (1990) has shown the advantages of using state estimation instead of the additive output disturbance commonly used in dynamic matrix control (DMC). A primary incentive for implementing MPC is for explicit constraint handling.

There are several options for implementing an MPC strategy on a CSTR with two temperature measurements and a single manipulated input. One option (perhaps the one most commonly used) is to use MPC on the "outer loop" (where jacket temperature setpoint is the manipulated variable and reactor temperature is the measured variable), and PI control on the inner loop (where jacket temperature is measured and coolant flow rate manipulated). This option would not be able to directly incorporate coolant flow rate constraints, however. Another option is to use MPC on both the outer and inner loops. This seems conceptually complex, compared to the next option. The third option is to use a single MPC strategy that incorporates both reactor and jacket temperature measurements, and manipulates the jacket flow rate; this is the approach used in this paper. Our formulation is different from a typical "non-square" MPC formulation, however. Standard MPC with more outputs than inputs will typically result in offset in all of the output variables. We develop an MPC formulation where only the reactor output is considered in the control objective function, but jacket temperature is used in the state estimation procedure to improve rejection of coolant feed temperature disturbances and outer loop disturbances. This results in a "square" formulation for MPC, but with the incorporation of information from secondary measurements. Two different approaches for MPC are presented; Section 3.1 covers the infinite horizon strategy, while Section 3.2 covers the finite horizon strategy. The design for classical cascade control is presented in Section 3.3. Since we are working with an open-loop unstable system, the guarantee of constrained stabilizability offered by the infinite horizon controller is appealing. The finite horizon model predictive controller provides a less computationally demanding alternative, but the controller must be tuned for stability. By conducting simulations with both model predictive controllers, we seek to compare their performance relative to each other in addition to exploring the trade-off in the computational requirements of the two controllers.

3.1. Infinite horizon MPC

We have used the approach of Muske and Rawlings (1993) for infinite horizon, state space-based MPC. The main advantage of the infinite over the finite horizon is elimination of the requirement of tuning for nominal stability. For unstable systems, the infinite horizon approach incorporates constrained stabilizability to bring unstable modes to the origin. Nominal stability is achieved by including a terminal state penalty term, which converts the infinite horizon objective function into an equivalent finite horizon objective function. The advantages of infinite horizon come with a high computational cost. Gilbert and Tan (1991) mention that the constraint horizon has to be chosen large enough that satisfying the constraints within the finite horizon implies the same for the infinite horizon. In the present paper, we use a linear control law on a nonlinear plant, since the theory of infinite horizon MPC for nonlinear systems is still under development. de Nicolao, Magni, and Scattolini (1998) have presented a nonlinear infinite horizon scheme which guarantees exponential stability of the equilibrium for any value of the horizon and avoids the use of equality constraints, thereby providing significant computational savings. Mayne, Rawlings, Rao, and Scokaert (2000) have presented the essential principles for the stability of model predictive control of constrained dynamical systems.

The discrete dynamical system model used by the controller is the state-space formulation in which y is the vector of outputs, u is the vector of inputs, and x is the vector of states.

$$\begin{aligned} x_{k+1} &= \Phi x_k + \Gamma u_k, \\ y_k &= C x_k. \end{aligned} \tag{4}$$

Muske and Rawlings (1993) express the infinite horizon open-loop objective function as a finite horizon open-loop objective function with the form

$$\begin{aligned} \min_{u^N} \phi_k = {} & x_{k+N}^{\mathrm{T}} \bar{Q} x_{k+N} \\ & + \Delta u_{k+N}^{\mathrm{T}} S \Delta u_{k+N} + \sum_{j=0}^{N-1} \left(x_{k+j}^{\mathrm{T}} C^{\mathrm{T}} Q C x_{k+j} \right. \\ & \left. + u_{k+j}^{\mathrm{T}} R u_{k+j} + \Delta u_{k+j}^{\mathrm{T}} S \Delta u_{k+j} \right). \end{aligned} \tag{5}$$

For tracking a non-zero target vector, the following quadratic objective function is used for the regulator:

$$\begin{aligned} \min_{u^N} \phi_k = {} & (x_{k+N} - x_S)^{\mathrm{T}} \bar{Q} (x_{k+N} - x_S) + \Delta u_{k+N}^{\mathrm{T}} S \Delta u_{k+N} \\ & + \sum_{j=0}^{N-1} ((x_{k+N} - x_S)^{\mathrm{T}} C^{\mathrm{T}} Q C (x_{k+N} - x_S) \\ & + (u_{k+j} - u_s)^{\mathrm{T}} R (u_{k+j} - u_s) + \Delta u_{k+j}^{\mathrm{T}} S \Delta u_{k+j}), \end{aligned} \tag{6}$$

where Q is a symmetric positive semi-definite penalty matrix on the outputs, R is a symmetric positive definite penalty matrix on the inputs, and S is a symmetric positive semi-definite penalty matrix on the rate of change in the inputs, with $\Delta u_{k+j} = u_{k+j} - u_{k+j-1}$ being the change in the input vector at time j. The vector u^N contains the N future open-loop control moves as shown below:

$$u^N = \begin{bmatrix} u_k \\ u_{k+1} \\ \vdots \\ u_{k+N-1} \end{bmatrix}. \tag{7}$$

The value of the state penalty matrix $\bar{Q}$ depends on the stability of the plant model. For stable systems $\bar{Q}$ is expressed as

$$\bar{Q} = \sum_{i=0}^{\infty} \Phi^{\mathrm{T}^i} C^{\mathrm{T}} Q C \Phi^i. \tag{8}$$

The infinite sum is determined as the solution of the following discrete Lyapunov equation for stable systems:

$$\bar{Q} = C^{\mathrm{T}} Q C + \Phi^{\mathrm{T}} \bar{Q} \Phi. \tag{9}$$

For unstable systems, the Jordan form of the Φ matrix is partitioned into stable and unstable parts. The unstable eigenvalues of Φ are contained in J_u and stable eigenvalues are in J_s.

$$\Phi = VJV^{-1} = [V_u V_s] \begin{bmatrix} J_u & 0 \\ 0 & J_s \end{bmatrix} \begin{bmatrix} \bar{V}_u \\ \bar{V}_s \end{bmatrix}. \tag{10}$$

For the unstable system, $\bar{Q}$ is represented as

$$\bar{Q} = \bar{V}_s^{\mathrm{T}} \sum \bar{V}_s,$$

$$\Sigma = V_S^{\mathrm{T}} C^{\mathrm{T}} Q C V_S + J_S^{\mathrm{T}} \Sigma J_S. \tag{11}$$

The main advantage of infinite horizon comes from the fact that it forces unstable modes to go to zero after the end of control horizon, N, at each time step k using the equality constraint (12) even though the solution with this constraint makes the problem computationally expensive.

$$\tilde{V}_u x_{k+N} = 0. \tag{12}$$

The input, output and velocity constraints are easily formed as $\tilde{G} \leqslant 0$, where $\tilde{G}$ is the matrix of constraints. The detailed formulation has been presented in Muske and Rawlings (1993).

3.2. Finite horizon MPC

There are many approaches to form the objective function for finite horizon MPC. Ricker (1990) presents an augmented state-space model approach. The formulation used in this paper for the finite horizon is similar to the infinite horizon approach, with the difference lying in the fact that the terminal state penalty matrix is not present. This means that nominal stability and constrained stabilizability cannot be guaranteed, but can only be judged based on proper selection of tuning parameters.

The objective function used for the finite horizon in this paper is

$$\min_{u^N} \phi_k = \sum_{j=1}^{N_1} ((x_{k+N} - x_S)^{\mathrm{T}} C^{\mathrm{T}} Q C (x_{k+N} - x_S) + (u_{k+j} - u_s)^{\mathrm{T}} R (u_{k+j} - u_s) + \Delta u_{k+j}^{\mathrm{T}} S \Delta u_{k+j}), \tag{13}$$

where N denotes the control horizon and N_1 denotes the output prediction horizon. Finite horizon MPC provides computational savings over infinite horizon MPC and is the most common MPC implementation in industry today. To get integral action, an input step disturbance model is used for the estimation of the states. We have used the step disturbance regulator to determine the input and state target vectors that can remove the step disturbance at steady state and maintain the steady state output at the desired state. Muske and Rawlings (1993) presented this regulator for the infinite horizon formulation, but it can be used for a finite horizon formulation as well. The minimization of the objective function in Eq. (13) is performed subject to manipulated variable (jacket flow rate, q_c) constraints.

3.3. State estimation

The linear observer is used for the system in which w_k and v_k are zero-mean, uncorrelated normally distributed, stochastic variables appended to the process model:

$$x_{k+1} = \Phi x_k + \Gamma u_k + G_w w_k,$$

$$y_k = C x_k + v_k. \tag{14}$$

The discrete time Kalman filter (Lewis, 1986) is used for state estimation.

The time update equations are

$$\text{Error covariance: } P_{k+1|k} = \Phi P_{k|k} \Phi^{\mathrm{T}} + G_w Q_w G_w^{\mathrm{T}},$$
$$\text{Estimate: } \hat{x}_{k+1|k} = \Phi \hat{x}_{k|k} + \Gamma u_k, \tag{15}$$

and the measurement update equations are

Error covariance:

$$P_{k+1|k+1} = P_{k+1|k} - P_{k+1|k} C^{\mathrm{T}} (C P_{k+1|k} C^{\mathrm{T}} + R_v)^{-1} C P_{k+1|k},$$

Estimate:

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + P_{k+1|k} C^{\mathrm{T}} R_w (z_{k+1} - C \hat{x}_{k+1|k}). \tag{16}$$

Q_w is the covariance of w_k, R_v is the covariance of v_k, P denotes the covariance of the state estimates and z is the vector of output measurements. This observer optimally reconstructs the states from the output measurements given the noise assumptions. Since not all the states are directly measured, the objective functions for the regulators in Eqs. (6) and (13) are modified with the true values of the states being replaced by the state estimates obtained from the discrete time Kalman filter. The optimal linear observer provides biased estimates when step disturbances affect the process. An appended state model is used to overcome this, where additional states (used to estimate the disturbances) are appended to the model. The disturbance can be appended as step input or step output disturbances. Since the operating point of the jacketed CSTR for the case dealt in the paper is unstable we cannot use the output step disturbance method to obtain integral action. This is because the observer poles will contain the plant poles and lead to instability in the regulator. The input disturbance model can be implemented in various ways. Muske and Rawlings (1993) present the case where the disturbance is assumed to be in the manipulated variable u_k. We have used the formulation where the disturbance enters the state equations as an additional input, and an additional state is appended to estimate the disturbance. The underlying assumption is that the difference between the predicted output and the measurement is caused by an input disturbance. The approach is formulated as

$$x_{k+1} = \Phi x_k + \tilde{\Gamma} \tilde{u},$$

$$z_{k+1} = z_k,$$

$$y_k = C x_k,$$

$$\tilde{u} = \begin{bmatrix} u_k \\ z_k \end{bmatrix},$$
$$\tilde{\Gamma}_1 = \Gamma,$$
$$\tilde{\Gamma} = [\Gamma \tilde{\Gamma}_2 \ldots \tilde{\Gamma}_{r+1}], \tag{17}$$

where n is the number of states in the system and r is the number of states appended as disturbances.

The augmented system is represented as

$$\bar{X}_{k+1} = \overline{\Phi X}_k + \bar{\Gamma} u_k,$$
$$y_k = \overline{CX}_k,$$
$$\bar{\Phi} = \begin{bmatrix} \Phi & \tilde{\Gamma} \\ 0 & I \end{bmatrix}, \quad \bar{\Gamma} = \begin{bmatrix} \Gamma \\ 0 \end{bmatrix},$$
$$\bar{C} = [C \quad 0], \quad \bar{\tilde{\Gamma}} = [\tilde{\Gamma}_2, \ldots, \tilde{\Gamma}_{r+1}], \quad \bar{X}_k = \begin{bmatrix} x_k \\ z_k \end{bmatrix}. \tag{18}$$

The above formulation when used on the jacketed CSTR defines the augmented state-space matrices (in continuous time) as

$$A = \begin{bmatrix} -q - \phi\kappa(x_2) & \dfrac{\kappa(x_2)}{(1 + x_{2s}/\gamma)^2} & 0 \\ \beta\phi\kappa(x_2) & -q - \delta + \dfrac{\beta\phi\kappa(x_2)x_{1s}}{(1 + x_{2s}/\gamma)^2} & \delta \\ 0 & \delta\delta_1\delta_2 & \delta_1(q_{cs} - \delta\delta_2) \end{bmatrix},$$

$$B = \begin{bmatrix} 0 \\ 0 \\ \delta_1(x_{3f} - x_{3s}) \end{bmatrix}, \quad C = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{19}$$

$$\bar{A} = \begin{bmatrix} -q - \phi\kappa(x_2) & \dfrac{\kappa(x_2)}{\left(1 + \frac{x_{2s}}{\gamma}\right)^2} & 0 & 0 & (x_{1f} - x_{1s}) \\ \beta\phi\kappa(x_2) & -q - \delta + \dfrac{\beta\phi\kappa(x_2)x_{1s}}{\left(1 + \frac{x_{2s}}{\gamma}\right)^2} & \delta & 0 & (x_{2f} - x_{2s}) \\ 0 & \delta\delta_1\delta_2 & \delta_1(q_{cs} - \delta\delta_2) & \delta_1 q_{cs} & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\bar{B} = \begin{bmatrix} 0 \\ 0 \\ \delta_1(x_{3f} - x_{3s}) \\ 0 \\ 0 \end{bmatrix}, \quad \bar{C} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}. \tag{20}$$

The state transition, input and output matrices for the discrete model can be obtained from the discretization of the continuous-time system. The state estimator uses an input step disturbance model, and for this particular example, we have chosen the jacket feed temperature and the reactor feed flow rate as the appended states. The input disturbance model, as opposed to an output disturbance model, must be chosen in order to stabilize open-loop unstable processes (Muske & Rawlings, 1993). Good state estimation is assured only when the disturbance structure assumed in the model corresponds with the effects of the actual disturbances affecting the plant. Since there are two measured outputs (reactor temperature x_2 and jacket temperature x_3), we are restricted to two appended disturbance states in the process model. The maximum number of appended disturbance states is equal to the number of measurements in the system (Kozub & MacGregor, 1992). The reason for choosing jacket feed temperature as the appended state is to reject the effect of disturbances in a manner similar to the use of an inner/secondary loop in cascade control. The choice of reactor feed flow rate as an augmented disturbance enables us to obtain unbiased state estimates for the reactor temperature in the presence of the disturbances in the reactor feed flow rate, reactor feed concentration and reactor feed temperature. The effect of disturbances in the reactor feed temperature or concentration on the estimate of reactor temperature is offset by including their effects in the effect of the disturbance state (reactor feed flow rate). This means that the reactor feed flow rate estimate will not be at its true value, but the reactor temperature estimate will be unbiased. This is because the effect of the true disturbances is handled by the disturbance state, which provides an additional degree of freedom. The choice of augmented states used to model disturbances was found to be optimal for the sets of actual disturbances that affected the plant in the simulations performed. Other disturbance models were tested, though results are not presented in the manuscript, and the performance of the estimation and control system was poorer.

Augmenting the system with a disturbance vector results in the inclusion of states that are uncontrollable and makes the augmented system non-stabilizable. Since the augmented states are observable, so we can design an observer to estimate and remove the effect of these states on the system. The input and the state target vectors (x_s and u_s) that remove the step disturbance at steady state and maintain the steady state output at the desired output (y_t) can be determined from the output target vector by the following quadratic program:

$$\min_{[x_s\ u_s]^{\mathrm{T}}} \quad \Psi = (y_t - Cx_s)^{\mathrm{T}} Q_s (y_t - Cx_s) \tag{21}$$

$$\text{s.t.} \quad [I - A - B - \hat{\tilde{B}}] \begin{bmatrix} \bar{X}_s \\ u_s \end{bmatrix} = 0. \qquad u_{\min} \leqslant u_s \leqslant u_{\max} \tag{22}$$

The above quadratic formulation will lead to a feasible solution as our formulation has only the reactor temperature in the control objective function.

3.4. "Classical" cascade control formulation

The MPC-based cascade strategy will be compared with "classical" cascade control designed using the state-space approach presented in Russo and Bequette (1997). They have shown that the traditional simulation methods based on series or parallel input/output relationships should not be used for open-loop unstable processes, as the true behavior of the process is not captured. An IMC-based feedback control system design procedure (Morari & Zafiriou, 1989) is used for the outer loop and a proportional controller is used in the inner loop. We emphasize that the conventional cascade control tuning procedure based on closing and tuning the inner loop first and then the outer loop cannot be used for our process, since closing the inner loop alone does not stabilize the system. In effect, we need to 'close both loops simultaneously' to rationally design a cascade controller for this system. We employ a proportional controller in the inner loop, and design the outer-loop controller based on knowledge of the dynamics of the system with the inner loop being closed. The outer-loop process model is developed using the three-state process and the inner-loop proportional controller, and the IMC-based feedback controller design procedure for unstable systems is used on the outer loop. A setpoint filter is used to remove the overshoot that results from the ISE-optimal design procedure. Although the resulting controllers are slightly more complex than standard PID, we feel that the design procedure is more transparent and less arbitrary, and yields better results than other PID controller tuning procedures. It should be noted that the unstable plant imposes limitations on the disturbance rejection performance which can be achieved by the standard IMC-based design. The disturbance rejection capability of IMC for stable systems can be improved by following the procedure of Horn, Arulandu, Gombas, VanAntwerp, and Braatz (1996). Their IMC filter design cancels the slow plant pole thereby increasing the speed of response. This approach does not provide much improvement in disturbance rejection for unstable systems, since λ (IMC- filter time constant) is restricted to being above a certain positive value (to avoid introducing non-minimum phase characteristics in the closed loop).

3.5. Tuning issues in MPC and Kalman filter

The MPC controller has a penalty matrix on input changes as an important tuning parameter. The tuning of the model predictive controller was based on the following considerations. The penalty matrix on Δu, S, was set at unity. Increasing the penalty on Δu decreases the oscillations but the output response slows down. The penalty on u, R, was kept zero for all calculations as increasing the penalty on the input leads to offset in the output response (there are no velocity constraints for our system). The input prediction horizon has to be at least equal to the number of unstable poles. For the augmented state formulation, we have three unstable poles (one from the process and other two from the augmented states), and so an input horizon of magnitude 3 was chosen. The objective function for optimization is formulated such that reactor temperature is the only state being optimized for future control moves, so the penalty on the jacket temperature in the objective function is zero. The formulation used is different from a typical "non-square" MPC (more outputs than inputs), and avoids offset in the output variables.

Increasing the penalty on the reactor temperature, Q, makes the input action fast so that the output tracks the setpoint aggressively. The Kalman filter was tuned to get an offset free estimate. The main tuning parameter in the Kalman filter is the assumed value of the state noise matrix. Noise-free outputs were assumed to be available, and so the error covariance for the measurement noise was taken to be zero. The state noise matrix G_w was assumed to be a diagonal matrix. For the case of disturbance rejection, only the diagonal element of G_w, which corresponds to the augmented state estimating the disturbance, has a non-zero value. The other augmented state may have nominal value of unity to avoid singularity. If G_w has non-zero contribution for other states, then the state estimation may not represent the true states of the plant for the disturbance rejection of the plant. Using a high value in G_w will give fast convergence of the estimated state to the true state but it will track the true states aggressively leading to oscillations. For the case of setpoint tracking, it was observed that the estimated states are close to plant states if non-zero state noise contribution was used for the measured outputs.

4. Results

The simulation results presented here are for the nonlinear plant using a linear controller. The finite horizon MPC approach is compared with classical cascade control (using the IMC-based procedure) for setpoint tracking and disturbance rejection. The state estimator used in the MPC strategy is a discrete dynamic Kalman filter with jacket feed temperature and reactor feed flow rate as appended state. The nonlinear plant is linearized at $x_2 = 2.6$ (in dimensionless units) to develop a linear model for controller design. The manipulated variable (jacket flow rate) is constrained between 0 and 1.55. The estimated states (in MPC) tracked the true values closely in all the simulations. Consequently, we only present the true values of the states and outputs in our simulations. However, we do include a typical case (Fig. 10) where we show both the estimated states and their true values. A sampling time of 0.05 was used for the MPC strategy. The representative set of tuning parameters used is given below. The IMC-based feedback controller had a filter time constant λ chosen as 0.2. The setpoint filter time constant τ_f is chosen as $\tau_f = 0.45 \cong 2\lambda$. The tuning parameters for IMC-based feedback control and MPC were held constant for all the cases studied. IMC-based feedback and MPC are tuned for similar performance under conditions of small setpoint changes, and these tuning parameters are then used in the entire set of simulations. The input and output prediction horizon used for finite horizon MPC is $N = 3$ and $N_1 = 10$, respectively. The values used for other tuning parameters (initial value of the error covariance matrix, process noise, etc.) are given below:

$$P_0 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad G_w = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 10 \end{bmatrix},$$

$$Q = \begin{bmatrix} 40 & 0 \\ 0 & 0 \end{bmatrix}, \quad Q_s = \begin{bmatrix} 10 & 0 \\ 0 & 0 \end{bmatrix},$$

$$\bar{R} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad S = 1, \ R = 0.$$

The input prediction horizon for the infinite horizon case was selected to be 12. This is the lowest input prediction horizon that admits a feasible solution to the stabilizability constraint of Eq. (12). The input horizon for the infinite horizon controller required to guarantee constrained stabilizability is thus much higher than that used for the finite horizon controller.

The first set of simulations presented here deals with the effect of unmeasured primary and secondary disturbances and setpoint changes on the performance of the cascade control and finite horizon-based state-space MPC on the nonlinear plant. The nominal setpoint is $x_2 = 2.6$ (which is open loop unstable and cannot be stabilized by the inner loop in cascade control).

Fig. 3 deals with the case of a small change in reactor temperature setpoint. In this case, the performance of MPC and cascade control is similar because the manipulated variable does not hit the constraint. The tuning for MPC and cascade control is based on these two sets of nominal conditions and it will remain fixed for the rest of the study. Fig. 4 deals with the case of small increase in the jacket feed temperature (x_{3f}) from -1 to -0.8. The performance of MPC and cascade control is comparable for such a small disturbance, since the manipulated variable is not close to constraints.

The IMC-based feedback controller provides worse disturbance rejection than MPC. The long tail in x_2 for cascade control is inherent to the disturbance rejection performance of IMC-based feedback control. As mentioned earlier, approaches that cancel the dynamics (Horn et al., 1996) cannot be used in this situation since the CSTR is open-loop unstable. The case dealt with shows that the cascade controller has been tuned for similar performance to MPC, for the nonlinear plant. Fig. 5 shows the response when an unmeasured disturbance in the dimensionless reactor feed concentration (primary disturbance, x_{1f}) occurs at time $\tau = 1$ (x_{1f} changes from 1 to 0.95). The presence of the appended state for the reactor feed flow rate in the model for MPC results in the estimation and rejection of the effect of the disturbance on reactor concentration (not shown in the figure) and reactor temperature. The appended state model results in rejection of primary and secondary disturbances in the loop.

The response to a large disturbance in x_{3f} from -1 to -0.4 is shown in Fig. 6. Fig. 7 shows the response for the case of a large setpoint change in reactor temperature x_2 from 2.6 to 2.9. Cascade control performs worse in the presence of the active manipulated variable constraints. Figs. 6 and 7 clearly show that traditional cascade control design limits satisfactory plant operation to small disturbances and small setpoint changes, where manipulated variable constraints are not active. MPC using state estimation performs better in servo and regulatory control when manipulated variable constraints are active, since the constraints are explicitly handled in MPC structure.

Fig. 8 shows the case of large primary disturbance occurring in the reactor feed flow rate. MPC performs better than cascade control. The simulation results show that finite horizon MPC with state estimation having appended states in the model (appended states are disturbances in the jacket feed temperature and disturbance in reactor feed flow rate) is better than cascade control for both primary and secondary disturbance rejections. Fig. 9 shows the rejection of multiple large primary and secondary disturbances, which appear as pulses. The unmeasured disturbance in the dimensionless

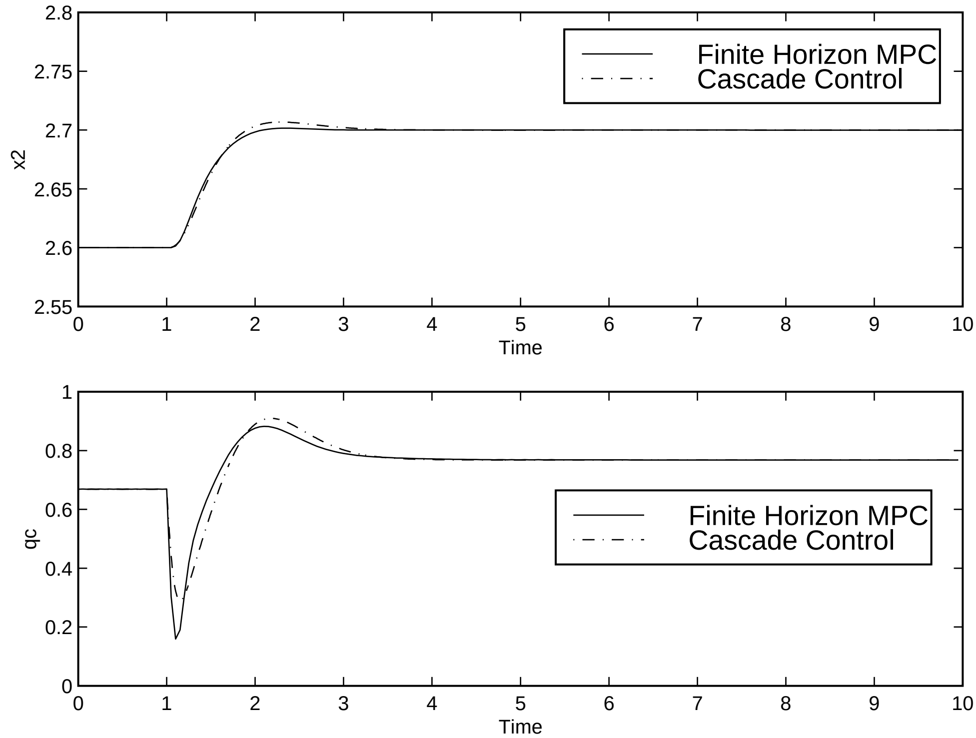

Fig. 3. Response to a small step setpoint change in reactor temperature. Comparison of MPC with classical cascade control.

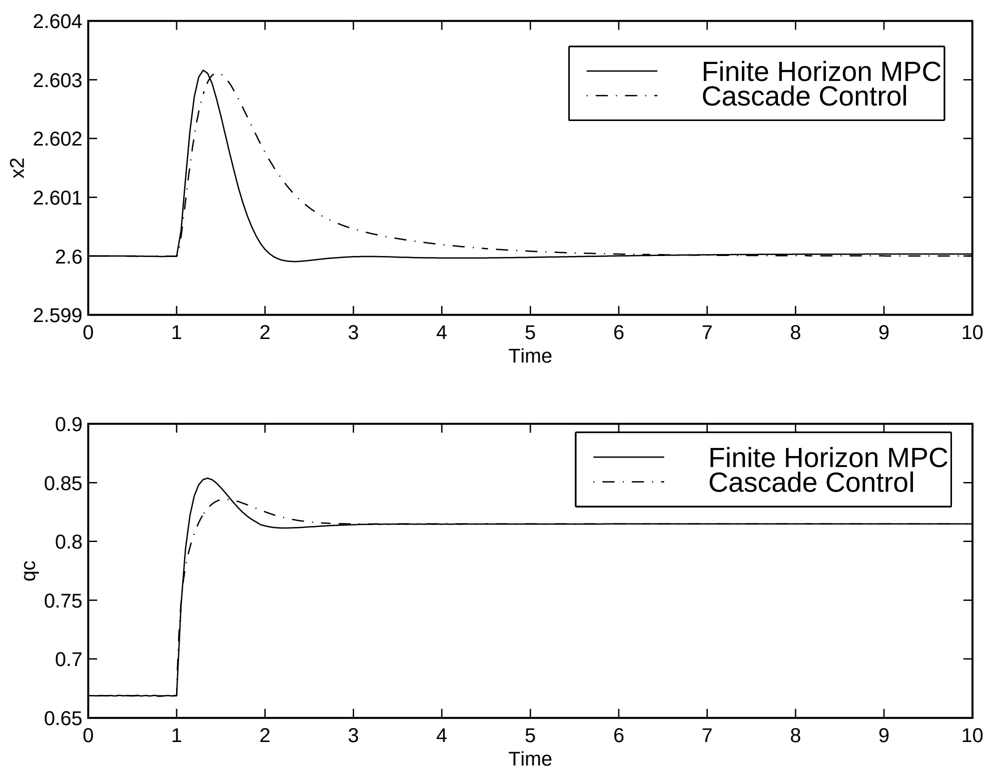

Fig. 4. Response to a small step increase in coolant feed temperature. Comparison of MPC with classical cascade control.

coolant feed temperature (secondary disturbance) occurs at $\tau = 1$ (x_{3f} changes from -1 to 0.4) and the change in reactor feed flow rate occurs at $\tau = 2$ (q changes from 1 to 0.91). The x_{3f} and q revert to their steady state values at $\tau = 3$. The response to this set of disturbances shows that cascade control performance degrades further as it stays at the satura-

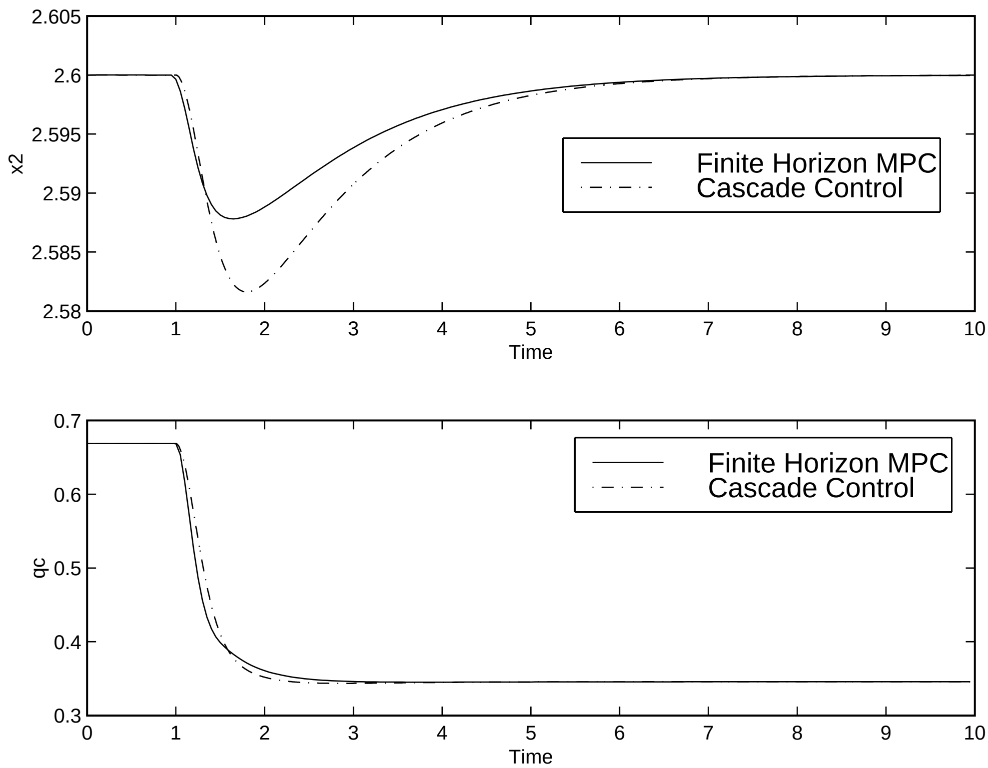

Fig. 5. Response to a small step decrease in reactor feed concentration. Comparison of MPC with cascade control.

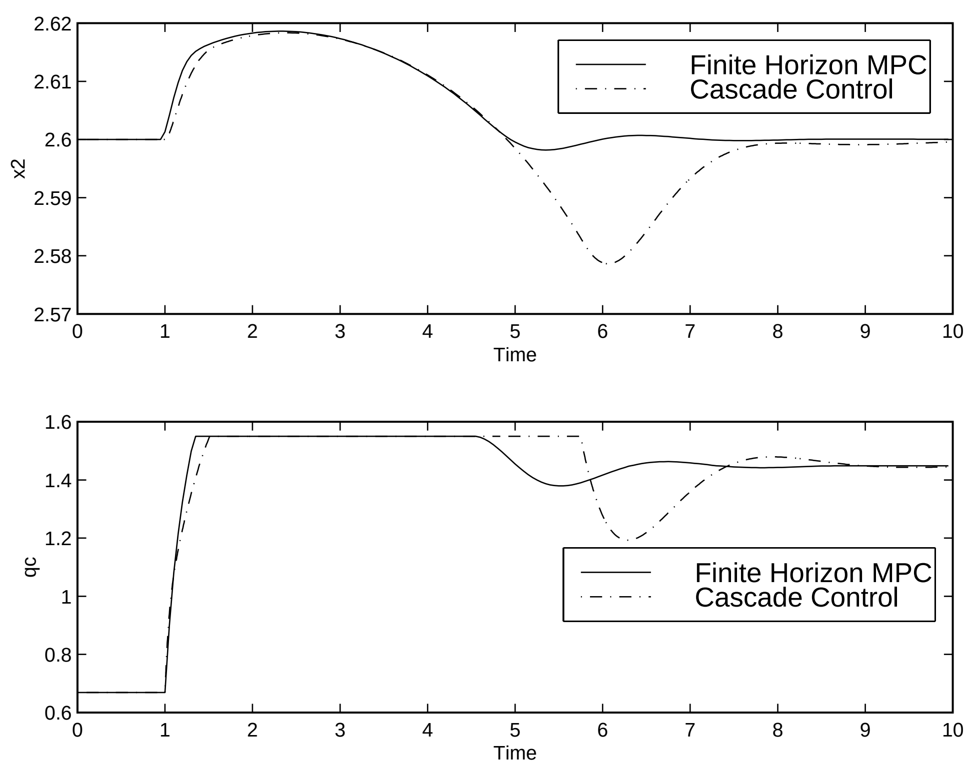

Fig. 6. Response to a large step increase in coolant feed temperature. Comparison of MPC with classical cascade control.

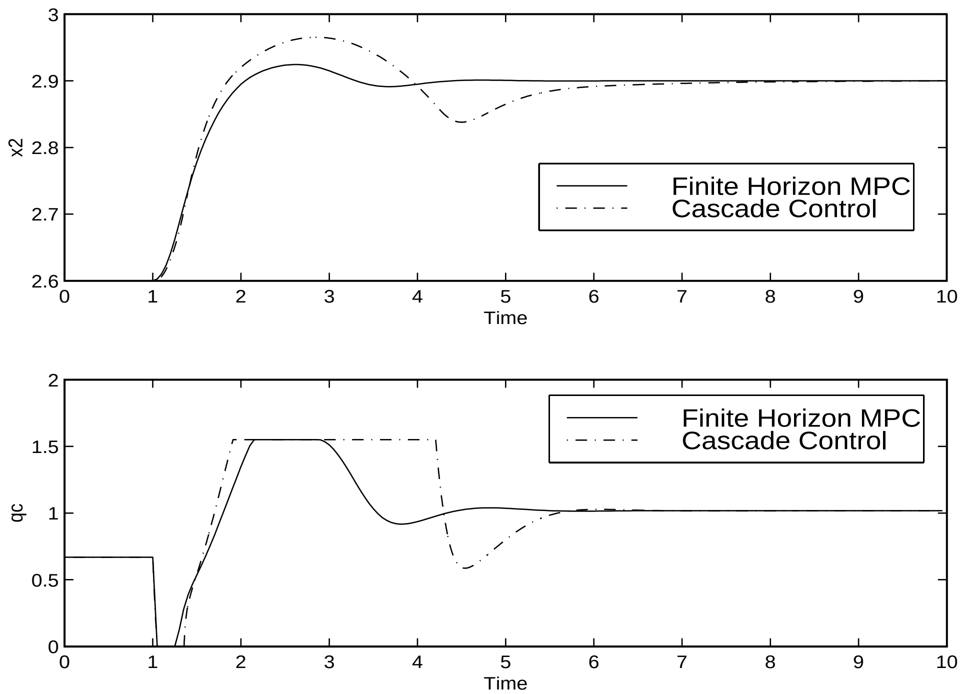

Fig. 7. Response to a large step setpoint change in reactor temperature. Comparison of MPC with classical cascade control.

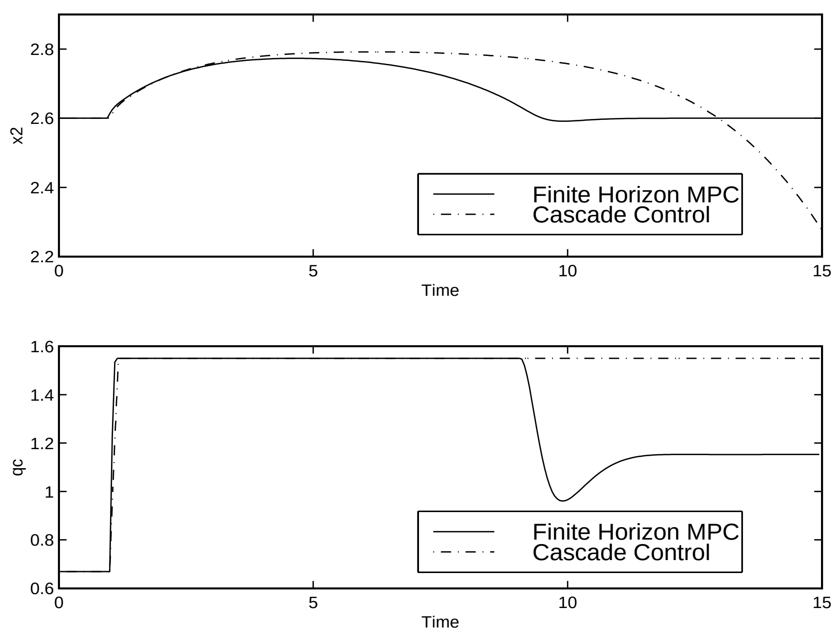

Fig. 8. Response to a large step decrease in reactor feed flow rate. Comparison of MPC with classical cascade control.

tion for a longer time. This result also shows that the infinite horizon MPC performance is similar to finite horizon MPC.

The second set of simulation in Fig. 10 is a typical case where small primary and secondary step disturbances occur in the system at different times. The unmeasured disturbance in the dimensionless coolant feed temperature (secondary disturbance) occurs at $\tau = 1$ (x_{3f} changes from -1 to 0.6). There is a step increase in reactor feed flow rate at $\tau = 2.5$ (q changes from 0 to 0.02), also at $\tau = 3.5$ there is a step increase in reactor feed concentration (x_{1f} changes from 1 to 1.01). The estimated states corresponding to reactor temperature and jacket temperature are identical to the actual outputs even though there is an offset in the estimation of reactor concentration (x_1). The offset in estimated x_1 is due to the

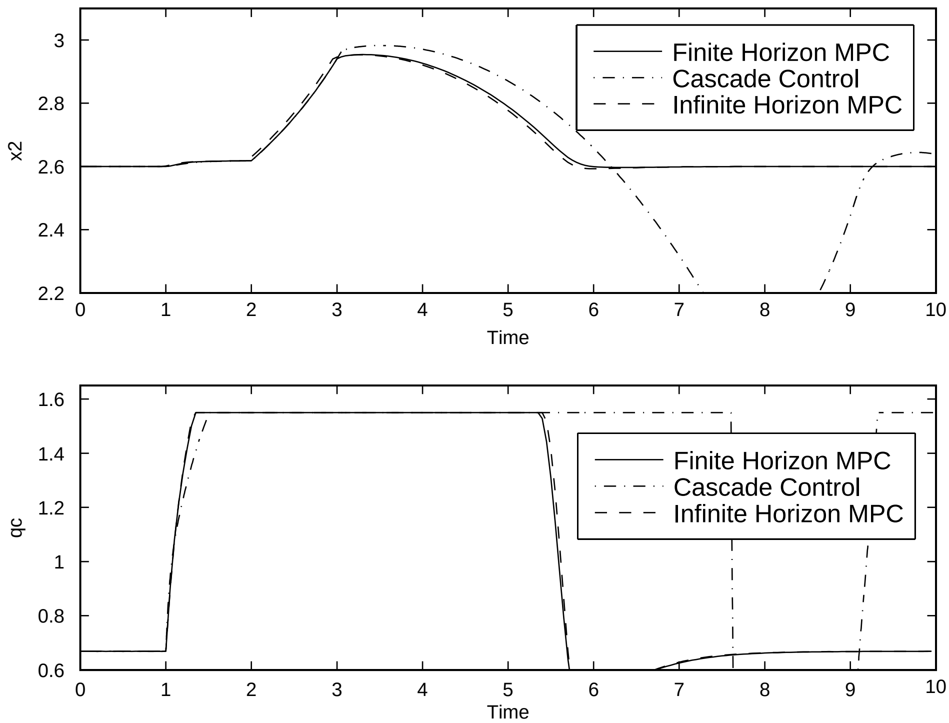

Fig. 9. Response to a large pulse increase in coolant feed temperature ($\tau = 1$ to 3) and large pulse decrease in reactor feed flow rate ($\tau = 2$ to 3). Comparison of MPC with classical cascade control.

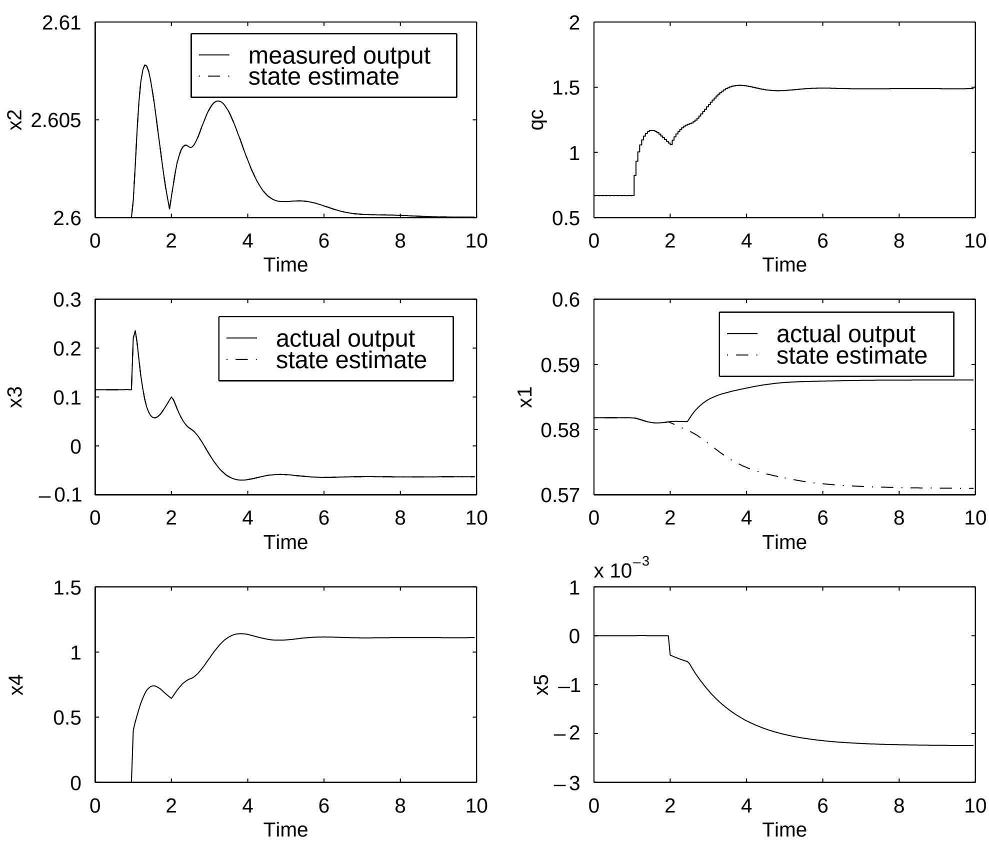

Fig. 10. Response of finite horizon MPC to a step increase in coolant feed temperature ($\tau = 1$), step increase in reactor feed concentration ($\tau = 2.5$) and step increase in reactor feed temperature ($\tau = 3.5$). States shown along with the actual output.

lack of state augmentation for x_1 and x_{2f}, leading to lack of observability of the entire set of disturbances. All the three disturbances cannot be estimated at the same time, since there are only two output measurements, which restricts the number of augmented disturbance states to two. The effect of disturbance gets distributed in augmented states x_4 (jacket feed temperature) and x_5 (reactor feed flow rate) due to the presence of nonlinearities in the system. Inaccurate estimates of the disturbance translates into inaccurate estimation of the state that the disturbance affects and finally into poor performance.

5. Conclusions

We have developed a model predictive control-based cascade control strategy and applied it to an open-loop unstable CSTR. A Kalman filter is used to estimate the coolant feed temperature and reactor flow rate disturbances, while a QP-based optimization for the predictive controller explicitly handles the manipulated variable (coolant flow rate) constraints. MPC outperforms classical cascade control whenever the manipulated variable constraints are active. There is an element of arbitrariness in the cascade control design, too, since the traditional tuning method of sequentially closing and tuning loops (inner and then outer) cannot be used for this class of open-loop unstable cascade systems. The model predictive cascade formulation presented in the article would be highly recommended for the systems having measurement lags and non-step types of disturbances. Though we do not present the results here, we have implemented our formulation on CSTR having measurement lags and a ramp disturbance (decrease in heat transfer coefficient because of fouling). For both cases, the response was better than classical cascade control.

Notation

G_w	state noise dynamics matrix
J_s	stable eigenvalue matrix of A
J_u	unstable eigenvalue matrix of A
N	number of future input moves to compute
P	error covariance matrix for states
q_c	dimensionless cooling jacket flow rate
Q	output penalty matrix
$\bar{Q}$	terminal state penalty matrix
Q_s	target tracking output penalty matrix
R	input state penalty matrix
$\bar{R}$	error covariance matrix for output noise vector
R_s	target tracking input penalty matrix
S	input rate of change penalty matrix
u	input vector
$\bar{u}$	desired input vector at steady state
u^N	vector of N future input vectors
v	zero mean, normal output noise vector
V	eigenvector matrix of A
V_s	stable eigenvector matrix of A
V_u	unstable eigenvector matrix of A
w	zero mean state, normal state noise vector
x_1	dimensionless reactor concentration
x_{1f}	dimensionless reactor feed concentration
x_2	dimensionless reactor temperature
x_{2f}	dimensionless reactor feed temperature
x_3	dimensionless cooling jacket temperature
x_{3f}	dimensionless cooling-jacket feed temperature
y	output vector
y_t	output target vector
z^s	stable modes of A
z^u	unstable modes of A
$\hat{z}$	estimated state step disturbance vector

Greek letters

β	dimensionless heat of reaction
γ	dimensionless activation energy
δ	dimensionless heat transfer coefficient
δ_1	reactor to cooling jacket volume ratio
δ_2	reactor to cooling-jacket density heat capacity ratio
$\kappa(x_2)$	dimensionless Arrhenius reaction rate non-linearity

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