Nonlinear Predictive Control of Uncertain Processes: Application to a CSTR

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Nonlinear predictive control (NLPC) is an effective strategy for controlling nonlinear chemical processes with constraints and time delays. In this article, a number of important issues in NLPC are addressed, emphasizing continuous stirred tank reactors (CSTR's) with parametric and model structure uncertainty. In particular, the effects of various choices for the initial conditions are discussed. The selection of initial conditions is particularly important in the presence of plant/model mismatch. A nonlinear programming-based approach is used for process identification. The effect of model structure uncertainty is included in our analysis by using a cascade control structure on the coolant temperature. Our CSTR results indicate that a simple PI (with anti-reset windup) cascade loop on coolant temperature is adequate for operation over a wide range of operating conditions. A particularly interesting result of this work is that a predictive controller based on an open-loop observer can be used to stabilize an open-loop unstable process, although this is not recommended in practice.

Introduction

Chemical processes have been traditionally operated using linear controllers, although it is well recognized that a characteristic of chemical processes presenting a challenging control problem is the inherent nonlinearity of the process. Linear controllers can yield satisfactory performance, if the process is operated "close" to a nominal steady state or is fairly "linear." Many times the process dynamic characteristics will change dramatically due to a large disturbance or due to significant setpoint changes from an on-line optimization routine. Also, batch processes typically operate over a large operating range, yielding a linear control strategy ineffective. Thus, there is an incentive to develop and implement nonlinear control strategies on chemical processes.

During the past five years, a number of nonlinear control system design techniques have been developed to control chemical processes including: differential geometric-based control, reference system synthesis, nonlinear internal model control, and nonlinear predictive control. A critique of differential geometric techniques was provided by Henson and Seborg (1990) and a tutorial by Kravaris and Kantor (1990a,b). McLellan et al. (1990) reviewed error trajectory control methods and detailed the similarities of the differential geometric, reference system synthesis (Bartusiak et al., 1989) and other model inverse-based techniques. Economou et al. (1986) and Li et al. (1990) extended linear internal model control (IMC) techniques (Garcia and Morari, 1982) to nonlinear systems to form nonlinear IMC (NLIMC). A comprehensive survey of nonlinear chemical process control techniques, with a perspective on future research needs, was provided by Bequette (1991a).

Limitations to model inverse-based approaches

There are a number of disadvantages to many of the techniques mentioned above. For example, the approaches based on differential geometry generally:

- Are developed for input-linear systems.
- Are based on a continuous time formulation; discrete time implementation issues in chemical process control have not been addressed.
- Constraints on manipulated, state or output variables are not handled explicitly; likewise, neither time delays nor nonminimum phase processes.
- May have controllers based on transformed variables. Good control of transformed variables may not assure good control of the physical (measured) variables.

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• Are based on theory that may not be easily understood by the personnel responsible for maintaining the control system.

Progress has been made recently in a number of areas mentioned above, which are limited to specific cases of SISO processes (as summarized by Bequette, 1991a). Most of the limitations to differential geometry-based techniques are avoided by using nonlinear predictive control (NLPC) techniques (Bequette, 1991b; Eaton and Rawlings, 1990a; Jang et al., 1987; Patwardhan et al., 1990), which are extensions of successful linear model-predictive control (LMPC) techniques.

Advantages to a nonlinear programming approach to process control

The advantages to nonlinear predictive control include the following.

• Time delays are explicitly handled.

• Manipulated and state variable constraints are explicitly handled.

• Nonminimum-phase processes are easily handled. A minimum prediction horizon is required.

• Knowledge of future setpoint changes is included (useful for batch control and scheduled, coordinated operational changes).

• NLPC approaches are intuitive and easy to understand (direct extensions of LMPC).

One goal of this article is to assess the capability of nonlinear predictive control to handle chemical processes with parametric and structural uncertainty. A number of predictive control approaches have been developed, but the issue of the proper choice of state variable initial conditions has not been given proper consideration; this important issue is addressed in this work. The effect of structural uncertainty is addressed by using a coolant temperature cascade control strategy on a CSTR. We find that the heat transfer nonlinearities cause a significant lag in the control response, even when the cooling jacket residence time is significantly smaller than that of the reactor residence time.

First, we review the general nonlinear predictive control optimization problem. We then detail the different approaches that can be used for open- and closed-loop state observers. An exothermic CSTR with multiple steady-state behavior is used to illustrate the effect of parametric and model structure uncertainty. We show conditions where an open-loop observer can be used when the CSTR is operated at an open-loop unstable operating point. A nonlinear programming approach is used for state variable and parameter estimation, which significantly improves the performance of NLPC on uncertain processes.

Nonlinear Predictive Control

Review of predictive control

During the past decade, linear model predictive control techniques [such as dynamic matrix control (DMC), Cutler and Ramaker, 1980] have been used successfully on a large number of industrial processes. At the same time, a number of theoretical papers have provided more insight on the properties of LMPC. A survey of model predictive control, including applied and theoretical papers, has been done by Garcia et al. (1989).

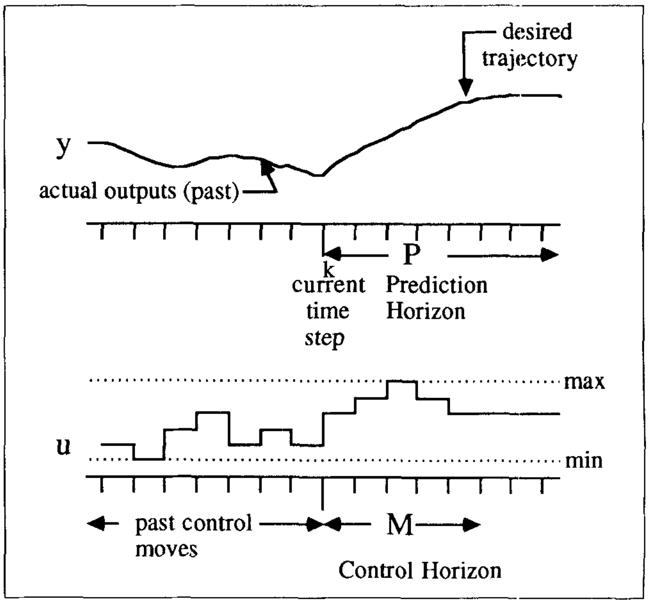


Figure 1. Predictive control approach.

One limitation to the LMPC methods is that they are based on linear systems theory and may not perform well on highly nonlinear systems. A direct extension of LMPC results, when a nonlinear dynamic process model is explicitly used in the control law formulation.

Nonlinear programming approach

The objective of nonlinear predictive control is to select a set of future control moves (control horizon) to minimize a function based on a desired output trajectory over a prediction horizon, as shown in Figure 1. A general mathematical formulation is (deadtime was not included for simplicity in notation):

$$\min_{u(k),\ldots,u(k+M-1)} \Phi(u) = \int_{t_k}^{t_k+T_p} e^2 dt = \sum_{i=k+1}^{k+P} [y_{sp}(i) - y_{\text{pred}}(i)]^2 \quad (1a)$$

subject to

$$\dot{x} = f(x,u,p,l) \quad (1b)$$

$$y_m = g(x) \quad (1c)$$

$$u_{\min} \le u(i) \le u_{\max} \quad (1d)$$

$$u(i-1) - \Delta u_{\max} \le u(i) \le u(i-1) + \Delta u_{\max} \quad (1e)$$

$$u(i) = u(k+M-1) \text{ for all } i > k+M-1 \quad (1f)$$

$$x_{\min} \le x(i) \le x_{\max} \quad (1g)$$

$$y_{\min} \le y(i) \le y_{\max} \quad (1h)$$

$$x(t_k) = x_k \quad (1i)$$

The objective function is the sum of the squares of the residuals between the model predicted outputs and the setpoint values over the prediction horizon of P time steps (Eq. 1a). It should be noted that the objective function can be much more general, including economic criteria or final condition relationships. The optimization decision variables are the control actions M time steps into the future; after the Mth time step, it is assumed that the control action is constant (Eq. 1f). Note that absolute (Eq. 1d) and velocity (Eq. 1e) constraints on the manipulated variables are explicitly included in this formulation. State and output variable constraints are included in Eqs. 1g and 1h.

Although the optimization is based on a control horizon, only the first control action is implemented. After the first control action is implemented, plant output measurements are obtained. Compensation of plant/model mismatch is performed, and the optimization is performed again.

There are a number of important issues that must be addressed in the solution of Eqs. 1a–1i. The choice of constrained optimization technique is one of the first decisions that must be made. Another major issue is how to solve the dynamic model constraints (Eq. 1b). Since many of the state variables are unmeasured, a decision must be made about the proper initial conditions for the state variables at the beginning of the prediction horizon (Eq. 1i). The model outputs (y_m) are a function of the state variables (Eq. 1c); however, a correction must be applied to y_m to account for plant/model mismatch and obtain a better prediction of the outputs (y_{pred}).

It should be noted that this predictive horizon approach is one of the distinguishing characteristics of model-predictive control. Other model-based control techniques do not allow the incorporation of future setpoint changes in the control algorithm. The knowledge of future setpoints is available typically in batch process control, and when scheduled, coordinated optimizing control is used on continuous processes.

Solution of the dynamic model equations

Several methods can be used to handle ordinary differential equation equality constraints (Eq. 1b) with a constrained nonlinear optimization program:

- Sequential
- Simultaneous
- Linear approximation.

The *sequential* solution techniques involves the iterative solution of the ordinary differential equations (ODE's) as an "inner loop" to evaluate the objective function (Jang et al., 1987), with an optimization code as the "outer loop." Jang et al. have used the generalized reduced gradient (GRG) optimization approach with a Runge-Kutta integration code for model solution. Bequette (1991b) used a sequential solution technique, transforming the ODE's into algebraic equations (AE's) (using orthogonal collocation on finite elements), which were solved as an "inner loop" using a sequential programming (SQP) code for optimization (Gill et al., 1986). The *simultaneous* solution involves the transformation of the ODE's into AE's using weighted residual techniques. Eaton and Rawlings (1990a) solved the AE's as equality constraints using SQP. A *linear approximation*, either by a single linearization over the prediction horizon or a linearization at a number of time steps in the prediction horizon, has been used by a number of researchers (Li and Biegler, 1989; Brengel and Seider, 1989). These various approaches are summarized by Bequette (1991a).

We feel that the approach used for the solution of the ODE's does not affect the performance of the controller. The computational efficiency of NLPC is influenced by the technique used to solve the ODE's. Sistu et al. (1991) addressed the computational aspects of the different solution techniques involved in the NLPC strategy. The other important issues involved in implementation of NLPC are the selection of the initial conditions for the model at each time step and the adjustments of the "tuning parameters." In this article we used the sequential simulation/optimization approach (orthogonal collocation on finite elements) to solve the model equality constraints. The primary advantage is that the optimization problem is much smaller than that in the simultaneous simulation/optimization method. This work focuses primarily on the various approaches that can be used to determine the model initial conditions for the optimization at each time step. In the next section, we outline the use of open-loop observers to determine the model initial conditions, and then develop a nonlinear programming approach to process identification.

Initial conditions and model output predictions.

Open-Loop Observer. If an open-loop observer is used, the initial conditions for the state variables (Eq. 1h) are obtained from the solution of the model over the previous time step, based on the manipulated action actually implemented on the plant. The DMC characterization of the future additive disturbances as the difference between the model output and the plant output at the current time step can be used to predict the output over the prediction horizon:

$$d(k) = y(k) - y_m(k) \tag{2}$$

$$y_{\text{pred}}(k+i) = y_m(k+i) + d(k) \quad \text{for } i = 1 \text{ to } P \tag{3}$$

For open-loop, unstable systems, a state variable identification procedure *should* be used (either explicitly or implicitly), so that the model state variables do not significantly diverge from the actual state variables. For linear, open-loop, unstable systems, a state variable estimation strategy *must* be used (either explicitly or implicitly), unless the model is open-loop stable.

Process Identification. Most nonlinear control strategies have assumed that all state variables are measured or are easily estimated. Even when all of the state variables are measured, the closed-loop performance may not be satisfactory if there are parametric or model structure errors, (as will be discussed later). Bequette (1991b) presented an approach for identification in a nonlinear, predictive control framework, while Sistu and Bequette (1990) developed a method to activate the process identification strategy. Jang et al. (1987) and Li and Biegler (1990) also presented nonlinear programming approaches for estimation. Jang et al. (1986) showed that a nonlinear programming approach is superior to Kalman filtering for a nonlinear dynamic system.

Nonlinear programming provides a natural formulation for process identification if nonlinear predictive control is used. The objective of the optimization-based approach is to minimize a measure of model-plant mismatch over an estimation horizon, by using process parameters, unmeasured states variables, and loads as decision variables.

The identification approach outlined below is presented in more detail by Sistu and Bequette (1990). The general process identification objective function is:

$$\min \Pi(x_o,p,l) = \sum_{j=1}^{N} \left\{ \sum_{i=k-E(j)*NS(j)}^{k} W_{ej}[y_j(i) - y_{mj}(i)]^2 \right\} \quad (4)$$

where $E(j)$ is the measurement estimation horizon (number of control sample times) for output j, W_{ej} is the weighting factor for output j, and $NS(j)$ is the number of measurement samples per control sample for output j. The objective function is based on the weighted least squares differences between the measured variables y and the values predicted by the process model y_m at each measurement time step t_i, where the current time step is represented by t_k. Note that the decision variables for this problem are the parameters p, load disturbances l as well as the initial unmeasured state variable values $x(k-E)$ at the beginning of the estimation horizon. The parameters and disturbances are assumed to be constant over the estimation horizon. The modeling equations are the same as those for the predictive control solution (Eqs. 1b and 1c).

If the measurements are perfect, the measured states are perfectly known at the beginning of the estimation horizon. The initial condition for the state variable vector $x(k-E)$ is then based on the values of the outputs at the beginning of the estimation horizon $t_o = t_k - T_E$:

$$0 = g[x(k-E)] - y(k-E) \quad (5)$$

In practice, there is measurement noise, so the measured state variables at the beginning of the time horizon are also estimated. Minimum and maximum bounds are placed on the estimates. Even when there is no measurement noise, there may be an incentive to estimate the measured state variables.

Since the model-predicted output is not exactly equal to the process output at the end of the time horizon, an additive output disturbance may be included after the process identification is performed:

$$d(k) = y(k) - g(x(k)) \quad (6)$$

$$y_{\text{pred}}(i) = y_m(i) + d(k) \quad (7)$$

for $i = k+1$ to $k+P$

The execution of the estimation scheme at each time step is not necessary and is computationally inefficient. It will result in erroneous estimates and hence poor control in the presence of noisy measurements if there is no process excitation. We have developed the following approach to activate the process identification phase.

Estimator Activation—Estimation Threshold. A statistical-analysis-based approach is developed to detect the presence of disturbances and activate the estimation mechanism. In this approach, a moving data window of past error estimates between model and process outputs at each measurement point is used to calculate a moving average $\mu_k(e)$ and a moving standard deviation $\sigma_k(e)$ based on a data window of W control samples for each output:

$$\mu_k(e) = \frac{1}{W^*NS} \sum_{j=1}^{W^*NS} e_{k-j+1} \quad (8)$$

$$\sigma_k(e) = \sqrt{\frac{1}{W^*NS-1} \sum_{j=1}^{W^*NS} (e_{k-j+1}) - \mu_k)^2} \quad (9)$$

A new term, $D_k = e_k - \mu_k(e)$, is used to determine if a disturbance has influenced the system.

The estimation scheme is activated if $|D_k| > s\,\sigma(e)$ for two successive measurements and if D_k has the same sign at both measurement times. Details involving the selection of s were discussed by Sistu and Bequette (1990). This approach for estimation is similar to that presented by Pavlechko et al. (1985) for linear adaptive-predictive control.

Tuning parameters

A number of "tuning" parameters can be used to adjust the desired speed of response of the closed-loop systems. For open-loop, stable, minimum-phase processes, longer prediction horizons P and shorter control horizons M add robustness and increase the closed-loop speed of response. For multi-output processes, the weights on each output can be adjusted depending on the relative importance of each output. Velocity constraints on the manipulated variable action can be used to minimize excessive control action. Bequette (1991b) has noted that, for unconstrained SISO systems, the control horizon can generally be set to one time step with the prediction horizon varied for performance and robustness. These results are consistent with linear MPC (Maurath et al., 1988).

CSTR Example

Ray (1982) has shown that a diabatic CSTR with an exothermic, first-order, irreversible reaction can have complex dynamic behavior which presents a challenging control problem. Several recent articles (for example, Limqueco and Kantor, 1990) have applied nonlinear control techniques to this process. We have extended the CSTR model to include cooling jacket dynamic effects to address the effect of model structure uncertainty. We will be considering two cases: (a) two-state (simplified) model (Eqs. 10 and 11) and (b) three-state (complete) model (Eqs. 10, 11 and 12).

$$\frac{dx_1}{d\tau} = -\phi x_1 \kappa(x_2) + q(x_{1f} - x_1) \quad (10)$$

$$\frac{dx_2}{d\tau} = \beta\phi x_1 \kappa(x_2) - (q+\delta)x_2 + \delta x_3 + q x_{2f} \quad (11)$$

$$\frac{dx_3}{d\tau} = \frac{q_c}{\delta_1}(x_{3f} - x_3) + \frac{\delta}{\delta_1 \delta_2}(x_2 - x_3) \quad (12)$$

where x_1 is the dimensionless concentration, x_2 is the dimensionless temperature (controlled variable), and x_3 is the dimensionless cooling jacket temperature. The relationship between the dimensionless parameters and variables and the physical variables are shown in Table 1; the nominal parameter values are shown in Table 2. For the simplified model, the dimensionless cooling jacket temperature x_3 is the manipulated variable. For the complete model, the dimensionless coolant flow rate q_c is the manipulated variable.

Table 1. Dimensionless Variables and Parameters for the CSTR Model

Simplified Model	
$\kappa(x_2) = \exp\left(\frac{x_2}{1+x_2/\gamma}\right)$	$\beta = \frac{(-\Delta H)C_f}{\rho C_p T_{f0}}\gamma$
$\gamma = \frac{E}{RT_{f0}}$	$\delta = \frac{UA}{\rho C_p Q_0}$
$\phi = \frac{V}{Q_0} k_0 e^{-\gamma}$	$q = \frac{Q}{Q_0}$
$\tau = \frac{Q_0}{V} t$	$x_1 = \frac{C}{C_{f0}}$
$x_2 = \frac{T-T_{f0}}{T_{f0}}\gamma$	$x_3 = \frac{T_c - T_{f0}}{T_{f0}}\gamma$
$x_{1f} = \frac{C_f}{C_{f0}}$	$x_{2f} = \frac{T_f - T_{f0}}{T_{f0}}\gamma$
Complete Model	
$x_{3f} = \frac{T_{cf} - T_{f0}}{T_{f0}}\gamma$	
$\delta_1 = \frac{V_c}{V}$	$\delta_2 = \frac{\rho_c C_{pc}}{\rho C_p}$

Table 2. Parameter Values (Case 2 from Limqueco and Kantor, 1990)

$\beta = 8.0$	$\phi = 0.072$
$\delta = 0.3$	$\gamma = 20.0$
$x_{1f} = 1.0$	$x_{2f} = 0.0$
$q = 1.0$	$x_3 = 0.0$

Lower steady state (SS1) $x^T = [0.8560, 0.8859]$ stable, overdamped
Middle steady state (SS2) $x^T = [0.5528, 2.7517]$ unstable
Upper steady state (SS3) $x^T = [0.2354, 4.7050]$ stable, underdamped

Simulation details

In all the simulations, three internal collocation points on each finite element are used for the process model. The length of each finite element is equal to the sample time of 0.25; the dominant time constant is approximately 2.5. NPSOL (Gill et al., 1986) is used for the optimization; HYBRD1 from MINPACK (More et al., 1980) is used to solve the AE's formed from the orthogonal collocation on the finite elements approximation of the model ODE's; and DASSL (Petzold, 1983) is used to solve the dynamic plant equations. All of the results presented are based on reactor temperature x_2 control.

Open-loop dynamic behavior

It is well-known that nonisothermal, exothermic chemical reactors (CSTR's) present some of the more challenging chemical process control problems. The characteristic nonlinear behavior includes multiple steady states, parametric sensitivity, and ignition extinction. Under the nominal parameter values, this system has three steady states. The lower- and upper-temperature steady states are stable, while the middle temperature steady state is unstable. An open-loop phase plane analysis is shown in Figure 2; the stable steady state obtained is a function of the initial condition as shown.

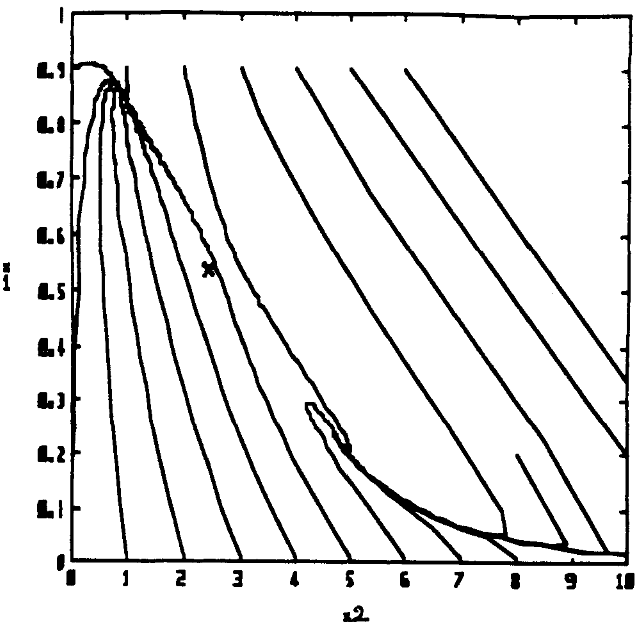


Figure 2. Open-loop phase plane, case 2 parameters.
x indicates open-loop unstable.

Two-State Simplified Model

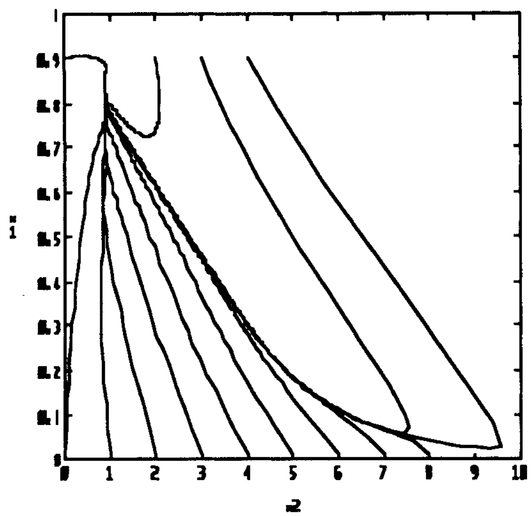
Perfect model

Open-Loop, Stable Setpoint, Open-Loop Observer. Initial results are based on a perfect model representation with an open-loop observer. A phase plane analysis is shown in Figure 3a for setpoint changes to the lower stable steady state. A change to the upper stable steady state is shown in Figure 3b. A prediction horizon of 5 and a control horizon of 1 are used in these simulations. We see that there is convergence to the desired steady states from any point in the phase plane.

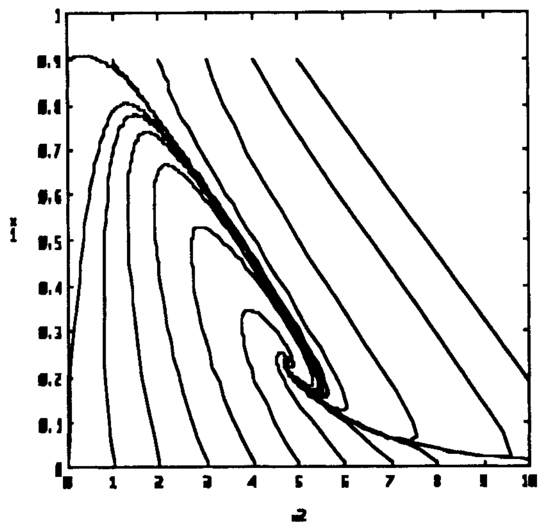
For linear, open-loop, unstable processes, an open-loop observer type of formulation cannot ordinarily be used because of internal stability considerations (Morari and Zafiriou, 1989). We have found that the open-loop observer approach can be used on certain nonlinear, unstable processes, as long as there also exist stable steady states for the model at the steady-state, manipulated variable value.

Open-Loop, Unstable Setpoint, Open-Loop Observer. A setpoint change from the lower open-loop, stable steady-state to the unstable steady-state is shown in Figure 4 for $P=5$ and $M=1$. Note that the model output begins to deviate from the plant output at $\tau=10$. This is due to the minor approximation error of the collocation solution, which accumulates over a period of time. The model goes to a stable steady state, while the plant is maintained at an open-loop, unstable steady state. This type of behavior has also been observed for a bioreactor system (Eaton and Rawlings, 1990b). An analysis based on linear systems theory shows that the open-loop, stable plant can be stabilized using an open-loop, stable model. (See the Appendix).

The steady-state operating curve for reactor temperature as a function of coolant temperature is shown in Figure 5. Note that the process gain is positive at the stable steady states and negative at the unstable steady state. The predictive controller based on the stable model is able to stabilize the unstable plant



(a) Lower Steady-State



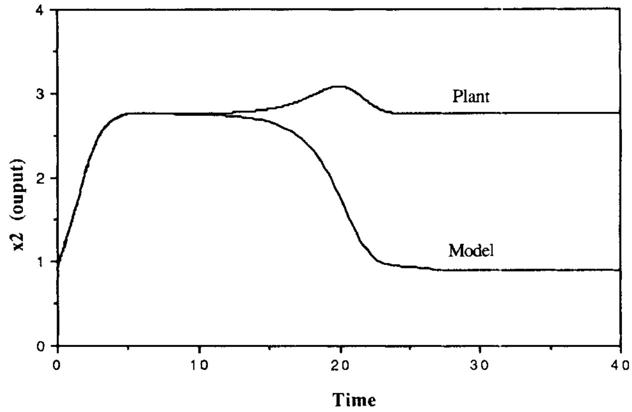
(b) Upper Steady-State

Figure 3. Phase plane analysis for a setpoint change to the open-loop stable steady states: perfect model.

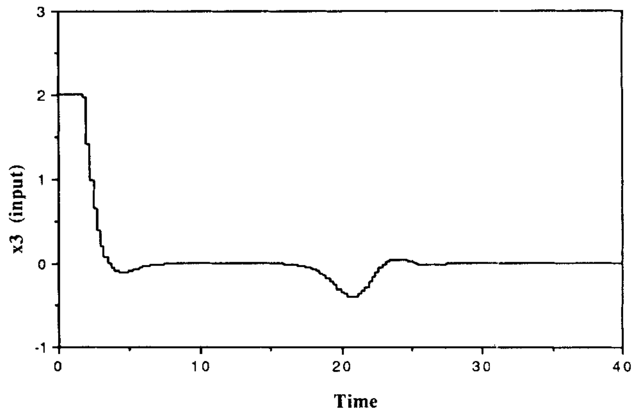
precisely because of the opposing gains. This is similar to the way that a proportional gain of opposite sign stabilizes a first-order, open-loop, unstable process.

Although process stability is achieved with an open-loop observer, this type of strategy should not be used for philosophical and practical reasons. Since the model states are not tracking the plant states, the true dynamic characteristics are not captured in the prediction optimization. Also, it should be obvious that state variable constraints cannot be successfully imposed in this situation.

The setpoint response for the case when both model states are perfectly known are excellent, but are not shown here since this is the expected result. This performance is achieved if both states are perfectly measured (as long as the model is perfect) or if the nonlinear state estimator is used. We will show in subsequent simulations that perfect measurements with an uncertain model can yield poor results.



(a) Output Response (reactor temperature)



(b) Input (coolant temperature)

Figure 4. Setpoint change to the open-loop unstable operating point, NLPC with open-loop observer: perfect model.

Parametric uncertainty

The static and dynamic behavior of this CSTR is a strong function of the parameter values. The steady-state operating curves for reactor temperature as a function of coolant tem-

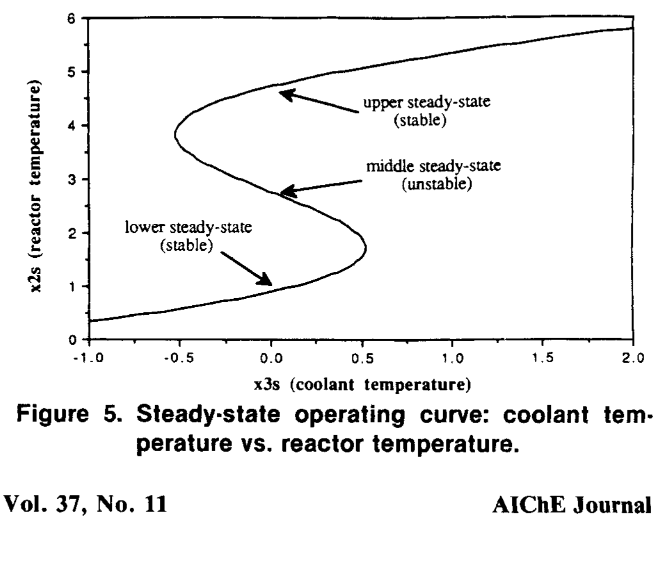


Figure 5. Steady-state operating curve: coolant temperature vs. reactor temperature.

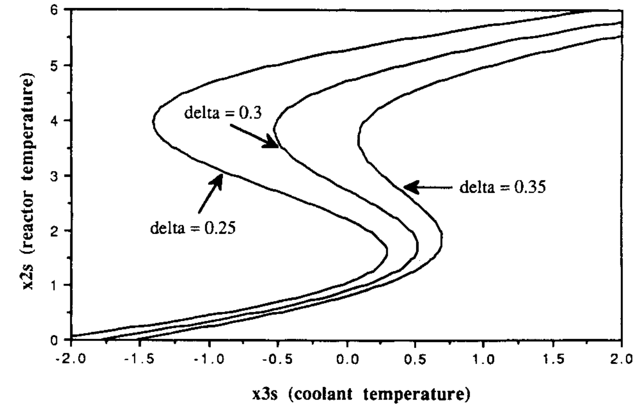


Figure 6. Sensitivity of the steady-state operating curve to δ (heat transfer coefficient).

perature are shown in Figure 6. If we assume that the coolant temperature x_3 is bounded between -1.0 and 2.0, we find that for certain parameter values there is a range of reactor temperatures that cannot be attained at steady state. For example, Figure 6 shows that if $\delta = 0.25$, then temperatures between $x_2 = 3.25$ and 4.5 cannot be attained (for $-1 \le x_3 \le 2$).

The majority of the nonlinear control techniques in the literature have assumed that all of the states were measured or perfectly estimated. One would believe that this would be the case that yields the best closed-loop performance. It turns out that this is only true if the process model is perfect. If there is model uncertainty, it may be better to perform state and parameter estimation to make the model as consistent with the process measurements as possible. Figure 7 shows results for a setpoint change to the open-loop, unstable operating point for the case where the model δ is 0.2 and the plant δ is 0.3. The open-loop observer is compared with state and parameter estimation (x_2 is measured), state variable resetting (the model initial conditions are set equal to the x_1 and x_2 measurements), and state variable estimation only. Note that an excellent response is obtained with state and parameter estimation even though only the temperature measurement is made, while state variable resetting has unsatisfactory performance (offset) with both temperature and composition measured. The strategy using only state variable estimation has extremely poor performance due to the parametric uncertainty. This illustrates the necessity of using both state and parameter estimation,

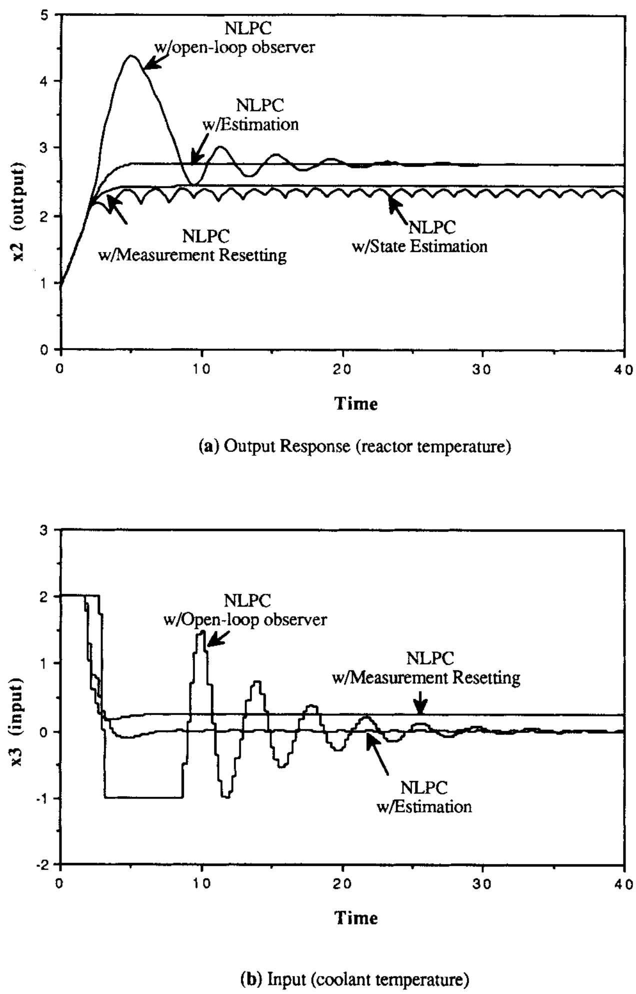


Figure 7. Setpoint change to unstable operating point with model uncertainty (plant $\delta = 0.3$, model $\delta = 0.2$).

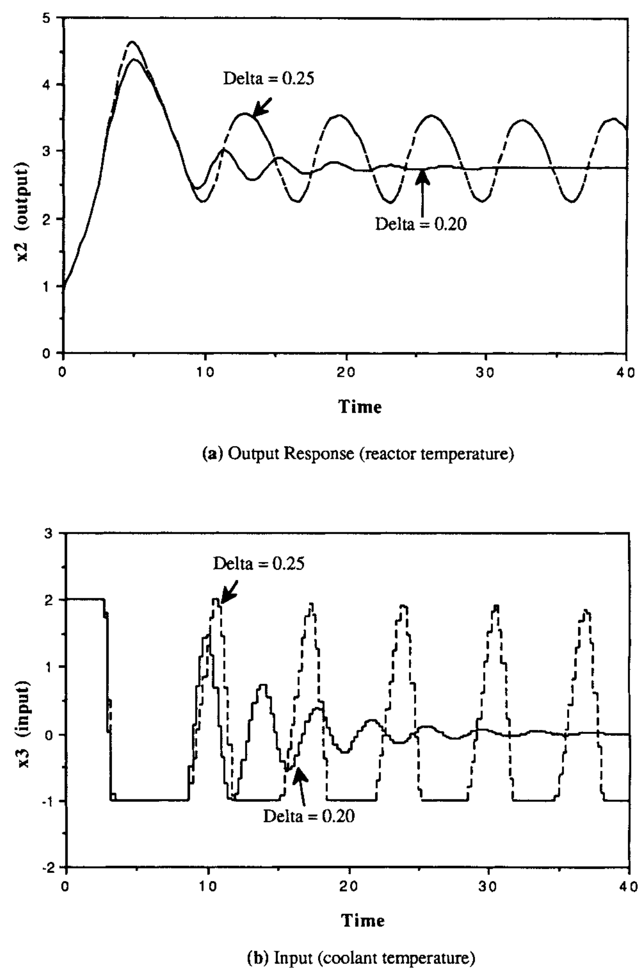


Figure 8. Setpoint change to unstable operating point, open-loop observer, model uncertainty (plant $\delta = 0.3$).

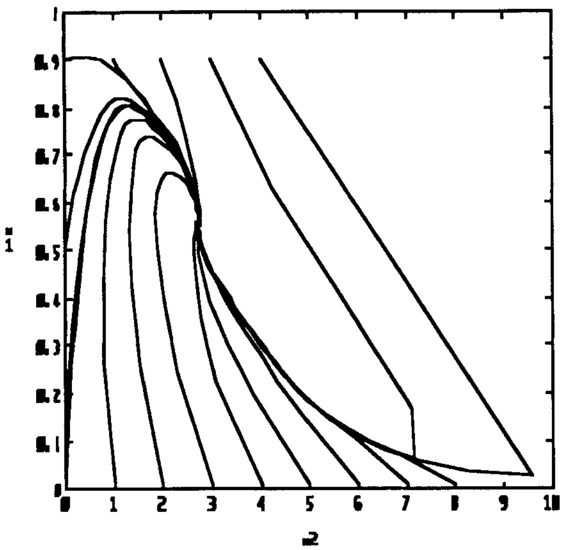


Figure 9. Phase plane for setpoint change to open-loop unstable point, NLPC with estimation.

rather than state estimation alone. The primary problem with control using only state estimation or measurement resetting, with this parametric uncertainty, is that the model has only one steady state while the plant has three steady states. In the estimation studies, we have used an estimation horizon of $E=2$ control samples, a measurement window of $W=10$ control samples, and 5 temperature measurements per control sample.

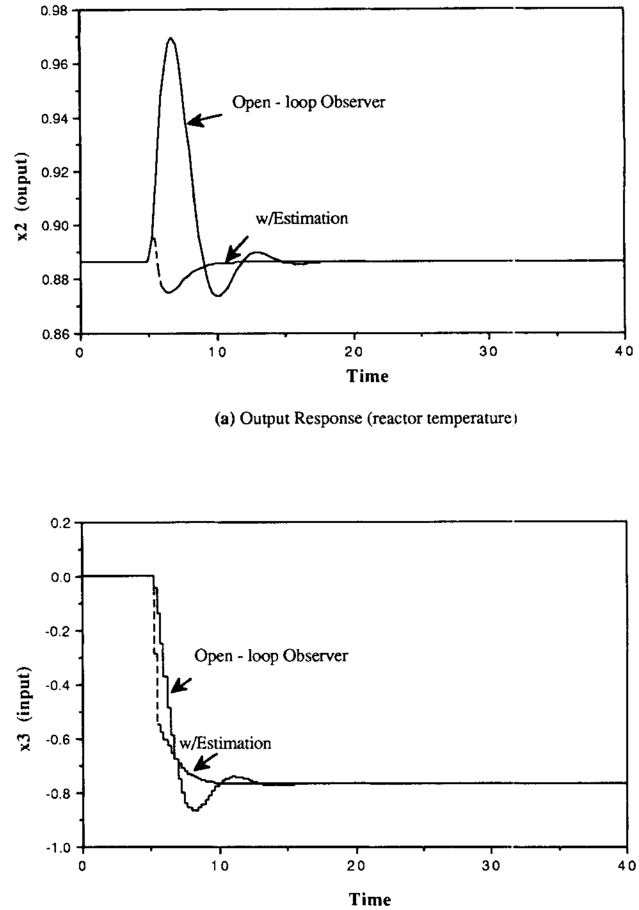
The parameter uncertainty effect on the behavior of open-loop, observer-based NLPC strategy is very interesting. Figure 8 shows that better control is actually obtained when there is more error in the heat transfer coefficient (δ). The plant δ is 0.3, while better closed-loop performance is obtained with a model δ of 0.2 than 0.25! Note that the control variable is constrained at the lower bound for $\delta=0.25$. Another reason for this interesting behavior of the closed-loop response is that the model with lower delta has real eigenvalues and the model with higher delta has complex eigenvalues. The results of NLPC with estimation strategy are not shown since the δ is perfectly estimated, yielding the same transient response as shown in Figure 7.

A phase plane analysis of the NLPC with estimation strategy for the open-loop, unstable setpoint is shown in Figure 9. Note that convergence is achieved from all the points in the operating region.

Figure 10 compares the disturbance rejection performance of NLPC with estimation to that of NLPC with an open-loop observer. The process is controlled at the lower stable steady state, with model mismatch in δ (model $\delta=0.2$, plant $\delta=0.3$). A feed composition disturbance of $+20\%$ occurs at $\tau=5$. The estimation strategy effectively results in feedforward control, so that much tighter control is achieved. The estimation strategy leads to a slightly higher magnitude of control action immediately after the disturbance enters, as shown in Figure 10b. Using measurement resetting leads to an undesirable response, which is not shown here.

Model Structure Uncertainty

The majority of the CSTR applications in the literature



(a) Output Response (reactor temperature)

(b) Input (coolant temperature)

Figure 10. Response to a 20% feed composition disturbance with uncertainty in δ.

assume that the cooling jacket temperature is the manipulated variable and that it can be changed instantaneously. Note that this is equivalent to specifying a perfect inner loop on a cascade control system. In practice, this inner loop may have significant dynamics or a constraint on jacket temperature may be encountered due to a coolant flow rate constraint. The purpose of this section is to illustrate the complications that may arise in a practical situation where there are jacket static and dynamic effects. In this study we assume that the jacket/reactor volume ratio (δ_1) is 1/20, the heat capacity ratio (δ_2) is 1, and the coolant feed temperature (x_{3f}) is -1.

Cascade control: two-state NLPC

When a two-state (simplified) model is used for the NLPC strategy and the plant is represented by three states, a cascade control loop must be used to regulate the coolant temperature. A cascade control structure is conceptually useful for disturbance rejection as the coolant temperature can be used as secondary measurement resulting in a better disturbance rejection. The coolant temperature setpoint is the manipulated variable, and the reactor temperature is the controlled variable for the outer (master) loop.

PI Control. The inner (slave) loop would normally be a PI controller, which is described by:

$$q_c = q_{co} + k_c(x_{3sp} - x_3) + \frac{k_c}{\tau_I}\int_0^t (x_{3sp} - x_3)d\mu \tag{13}$$

RSS Control. Another option is to use a gain-scheduled, adaptive or other type of nonlinear control on the inner loop. One example that we show involves an RSS controller for the inner loop. As developed by Bartusiak et al. (1989), in the RSS approach the dynamic equation for the controlled state variable is first written:

$$\dot{x}_3 = \frac{q_c}{\delta_1}(x_{3f} - x_3) + \frac{\delta}{\delta_1\delta_2}(x_2 - x_3) \tag{14}$$

A controller of PI form is used as a reference trajectory, based on a difference between the desired output (that is, the setpoint) and the actual measurement. The advantage of this approach is that the nonlinear heat transfer behavior is explicitly handled. Note that the RSS controller is implicitly based on differential geometric concepts (McLellan et al., 1990). The form of RSS-PI controller is:

$$\dot{x}_{3r} = k_c(x_{3sp} - x_3) + \frac{k_c}{\tau_I}\int_0^t (x_{3sp} - x_3)d\mu \tag{15}$$

Equating Eqs. 14 and 15 results in the final control calculation of:

$$q_c = \frac{k_c(x_{3sp} - x_3) + \frac{k_c}{\tau_I}\int_0^t (x_{3sp} - x_3)d\mu - \frac{\delta}{\delta_1\delta_2}(x_2 - x_3)}{\frac{(x_{3f} - x_3)}{\delta_1}} \tag{16}$$

Note that, if the coolant inlet temperature (x_{3f}) is measured, then feedforward control of coolant inlet temperature disturbances is explicitly handled in this approach. A singularity occurs if the coolant inlet temperature is momentarily equal to the cooling jacket temperature due to a sudden disturbance. This is a problem with many approaches that are based on an instantaneous model inverse.

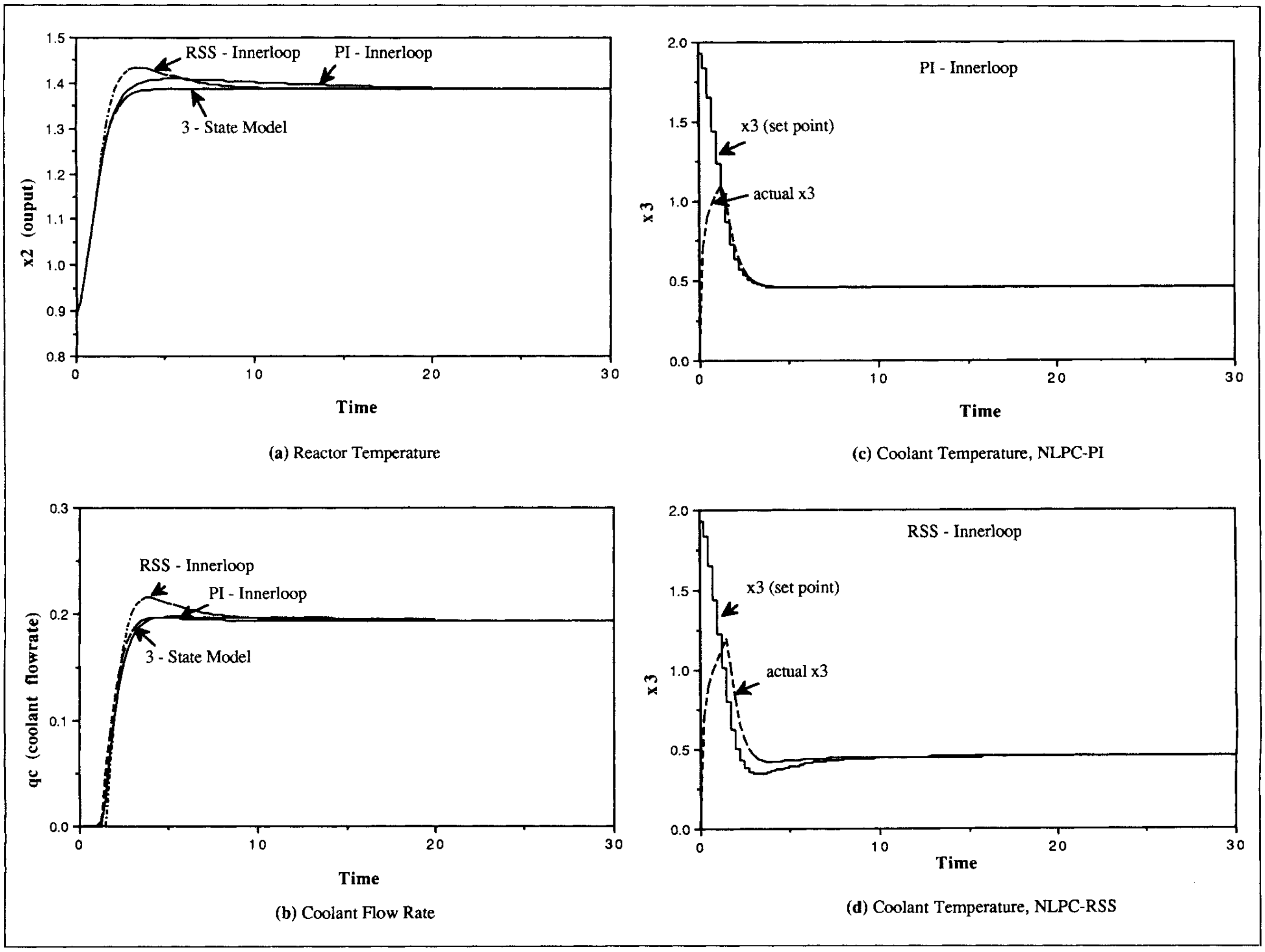


Figure 11. Comparison of two-state NLPC-RSS and NLPC-PI with three-state NLPC for a setpoint change.

Three-state NLPC

A major disadvantage to the cascade type of control approaches is that they do not explicitly account for possible constraints (velocity or absolute) on the coolant flow rate. If the NLPC is based on the complete (three-state) model, then constraints on the coolant flow rate are explicitly handled. If the coolant inlet temperature is measured, then feedforward control of coolant inlet temperature disturbances is explicit. Also using a full model representation of the plant results in a better setpoint tracking. The major advantage to the cascade controllers is that we are assuming that the inner loop is sampled very frequently, giving them the capability to quickly reject inner-loop disturbances. Also, the three-state NLPC requires more computation time than the two-state NLPC to calculate the optimal control moves.

Tuning the cascade controllers

The RSS and PI cascade controllers are implemented in discrete (velocity) form, with a sample time of 0.0125 (the outer loop had a sample time of 0.25); they were tuned to achieve similar closed-loop control of the cooling jacket temperature for small setpoint changes around the nominal setpoint. The IMC-based PI tuning parameters (Rivera et al., 1986) for the linearized jacket energy balance were used as the initial guesses. These parameters were detuned to give first-order responses for small setpoint changes on the nonlinear process. The PI parameters used were $k_c = -0.5$ and $\tau_I = 0.1$, while the RSS parameters were $k_c = 3.0$ and $\tau_I = 0.2$. For a large setpoint change in the reactor temperature, the responses are significantly different, as shown in Figure 11a. The performance of the three-state NLPC strategy (with $P=5$, $M=1$) is superior to the two-state NLPC strategies with RSS and PI inner loops. Figure 11b shows the coolant flow rate implemented by each controller, while Figures 11c and 11d show the actual x_3 tracking for PI and RSS, respectively. The lag for the cascade control strategies is due primarily to the heat exchanger nonlinearities; the two-state model cannot compensate for these nonlinearities.

Coolant feed temperature disturbances

The coolant feedstream in a typical process plant is subject to frequent temperature disturbances. To compare the performance of the NLPC strategies, a step coolant inlet temperature (x_{3f}) disturbance occurs at $\tau = 5$. We will compare the performance of these strategies when the coolant feed temperature is measured (feedforward) and when it is unmeasured.

Coolant Inlet Temperature Unmeasured. If the coolant inlet temperature is unmeasured then the two-state NLPC-PI strategy has better performance than the two-state NLPC-RSS or three-state NLPC approaches, as shown in Figure 12a. This is not surprising, since the RSS and three-state NLPC methods use a incorrect temperature for the control calculation, while the PI controller calculations are based on the deviation of the coolant temperature from setpoint.

Coolant Inlet Temperature Measured. When the coolant inlet temperature is measured, the two-state NLPC with both RSS and PI inner loop has better performance than the three-state NLPC, as shown in Figure 13. Note difference in the scales for Figures 12a and 13a. The responses for a measured disturbance are much better than for an unmeasured disturbance, as expected. The NLPC-RSS has almost perfect disturbance rejection, since it is based on a rapidly sampled inner loop. The three-state NLPC does not perform as well, because of the jacket dynamics in the discrete implementation of the control moves; perfect disturbance rejection can be achieved with fast jacket dynamics and smaller sampling times.

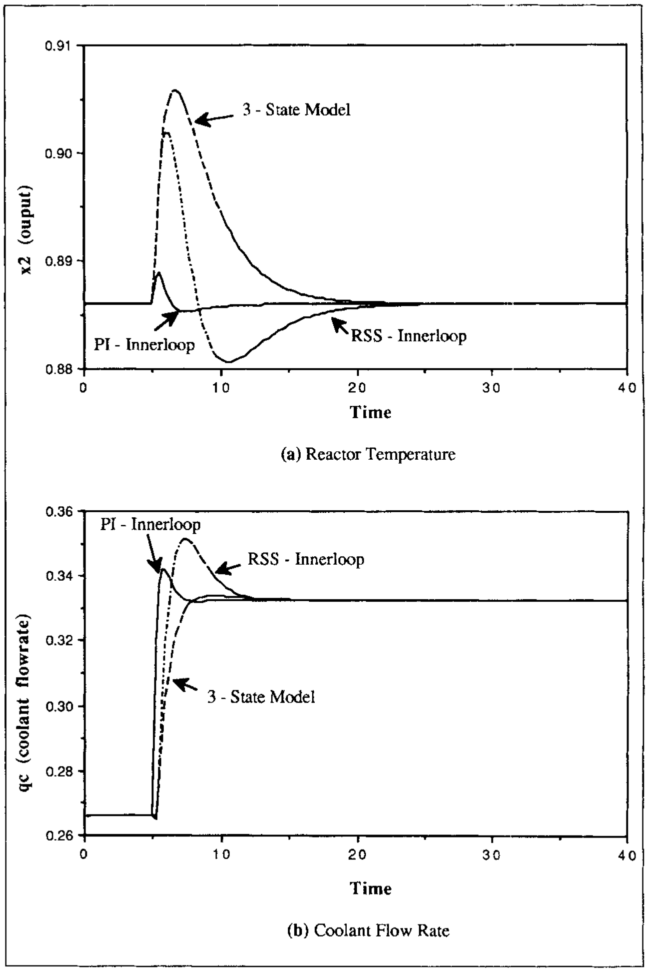
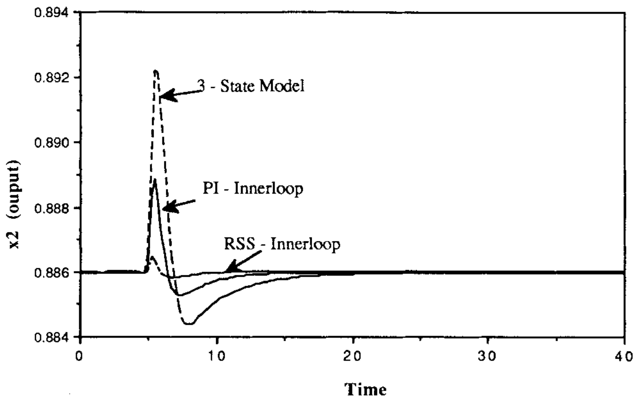


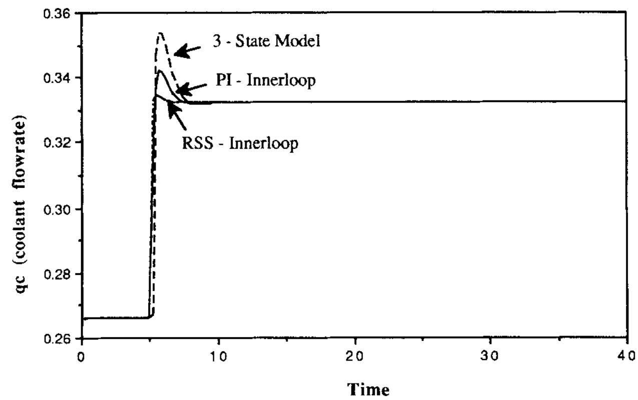
Figure 12. Unmeasured coolant feed temperature disturbance.

Parameter uncertainty

The responses for a setpoint change with uncertainty in δ (model $\delta = 0.2$, plant $\delta = 0.3$) are shown in Figure 14. The inner-loop process gain is a strong function of δ, and the continuous PI controller has poor performance due to reset wind-up, as shown. These simulations indicate that the three-state NLPC (without estimation) performs satisfactorily even in the presence of unmeasured disturbances and model uncertainty. For the two-state NLPC strategy, PI on the inner loop is preferred over RSS in the presence of model uncertainty. The best performance is by the discrete NLPC-PI controller, since it is not as dependent on δ and the velocity form prevents reset windup. Although not shown here, all of the NLPC strategies with estimation exhibit good performance.

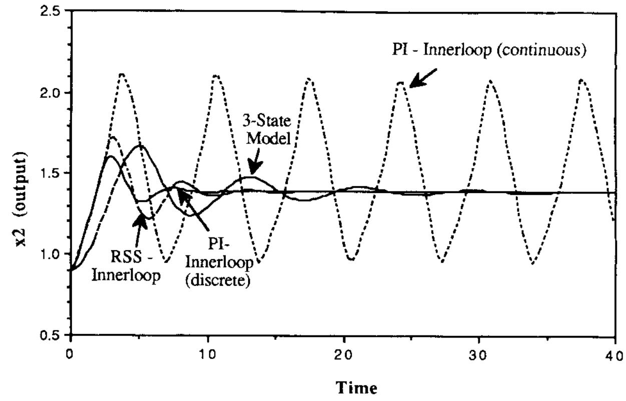


(a) Reactor Temperature

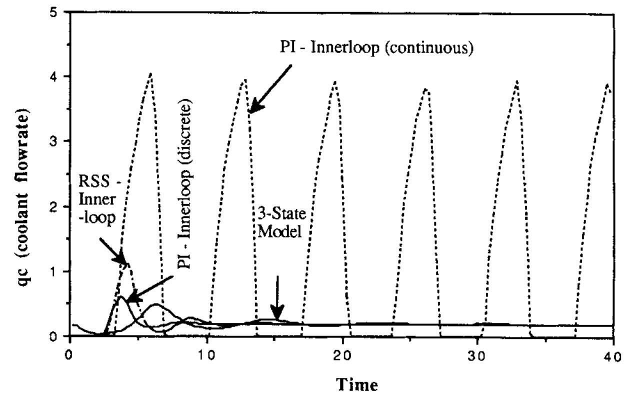


(b) Coolant Flow Rate

Figure 13. Measured coolant feed temperature disturbance.



(a) Reactor Temperature



(b) Coolant Flow Rate

Figure 14. Setpoint change in reactor temperature, open-loop observer: model uncertainty (plant $\delta = 0.3$, model $\delta = 0.2$).

Summary

A number of important issues in nonlinear predictive control of uncertain chemical processes were studied. The classical CSTR with a first-order, irreversible, exothermic reaction was used as the process example. It was shown that an open-loop observer can be used on an open-loop, unstable process, as long as a stable model steady state at the same manipulated variable value exists; this strategy is not recommended in practice. With plant/model mismatch, a nonlinear programming-based process identification scheme is used in combination with NLPC to achieve much tighter performance than is possible without estimation. We found that setting the model initial conditions equal to the process measurements can yield very poor performance if there is a plant/model mismatch. We also found that nonlinear control with state estimation may have unsatisfactory performance when there is parametric uncertainty; it is necessary to include parameter estimation for good performance. Our results also indicate that NLPC based on a two-state model with a simple (velocity-form) discrete PI cascade loop on coolant temperature is sufficient for operation over a wide range of operating conditions. In this work we have not addressed deadtime and measurement noise issues, which we feel could present significant challenges at the open-loop unstable operating point.

Acknowledgment

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Notation

e = error
E = estimation horizon
k = current time step
l = load disturbance
M = control horizon
N = number of outputs
NS = number of measurement samples/control sample
P = prediction horizon
u = manipulated variable
W = data window
x = state variable
y = output variable

Parameters and variables

C = reactor composition
C_f = feed composition
Q = feed flowrate
Q_c = coolant flowrate
q = dimensionless reactor feed flowrate

q_c = dimensionless coolant flowrate
T = reactor temperature
T_c = coolant temperature
UA = heat transfer coefficient* heat transfer area
V = reactor volume
V_c = cooling jacket volume
x_1 = dimensionless reactor concentration
x_2 = dimensionless reactor temperature
x_3 = dimensionless cooling jacket temperature
x_{1f} = dimensionless feed concentration
x_{2f} = dimensionless feed temperature
x_{3f} = dimensionless coolant feed temperature

Greek letters

β = dimensionless heat of reaction
ϕ = damkohler number (at nominal flowrate)
δ = dimensionless heat transfer coefficient
δ_1 = dimensionless volume ratio
δ_2 = dimensionless density* heat capacity ratio
ρC_p = density* heat capacity
$\rho_c C_{pc}$ = density* heat capacity of coolant
γ = dimensionless activation energy
τ = dimensionless time
σ = standard deviation
μ = mean

Literature Cited

Bartusiak, R. D., C. Georgakis, and M. J. Reilly, "Nonlinear Feedforward/Feedback Control Structures Designed by Reference System Synthesis," *Chem. Eng. Sci.*, **44**, 1837 (1989).

Bequette, B. W., "Nonlinear Control of Chemical Processes—a Review," *Ind. Eng. Chem. Res.*, **30**, 1391 (1991a).

Bequette, B. W., "Nonlinear Predictive Control Using Multirate Sampling," *Can. J. Chem. Eng.*, **69**, 136 (1991b).

Brengel, D. D., and W. D. Seider, "Multistep Nonlinear Predictive Controller," *Ind. Eng. Chem. Res.*, **28**, 1812 (1989).

Cutler, C. R., and B. L. Ramaker, "Dynamic Matrix Control—a Computer Control Algorithm," *Proc. Amer. Control Conf.*, WP5-B (1980).

Eaton, J. W., and J. B. Rawlings, "Feedback Control of Nonlinear Processes Using On-Line Optimization Techniques," *Comp. Chem. Eng.*, **14**, 469 (1990a).

Eaton, J. W., and J. B. Rawlings, "Model Predictive Control of Chemical Processes," *Chem. Eng. Sci.*, in press (1990b).

Economou, C. G., M. Morari, and B. O. Palsson, "Internal Model Control: 5. Extension to Nonlinear Systems," *Ind. Eng. Chem. Process Des. Dev.*, **25**, 403 (1986).

Garcia, C. E., and M. Morari, "Internal Model Control: a Unifying Review and Some New Results," *Ind. Eng. Chem. Process Des. Dev.*, **21**, 308 (1982).

Garcia, C. E., D. M. Prett, and M. Morari, "Model Predictive Control: Theory and Practice—a Survey," *Automatica*, **25**, 335 (1989).

Gill, P. E., W. Murray, M. A. Saunders, and M. H. Wright, "User's Guide for NPSOL (Version 4.0): a Fortran Program for Nonlinear Programming," Technical Report SOL 86-2, Dept. of Operations Research, Stanford Univ. (1986).

Henson, M. A., and D. E. Seborg, "A Critique of Differential Geometric Control Strategies for Nonlinear Process Control," IFAC World Congress, Tallin, Estonia (1990).

Jang, S., B. Joseph, and H. Mukai, "Comparison of Two Approaches on On-Line Parameter and State Estimation of Nonlinear Systems," *Ind. Eng. Chem. Process Des. Dev.*, **25**, 809 (1986).

Jang, S., B. Joseph, and H. Mukai, "Control of Constrained Multivariable Nonlinear Process Using a Two-Phase Approach," *Ind. Eng. Chem. Res.*, **26**, 2106, (1987).

Kravaris, C., and J. C. Kantor, "Geometric Methods for Nonlinear Process Control: I. Background," *Ind. Eng. Chem. Res.*, **29**, 2295 (1990a).

Kravaris, C., and J. C. Kantor, "Geometric Methods for Nonlinear Process Control: II. Controller Synthesis," *Ind. Eng. Chem. Res.*, **29**, 2310 (1990b).

Limqueco, L. C., and J. C. Kantor, "Nonlinear Output Feedback Control of an Exothermic Reactor," *Comp. Chem. Eng.*, **14**, 427 (1990).

Li, W. C., and L. T. Biegler, "Multistep, Newton-type Control Strategies for Constrained, Nonlinear Processes," *Chem. Eng. Res. Des.*, **67**, 562 (1989).

Li, W. C., L. T. Biegler, C. G. Economou, and M. Morari, "A Constrained Pseudo-Newton Control Strategy for Nonlinear Systems," *Comp. Chem. Eng.*, **14**, 451 (1990).

Li, W.-C., and L. T. Biegler, "Newton-Type Controllers for Constrained Nonlinear Processes with Uncertainty," *Ind. Eng. Chem. Res.*, **29**, 1647 (1990).

Maurath, P. R., D. A. Mellichamp, and D. E. Seborg, "Predictive Controller Design for Single-Input/Single-Output (SISO) Systems," *Ind. Eng. Chem. Res.*, **27**, 956 (1988).

McLellan, P. J., T. J. Harris, and D. W. Bacon, "Error Trajectory Descriptions of Nonlinear Controller Designs," *Chem. Eng. Sci.*, **45**, 3017 (1990).

Morari, M., and E. Zafiriou, *Robust Process Control*, Prentice Hall, Englewood Cliffs, NJ (1989).

More, J. J., B. S. Garbow, and K. E. Hillstrom, "User Guide for Minpack-1," Technical Report ANL-80-74, Argonne National Laboratory, Argonne, IL (Aug. 1980).

Patwardhan, A. A., J. B. Rawlings, and T. F. Edgar, "Nonlinear Model Predictive Control," *Chem. Eng. Comm.*, **87**, 123 (1990).

Pavlechko, P. A., M. C. Wellons, and T. F. Edgar, "An Approach for Adaptive-Predictive Control," *Adaptive Control of Chemical Processes*, p. 37, IFAC Workshop, Frankfurt, Germany (1985).

Petzold, L. R., "A Description of DASSL: a Differential-Algebraic System Solver," *Scientific Computing*, p. 65, R. S. Stepleman, ed., North-Holland (1983).

Ray, W. H., "New Approaches to the Dynamics of Nonlinear Systems with Implications for Process and Control System Design," *Chemical Process Control 2*, p. 246, D. E. Seborg and T. F. Edgar, eds., United Engineering Trustees, New York (1982).

Rivera, D. E., S. Skogestad, and M. Morari, "Internal Model Control: 4. PID Controller Design," *Ind. Eng. Chem. Proc. Des. and Dev.*, **25**, 252 (1986).

Sistu, P. B., and B. W. Bequette, "Process Identification using Nonlinear Programming Techniques," *Proc. Amer. Control Conf.*, 1534 (1990).

Sistu, P. B., R. S. Gopinath, and B. W. Bequette, "Implementation Issues in Nonlinear Predictive Control," *Proc. Amer. Control Conf.*, 2361 (1991).

APPENDIX

Consider the regulation of the plant around an open-loop unstable operating point. Under these conditions, the nonlinear plant can be described by a locally linearized discrete input—output representation as:

$$y(k+1) = -a_1 y(k) - a_2 y(k-1) + b_1 u(k) + b_2 u(k-1) \quad \text{(A1)}$$

Similarly, the model is represented by a discretized linear input—output relationship at an open-loop, stable operating point:

$$y_m(k+1) = -a_{m1} y_m(k) - a_{m2} y_m(k-1) + b_{m1} u(k) + b_{m2} u(k-1) \quad \text{(A2)}$$

Now, at the kth time step the control move $u(k)$ to be implemented is the solution of the open-loop, optimal control problem for a control horizon of 1:

$$\min \sum_{i=1}^{P} [y_m(k+i) + d(k) - y_{set}]^2 \quad \text{(A3)}$$

where

$$d(k) = y(k) - y_m(k)$$
$$y_m(k+i) = \text{model predicted output at the } (k+i)\text{th time step}$$

From Eq. A2 the model predictions over the prediction horizon P are given by:

$$Y_m(k) = \underline{\mathbf{A}}y_m(k-1) + \underline{\mathbf{B}}y_m(k) + \underline{\mathbf{C}}u_m(k-1) + \underline{\mathbf{D}}u(k)$$

where $\underline{\mathbf{A}}$, $\underline{\mathbf{B}}$, $\underline{\mathbf{C}}$, $\underline{\mathbf{D}}$ are $P \times P$ matrices whose elements are functions of the model coefficients, and $Y_m(k)$ is the vector of model-predicted outputs $y_m(k+i)$ over the prediction horizon P.

$u(k)$, the optimal solution to the optimization problem (Eq. A3), for unbounded case is obtained by applying the first derivative optimality conditions and is given by:

$$u(k) = \frac{\sum_{i=1}^{P} D_{Pi}[y_{\text{set}} - d(k)]}{\sum_{i=1}^{P} D_{Pi}[D_{Pi} + C_{Pi}u(k-1) + A_{Pi} + B_{Pi}]}$$

where A_{Pi}, B_{Pi}, C_{Pi}, and D_{Pi} are the Pth row of the respective matrices. The closed-loop characteristic equation in the feedback form is given by:

$$1 + G_P(z)G_c(z) = 0$$

where

$$G_c(z) = \frac{u(z)}{e(z)} = \frac{u(z)}{y_{\text{set}} - y}$$
$$= \frac{\sum_{i=1}^{P} D_{Pi}}{\sum_{i=1}^{P} D_{Pi}[D_{Pi} + C_{Pi} + (A_{Pi} + B_{Pi} - 1)G_m(z)]}$$

where G_p and G_m are z transform representations of the plant and the model, respectively.

The coefficients of this polynomial in the variable z are complicated functions of plant and model parameters and the prediction horizon. Therefore, it is not possible to analytically calculate the stability limits as a function of these parameters. The closed-loop characteristic equation allows us to numerically determine whether a particular closed-loop system is stable or not by examining the roots of the equation. For a stable system, the roots of this equation should lie within the unit circle. Simulations presented in this study confirm the closed-loop stability predicted by the above analysis.

Similarly, the convergence of the plant output to the setpoint at the open-loop, unstable operating point can be verified using the final value theorem. The closed-loop relationship between setpoint and plant output is given by:

$$\frac{y(z)}{y_{\text{set}}} = \frac{G_p(z)G_c(z)}{1 + G_p(z)G_c(z)}$$

Using the final value theorem we can verify that y/y_{set} goes to 1 as z goes to one.

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