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Gain-scheduling trajectory control of a continuous stirred tank reactor

K.-U. Klatt* and S. Engell

Process Control Group, Department of Chemical Engineering, University of Dortmund, D-44221 Dortmund, Germany

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Abstract

The control of continuous stirred tank reactors is often a challenging problem because of the strong pronounced nonlinearity of the process dynamics. Exact feedback linearization and gain-scheduling are two well-known approaches to the design of nonlinear process control systems. The basic idea in this paper is to combine these techniques to obtain a control structure which preserves the advantages and overcomes some of the problems of the two concepts. In a first step, a nonlinear state feedback controller is computed by exact linearization of the process model to shape the nominal closed-loop system. The required unmeasurable state variables are obtained by simulation of the process model. This part of the controller thus is a pure nonlinear feedforward compensator for the nominal plant. To act against disturbances and model uncertainty, a nonlinear gain-scheduled controller is designed by approximately linearizing the process model not for a number of operating points as in the standard gain-scheduling approach but around the nominal trajectory generated by the nonlinear feedforward controller. The design approach is applied to a non-trivial concentration control problem in a continuous stirred tank reactor with non-minimum phase behaviour, unmeasurable states, and model uncertainties as well as unknown disturbances. The nonlinear control structure is compared to a linear controller and to a pure gain-scheduling controller and shows excellent performance even for worst case disturbances and model uncertainties.

Keywords: nonlinear process control; gain-scheduling; exact linearization; continuous stirred tank reactor

Nomenclature

Roman Symbols:

A,B,C,D = linear system matrices, bodies
A_R = reactor surface
c = concentration, parameter
C_P = heat capacity
E_A = activation energy
e = error
F = normalized process stream inflow
$f(\cdot),g(\cdot)$ = vector fields
$G(s)$ = transfer function
ΔH_R = reaction enthalpy
$h(\cdot)$ = vector function
K,L = linear controller matrices
K_I,K_P = PI-controller parameters
k_0 = activation factor
k_i = rate coefficients
k_W = heat transfer coefficient
$k(\cdot),l(\cdot)$ = vector functions
m_K = coolant mass
$\dot{Q}_K$ = cooling rate
OP = family of operation points
r = relative degree
s = Laplace transform variable
T = time constant
t = time
u = manipulated input
V_R = reactor volume
$\dot{V}$ = volume flow
v,w = exogenous inputs
x = state (vector)
y = output
z = state (vector)

Greek Symbols:

α = parameter
β = scheduling variable
η = zero dynamics state
ϑ = temperature

* Author to whom correspondence should be addressed. E-mail: karsten@ast.chemietechnik.uni-dortmund.de.

$\lambda(\cdot)$ = vector function
ϱ = density
ϕ = nonlinear coordinate transformation

Essential Indices:

0 = initial value, point on a trajectory
A = reaction educt (cyclopentadiene)
B = desired product (cyclopentenol)
K = coolant
R = reactor, reaction
S = steady-state
δ = reference controller output

1. Introduction

Continuous stirred tank reactors (CSTRs) often exhibit highly nonlinear dynamics, especially when consecutive and side reactions are present. Bifurcations to multiple steady states or periodic limit cycles may appear (Uppal *et al.*, 1974; Doyle *et al.*, 1989). In addition, the mathematical model of the process in most cases is only known with limited accuracy so that the robustness demands on the process control scheme are very high. Classical linear (PID-)feedback often does not achieve satisfactory performance.

In the last decade, significant developments have been made in the field of nonlinear process control. A detailed review of various methods is presented in Bequette (1991). Two important approaches to the design of nonlinear control structures for nonlinear systems are exact feedback linearization (e.g. Kravaris and Kantor, 1990; Henson and Seborg, 1990a) which is based on the differential geometric control theory (Isidori, 1989; Nijmeijer and van der Schaft, 1990) and gain-scheduling techniques based on approximate linearization of the process model and the concept of linearization families (Wang and Rugh, 1987; Rugh, 1991; Lawrence and Rugh, 1995).

The idea of exact feedback linearization is to transform a nonlinear system to a (fully or partly) linear one by means of a coordinate transformation and/or nonlinear feedback. Then linear control techniques can be applied and stability and performance of the resulting control scheme are ensured a priori for the nominal system. However, there are also shortcomings and limitations associated with the feedback linearization approach. One problematic issue of exact feedback linearization is that the complete state of the nonlinear process has to be measured for the implementation of the control structure. In general, this is not possible and an observer must be used for state estimation, which may cause problems because the separation principle does not hold in the nonlinear case. Another problem is due to the fact that an exact model of the nonlinear process is generally not available. Thus robustness cannot be guaranteed in the presence of parameter uncertainty and unmodelled dynamics. This may give rise to steady-state offset or deviations from the specified closed-loop dynamics.

Gain-scheduling is an attempt to apply the well-known linear control methodology directly to the control of nonlinear systems. The main idea is to select a set of constant operating points which covers the intended range of process operation. The linear time-invariant approximation of the process at these points is parametrized and a linear controller for each operating point is designed, this yields a parametrized linear control law. Between the operating points the parameters of the controller are interpolated, or *scheduled*. The approximate linearization of this global nonlinear compensator at each operating point should give the corresponding linear controller which was designed in the first step. Although this often results in a satisfactory control of nonlinear processes, gain-scheduling is inherently local in nature so that global stability and performance statements are rarely possible. Furthermore, the scheduled controller parameters are chosen for constant operating points, which are steady-states of the system, but on a transient trajectory the system operates more or less far from the operating point which corresponds to the actual values of the scheduling variables (Klatt and Engell, 1995a). In Shamma and Athans (1991) Shamma and Athans (1992) the limitations and potential hazards of common gain-scheduling approaches were analyzed in the context of linear parameter-varying systems. They state that if the characteristics of the parameter variations are not addressed correctly in the design process, guaranteed properties of the overall gain-scheduled design cannot be established.

In Klatt and Engell (1995b) we presented gain-scheduling trajectory control (GSTC), a new control scheme which combines exact feedback linearization and gain-scheduling to make use of the advantages and reduce or even overcome some of the disadvantages of both single concepts. In a first step, the nonlinear process model is used to design a nominal nonlinear state feedback controller using exact linearization techniques which specifies a nominal closed-loop trajectory. The on-line simulation of the process model forced by the output of the feedback linearizing controller is used to calculate the nominal state variables for the state feedback controller. Then a nonlinear gain-scheduling reference controller is designed by approximately linearizing the process model around the nominal trajectory generated by the nonlinear controller, whereas fixed operating points are assumed in the standard gain-scheduling approach. The linearization of the trajectory control loop meets the specifications of a robust linear design and the gain-scheduling reference controller forces the process output to follow the desired nominal trajectory even in the case of modeling errors and disturbances.

In Engell and Klatt (1993a) a mathematical model for a complex chemical reaction in a CSTR was introduced as a benchmark problem for nonlinear process control design. This control problem was first presented in abstract form by Kantor (1986) for the reaction mechanism attributed to van de Vusse (1964). As a concrete example, we consider the production of cyclopentenol from cyclopentadiene. The resulting mathematical model is a fourth order nonlinear dynamical system which has unstable zero dynamics in the considered range of operation. The model parameters are only known with limited accuracy and not all states can be measured. The control problem is described in detail in Section 4.

This paper is organized as follows. In Section 2 we present the theoretical background of the proposed approach reviewing the basic concepts of exact feedback linearization and standard gain-scheduling. In Section 3 the concept of gain-scheduling trajectory control is explained. We then treat the concentration control problem for the reaction system with the GSTC approach (Section 4). The performance of the resulting controller is tested and compared to that of a standard gain-scheduling controller and a classical linear controller by means of simulations.

2. Theoretical background

In this paper we focus on open-loop stable, single input/single output analytical nonlinear systems of the form

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)) \\ y(t) &= h(x(t)) \end{aligned} \tag{1}$$

where x is the n-dimensional state vector, u is a scalar manipulated input and y is a scalar output. f denotes a smooth vector field on $\mathbb{R}^{n\times 1}$ and h denotes a smooth vector function on $\mathbb{R}^n$. The Lie derivative of a vector function $\lambda(x)$ along a vector field $g(x)$ is defined as:

$$L_g\lambda = \frac{\partial\lambda(x)}{\partial x}\cdot g(x) = \sum_{i=1}^{n} \frac{\partial\lambda(x)}{\partial x_i} g_i(x).$$

Since the Lie derivative is also a vector function, repeated use of this operation is possible. In terms of this differential operator the relative degree r of the nonlinear system (1) is defined as:

$$r = \min\left\{k : \frac{\partial}{\partial u}[L_f^k h] \neq 0\right\}.$$

2.1. Exact feedback linearization

The design of exact linearizing controllers has been described in numerous papers and textbooks. For the sake of clarity of the expositions following we shortly sketch the basic ideas of input/state and input/output linearization.

Input/state linearization is usually applied to nonlinear systems with state equations which are affine in the input

$$\dot{x} = f(x) + g(x)u.$$

The procedure consists of two steps. First, a smooth nonlinear coordinate transformation (local diffeomorphism)

$$z = \phi(x);\ x = \phi^{-1}(z) \tag{2}$$

is used to transform the nonlinear state equations to the following normal form:

$$\begin{aligned} \dot{z}_1 &= z_2 \\ \dot{z}_2 &= z_3 \\ &\vdots \\ \dot{z}_n &= a(z) + b(z)u \end{aligned} \quad . \tag{3}$$

The coordinate transformation of (2) is the solution of a set of first order partial differential equations (for details see Isidori, 1989; Nijmeijer and van der Schaft, 1990). In the second step, a static nonlinear state feedback law

$$u = \frac{v - a(z)}{b(z)} = \frac{v - L_f^n\phi_1(x)}{L_g L_f^{n-1}\phi_1(x)} \tag{4}$$

compensates the nonlinearities and leads to a linear system which consists of a chain of n integrators. It can be stabilized and controlled by a linear state feedback of the form $v = -k^{\mathrm{T}}z$. Note that only the dynamics from the new input v to the transformed state z is linearized but not the real input/output behaviour of the system. This may lead to unsatisfactory control of the output y. The computation of the state transformation (2) is only possible under certain conditions which can be quite restrictive for systems with more than two states.

Input/output linearization can be applied under less restrictive conditions and provides direct control of the desired process output y. Suppose that the nonlinear system of (1) has a well-defined relative degree r. Thus the first $r-1$ Lie derivatives are independent of u but not $L_f^r h$. By solving the nonlinear algebraic equation

$$[L_f^r h](x, u) = y^{(r)} = v \tag{5}$$

for u, we get the static nonlinear state feedback

$$u = g(x, v) \tag{6}$$

which leads to a linear map from the new input v to the output: $y^{(r)} = v$ (see e.g. Henson and Seborg (1990b) for details). The linear input/output map is a chain of r integrators and one can use linear feedback in order to assign a desired closed-loop behaviour. The nonlinear state feedback (6) linearizes only a r-dimensional part of the nonlinear system of (1). The other part of the system dynamics is rendered unobservable by the linearizing feedback and for zero (or constant) input represents the *zero dynamics* of the system. By analogy to linear systems the nonlinear system is called *minimum-phase* if its zero dynamics is stable. The state feedback (6) will provide internal stability of the closed-loop system only if the system of (1) is minimum-phase.

The combined synthesis of input/output linearizing feedback and linear control for nonlinear systems which are affine in the input was originally presented in Kravaris and Chung (1987) and is known as global linearizing control (GLC). Exact input/output linearization can be applied for a broader class of processes because the necessary conditions are less restrictive. Both exact input/state and input/output linearization can be applied to multivariable systems in a straightforward manner but the computation of the linearizing feedback may become more complicated. The major advantage of exact feedback linearization is that stability and performance of the nominal closed-loop system can be ensured a priori by design.

2.2. Gain-scheduling

The goal of the standard gain-scheduling approach is to compute a nonlinear output control law of the form

$$\begin{aligned} \dot{z}(t) &= l(z(t), e(t), u(t)) \\ u(t) &= k(z(t), e(t)) \end{aligned} \tag{7}$$

such that the linear approximation (Taylor-linearization) of the closed-loop system at each constant operating point has prescribed dynamical characteristics (eigenvalues, gain margin, etc.). Here, z represents the state vector of the controller and $e=w-y$ denotes the difference between a scalar exogenous input w (e.g. a reference signal) and the process output y. Suppose that (1) has a parametrized family of constant operating points

$$OP(\alpha)=\{u_S(\alpha), x_S(\alpha), y_S(\alpha)\}. \tag{8}$$

The corresponding steady-state linearization family of the nonlinear system (1) is

$$\begin{aligned} \Delta\dot{x} &= A(\alpha)\Delta x+B(\alpha)\Delta u \\ \Delta y &= C(\alpha)\Delta x, \end{aligned} \tag{9}$$

where Δ denotes small deviations from the respective operating point (e.g. $\Delta x=x-x_S(\alpha)$) and $A(\alpha)$, $B(\alpha)$ and $C(\alpha)$ are the parametrized Jacobians. For each α, a linear controller for (9) is computed which achieves a specified dynamical behaviour of the linearized closed-loop system. This yields a parametrized linear controller:

$$\begin{aligned} \Delta\dot{z} &= L_1(\alpha)\Delta z+L_2(\alpha)\Delta e \\ \Delta u &= K_1(\alpha)\Delta z+K_2(\alpha)\Delta e. \end{aligned} \tag{10}$$

From this parametrized linear controller a nonlinear controller (7) is constructed so that its linear approximation at a certain operating point in $OP(\alpha)$ yields the linear controller. There is no unique solution of this problem. One possibility is to substitute the parameter α by a suitable measurable exogenous or endogenous variable $\beta(t)$ (*scheduling variable*) of the control loop such that $\beta=\alpha$ holds for each operating point of $OP(\alpha)$. Thus one gets the resulting nonlinear control law:

$$\begin{aligned} \dot{z} &= L_1(\beta)[z-z_S(\beta)]+L_2(\beta)[e-e_S(\beta)] \\ u &= u_S(\beta)+K_1(\beta)[z-z_S(\beta)]+K_2(\beta)[e-e_S(\beta)] \end{aligned} \tag{11}$$

The linearization of this nonlinear controller at each operating point of $OP(\alpha)$ yields the corresponding linear controller from (10) if certain linearization conditions are met. These conditions result from computing the partial derivatives of (11) and comparing them with the corresponding terms of the parametrized linear control law (10) (for details see Wang and Rugh, 1987; Lawrence and Rugh, 1995). The major advantage of this standard gain-scheduling approach is that one can use well-known techniques for linear controller design to compute a nonlinear controller for a nonlinear process in a straightforward way.

3. Gain-scheduling trajectory control

Exact feedback linearization as well as standard gain-scheduling for a family of operating points have certain drawbacks. Robustness against model uncertainties and unknown disturbances is a critical issue in the exact linearization approach, especially for its implementation in real processes. In the GLC approach (Kravaris and Chung, 1987), the error $e=w-y$ is fed to an integral part added to the feedback control law in order to achieve convergence to the reference signal. However, this slows down the closed-loop response considerably even if there is no model mismatch or disturbance and may lead to stability problems and windup effects in the case of manipulated variable constraints.

Gain-scheduling for a family of operating points often leads to nonlinear controllers which show satisfactory performance even for fast transient processes although the design approach is valid only in the vicinity of steady-state operating points. For transient moves the controller parameters are scheduled by a projection onto the corresponding operating points. However, on an arbitrary transient trajectory the linearized dynamics of the gain-scheduling controller are different from their steady-state linearization. For example, consider a simple PI-controller which is parametrized in its steady-state output u_S in the following way:

$$\begin{aligned} \Delta\dot{z} &= K_I(u_S)\Delta e \\ \Delta u &= \Delta z+K_P(u_S)\Delta e. \end{aligned} \tag{12}$$

Because of the integral action we get $e_S=0$ and $u_S=z_S$ for each steady-state operating point. Therefore the controller state $z(t)$ can be chosen as the scheduling variable. This results in the following nonlinear gain-scheduling controller:

$$\begin{aligned} \dot{z} &= K_I(z)e \\ u &= z+K_P(z)e. \end{aligned} \tag{13}$$

Linearization of the nonlinear controller (13) at a steady-state operating point leads to the respective linear controller (12) by construction, but linearizing (13) around an arbitrary transient trajectory ($e_0\neq 0$) yields

$$\Delta\dot{z}=K_I(z_0)\Delta e+\left.\frac{\partial K_I(z)}{\partial z}\right|_{z_0} e_0\Delta z \tag{14}$$

$$\Delta u=\left[1+\left.\frac{\partial K_P(z)}{\partial z}\right|_{z_0} e_0\right]\Delta z+K_P(z_0)\Delta e.$$

Thus the dynamics of the closed-loop system differ more or less from their specifications when not operating in the vicinity of the steady-state points and this may lead to bad performance or even to instability of the overall control scheme for fast transients. Linearization around transient trajectories is much more meaningful to compute gain-scheduled controllers for systems which are not operated only in the neighbourhood of steady-state operating points. Such a transient trajectory has to be generated by suitable nonlinear control techniques.

These considerations motivated the idea of gain-scheduling trajectory control (GSTC) for nonlinear processes described by (1). First, a nominal exact linearizing controller is determined for the process model which generates a desired nominal trajectory. The process model (1) is assumed to be open-loop stable, therefore the states can be reconstructed by using an on-line simulation of the process model (1), forced by the output $\tilde{u}$ of the nominal nonlinear controller, which is a standard technique in nonlinear process control. This part of the controller thus is a nonlinear feedforward compensator for the nominal plant. If the model is perfect and no disturbances are present, it forces the closed-loop dynamics to track a nominal trajectory $(\tilde{u}(t), \tilde{x}(t), \tilde{y}(t))$ and nominal stability and performance are guaranteed. Of course, these assumptions generally do not hold for real processes. Therefore, the tracking error $e=\tilde{y}-y$ is fed to a nonlinear gain-scheduled reference controller whose output u_δ is added to $\tilde{u}$ to force the process output y to converge asymptotically to the nominal trajectory. The resulting control structure is shown in Fig. 1. In contrast to the standard gain-scheduling approach presented in Section 2.2, the reference controller here is developed from the linear approximation around the nominal trajectory generated by the nominal nonlinear control scheme. The transient dynamics is thus correctly represented in the gain-scheduling controller design. The design of the gain-scheduling reference controller is explained in the sequel.

The linear approximation of the nonlinear system (1) at an arbitrary point $(\tilde{x}_0, \tilde{u}_0)$ of the nominal trajectory yields

$$\Delta\dot{x}=\frac{\partial f}{\partial x}(\tilde{x}_0, \tilde{u}_0)\Delta x+\frac{\partial f}{\partial u}(\tilde{x}_0, \tilde{u}_0)\Delta u \qquad (15)$$

$$\Delta y=\frac{\partial h}{\partial x}(\tilde{x}_0)\Delta x$$

where Δ denotes small deviations from the nominal trajectory. The parametrized linear reference controller then is designed for this linear approximation, such that the tracking error e converges to zero with specified dynamics. The reference controller can be written as

$$\begin{aligned}\Delta\dot{z} &= L_1(\alpha)\Delta z+L_2(\alpha)\Delta e\\ \Delta u_\delta &= K_1(\alpha)\Delta z+K_2(\alpha)\Delta e.\end{aligned} \qquad (16)$$

As pointed out in Lawrence and Rugh (1995) for the standard gain-scheduling approach, the existence of an integral error component in the gain-scheduling control loop is essential for the existence of a nonlinear gain-scheduling controller the linear approximation of which gives the corresponding linear controller. Thus the reference controller has to satisfy $z_0=0$ and $e_0=0$ for each point on the nominal trajectory in order to satisfy this condition.

As in the standard approach, the parameter vector α is substituted by an appropriate vector of scheduling variables $\beta(t)$ such that for each point on the nominal trajectory $\beta=\alpha$ holds. This results in the nonlinear gain-scheduling reference controller:

$$\begin{aligned}\dot{z}(t) &= L_1(\beta(t))z(t)+L_2(\beta(t))e(t)\\ u_\delta(t) &= K_1(\beta(t))z(t)+K_2(\beta(t))e(t).\end{aligned} \qquad (17)$$

Linearizing this nonlinear reference controller at an arbitrary point of the nominal trajectory we get

$$\begin{aligned}\Delta\dot{z}=&\left[L_1(\beta_0)+\frac{\partial L_1}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial z}\bigg|_p z_0+\frac{\partial L_2}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial z}\bigg|_p e_0\right]\Delta z\\ &+\left[L_2(\beta_0)+\frac{\partial L_1}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial e}\bigg|_p z_0+\frac{\partial L_2}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial e}\bigg|_p e_0\right]\Delta e\\ =&L_1(\alpha)\Delta z+L_2(\alpha)\Delta e,\end{aligned}$$

$$\begin{aligned}\Delta u_\delta=&\left[K_1(\beta_0)+\frac{\partial K_1}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial z}\bigg|_p z_0+\frac{\partial K_2}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial z}\bigg|_p e_0\right]\Delta z\\ &+\left[K_2(\beta_0)+\frac{\partial K_1}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial e}\bigg|_p z_0+\frac{\partial K_2}{\partial\beta}\bigg|_p\frac{\partial\beta}{\partial e}\bigg|_p e_0\right]\Delta e\\ =&K_1(\alpha)\Delta z+K_2(\alpha)\Delta e.\end{aligned}$$

Thus, the linear approximation of the trajectory control loop around an arbitrary point of the nominal trajectory exhibits the dynamics specified by the linear controller design. The actual value of the manipulated variable $u(t)$ is the sum of the output $\tilde{u}$ of the nominal linearizing controller and the output u_δ of the gain-scheduling reference controller (17)

$$u(t)=\tilde{u}(t)+u_\delta(t). \qquad (18)$$

Note that the linear approximation of the nonlinear reference control loop around the nominal trajectory gives a time-varying linear system but the design of the reference controller is based on a family of linear systems with "frozen coefficients". The stability of the overall nonlinear control scheme thus can be guaranteed in the first approximation for a neighbourhood of the nominal trajectory only if

1. The overall control scheme is properly initialized.
2. The dynamics of the nominal trajectory is sufficiently slow compared with the dynamics of the reference control loop in order to justify the time-invariant design of the gain-scheduling controller.

Condition 2 directly corresponds to the slow variation assumption for the scheduling parameters of common gain-scheduling controllers (Lawrence and Rugh, 1990; Shamma and Athans, 1990). It is based on the fundamental results for time-varying linear systems with slowly varying parameters presented in Desoer (1969) which, together with Lyapunov's linearization method for non-autonomous systems (Slotine and Li (1991)), guarantee stability of the nonlinear control loop provided that the parameter variations are sufficiently slow compared to the specified closed-loop dynamics. Within the GSTC framework, the relation between the nominal dynamics and the reference control dynamics can be directly addressed by the designer in a transparent way. Unfortunately, no general quantitative measure can be established to guarantee global stability directly within the design step. However, for chemical processes the nominal transient dynamics generally are specified

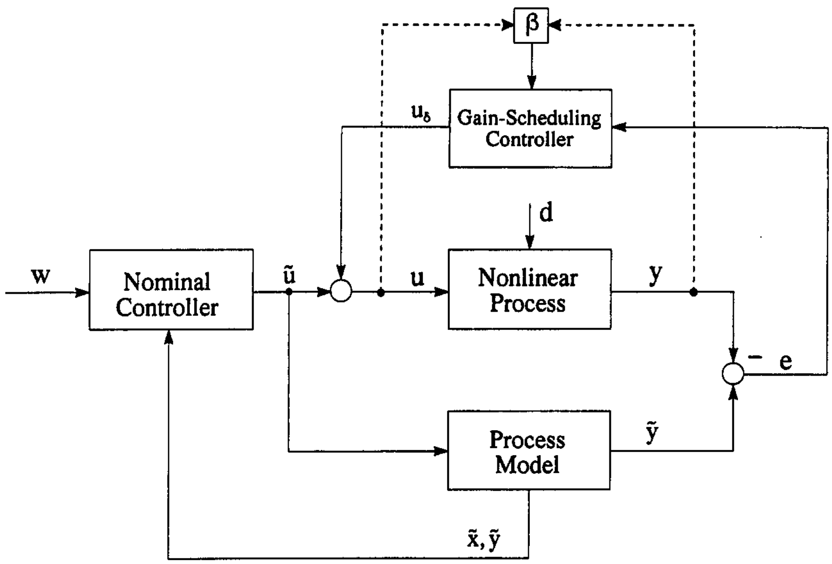

Fig. 1. Gain-scheduling trajectory control (overall structure).

rather slow so that in many practically relevant cases the slow variation assumption will hold.

Manipulated variable constraints can be treated within the GSTC approach in a very straightforward manner. The output of the nominal feedforward control $\tilde{u}$ should be restricted to a certain fraction of the overall range of the manipulated variable in order to provide a sufficiently large range for the reference controller output at any time. Windup effects then are more unlikely than in the GLC framework where the full tracking error is fed to the integral part and not only the error between the nominal and the actual trajectory. Should windup problems arise for gain-scheduling trajectory control, any standard technique of linear anti-reset windup compensation can be employed for the reference controller. This is in our opinion an advantage of the GSCT approach because, as far to our knowledge, within the common exact feedback linearizing control framework this is possible only for input/output linearizing control but not for state linearizing control in a straightforward way.

4. Design example

4.1. Control problem

We consider the production of cyclopentenol (B) from cyclopentadiene (A) by acid-catalysed electrophilic addition of water in dilute solution as presented in Engell and Klatt (1993a). Due to the strong reactivity of both the educt and the product, dicyclopentadiene (D) is produced by the Diels–Alder reaction as a side product, and cyclopentanediol (C) as a consecutive product by addition of another water molecule. The complete reaction scheme is

$$\underset{\text{Cyclopentadiene(A)}}{\mathbf{C_5H_6}} \xrightarrow{+H_2O/H^{\oplus}} \underset{\textit{Cyclopentenol (B)}}{C_5H_7OH}$$

$$\xrightarrow{+H_2O/H^{\oplus}} \underset{\textit{Cyclopentanediol (C)}}{C_5H_8(OH)_2}$$

$$\underset{\textit{Cyclopentadiene (A)}}{2\,C_5H_6} \longrightarrow \underset{\textit{Dicyclopentadiene (D)}}{C_{10}H_{12}}$$

Fig. 2 schematically shows the CSTR. The reactor inflow contains only the educt A in low concentration c_{A0}. Assuming constant density and an ideal residence time distribution within the reactor, the balance equations

$$\frac{dc_A}{dt} = \frac{\dot{V}}{V_R}(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2 \tag{19}$$

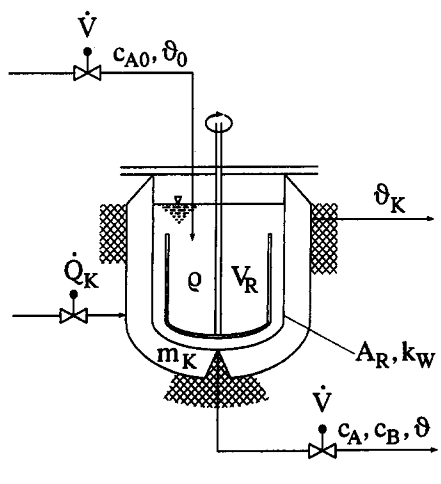

Fig. 2. Continuous stirred tank reactor.

$$\frac{dc_B}{dt} = -\frac{\dot V}{V_R}c_B + k_1 c_A - k_2 c_B \tag{20}$$

$$\frac{d\vartheta}{dt} = \frac{\dot V}{V_R}(\vartheta_0 - \vartheta) + \frac{k_W A_R}{\varrho C_p V_R}(\vartheta_K - \vartheta) - \frac{k_1 c_A \Delta H_R^{AB} + k_2 c_B \Delta H_R^{BC} + k_3 c_A^2 \Delta H_R^{AD}}{\varrho C_p} \tag{21}$$

$$\frac{d\vartheta_K}{dt} = \frac{1}{m_K C_{pK}}[\dot Q_K + k_W A_R(\vartheta - \vartheta_K)] \tag{22}$$

constitute a fourth order nonlinear system. Here c_A and c_B represent the concentrations of the educt A and the desired product B within the reactor, ϑ denotes the reactor temperature and ϑ_K the coolant temperature. The rate coefficients k_1–k_3 depend exponentially on the reactor temperature ϑ via Arrhenius' law

$$k_i(\vartheta) = k_{0i} \cdot \exp\left(\frac{-E_{Ai}}{R(\vartheta + 273.15)}\right). \tag{23}$$

For the reaction system at hand $k_1 = k_2$. The control of the product concentration c_B is specified such that any value in the range $0.7\ \text{mol/l} \le c_B \le 0.95\ \text{mol/l}$ can be attained without steady-state error for all values of the unmeasured inflow concentration, which is nominally $c_{A0} = 5.1$ mol/l but can vary in the range $4.5\ \text{mol/l} \le c_{A0} \le 5.7$ mol/l. The reactor temperature ϑ and the product concentration c_B are assumed to be available from measurements, but not c_A and ϑ_K. The inflow normalized by the reactor volume, F, and the amount of heat removed by the coolant, $\dot Q_K$, are available as manipulated variables subject to the following constraints:

$$5h^{-1} \le F = \frac{\dot V}{V_R} \le 35h^{-1},\ -8500\frac{kJ}{h} \le \dot Q_K \le 0\frac{kJ}{h}.$$

The values of the model parameters and their uncertainties as well as the steady-state values of the main operating point of the reactor are given in Table 1. A detailed discussion of the chemical background of the process model is given in Klatt *et al.* (1995). Different control problems for this reaction system in a CSTR were considered, e.g. concentration control for a fixed amount of the cooling rate (Engell and Klatt, 1993b) or control for maximal yield (Chen *et al.*, 1995). For the problem described above, a standard gain-scheduling controller design was presented in Engell and Klatt (1993a) which achieved satisfactory control and was superior to a linear PI-controller with fixed parameters.

Table 1. Model parameters and main operating point

Model parameters	
	$V_R = 10.01$
	$m_K = 5.0$ kg
$k_{0_{1,2}} = (1.287 \pm 0.04)\ 10^{12}\ \text{h}^{-1}$	$\vartheta_0 = 130.0$°C
$k_{0_3} = (9.043 \pm 0.27)\ 10^9$ l/molA h	$k_W = 4032 \pm 120$ kJ/h m^2 K
$E_{A_{1,2}}/R = 9758.3\ \text{K} \pm \Delta$	**Main operating point**
$E_{A_3}/R = 8560.0\ \text{K} \pm \Delta$	$c_A\vert_S = 1.235$ mol/l
$\Delta H_R^{AB} = 4.2 \pm 2.36$ kJ/molA	$c_B\vert_S = 0.9$ mol/l
$\Delta H_R^{BC} = -11.0 \pm 1.92$ kJ/molB	$\vartheta\vert_S = 134.14$°C
$\Delta H_R^{AD} = -41.85 \pm 1.41$ kJ/molA	$\vartheta_K\vert_S = 128.95$°C
$\varrho = 0.9342 \pm 4 \cdot 10^{-4}$ kg/l	$F\vert_S = 18.83\ \text{h}^{-1}$
$C_p = 3.01 \pm 0.04$ kJ/kg K	$\dot Q_K\vert_S = -4495.7$ kJ/h
$C_{pK} = 2.0 \pm 0.05$ kJ kg^{-1} K^{-1}	$c_{A0}\vert_S = 5.1$ mol/l
$A_R = 0.215$ m^2	

4.2. System reduction and analysis

The complete process model of eqns. (19)(20)(21)(22) is a fourth order analytical nonlinear system which is open-loop stable and affine in the input variables. Eqns. (19)(20) describe the chemical part of the system which is strongly influenced by the reactor temperature. A steady-state analysis of the process shows that the concentration control problem is solvable if the reactor temperature ϑ is kept in a narrow range around its value at the main operating point $\vartheta|_S = 134.14$°C. Using frequency domain design methods for the linearized heat transfer model of the process and taking its variations over the range of operation into account, a second order linear controller

$$G_\vartheta(s) = 986 \cdot \frac{(s + 16.4)(s + 77.8)}{s(s + 125.2)} \tag{24}$$

was designed to assure fast temperature control by manipulating the cooling rate $\dot Q_K$. Under the assumption of constant temperature the relevant dynamics can be reduced to the chemical part of the system, (19)(20) which is a single input/single output nonlinear system of the form

$$\dot x(t) = f(x(t)) + g(x(t))u(t) \tag{25}$$
$$y(t) = h(x(t)),$$

where $x_1 = c_A$, $x_2 = y = c_B$, $u = F$ and

$$f(x) = \begin{bmatrix} -k_1 c_A - k_3 c_A^2 \\ k_1(c_A - c_B) \end{bmatrix},\ g(x) = \begin{bmatrix} c_{A0} - c_A \\ -c_B \end{bmatrix},\ h(x) = c_B.$$

The relative degree between the output $y = c_B$ and the input $u = F$ is $r = 1$, the order of the reduced system is $n = 2$. Fig. 3 shows the steady-state behaviour of the system for constant reactor temperature $\vartheta = \vartheta_S$ within the given range of the manipulated variable. If the range of the manipulated variable F would be extended, at $F^* = k_1$ the reactor reaches the peak production rate of B and shows an input multiplicity for larger values of the manipulated variable. This can be directly related to a sign change of the steady-state gain and thus to a sign change of the transfer function zero of the linearized process (Sistu and Bequette, 1995). At maximum yield the steady-state gain is zero so that the process is neither invertible nor integral controllable at this point. The zero-dynamics of the reduced reactor model is described by

$$\dot\eta = -\left(1 + \frac{k_3 c_B}{k_1}\right) \cdot \eta^2 + \left(\frac{k_1 c_{A0}}{c_B} - 2k_1 - 2k_3 c_B\right) \cdot \eta - k_1^2 - k_1 k_3 c_B \tag{26}$$

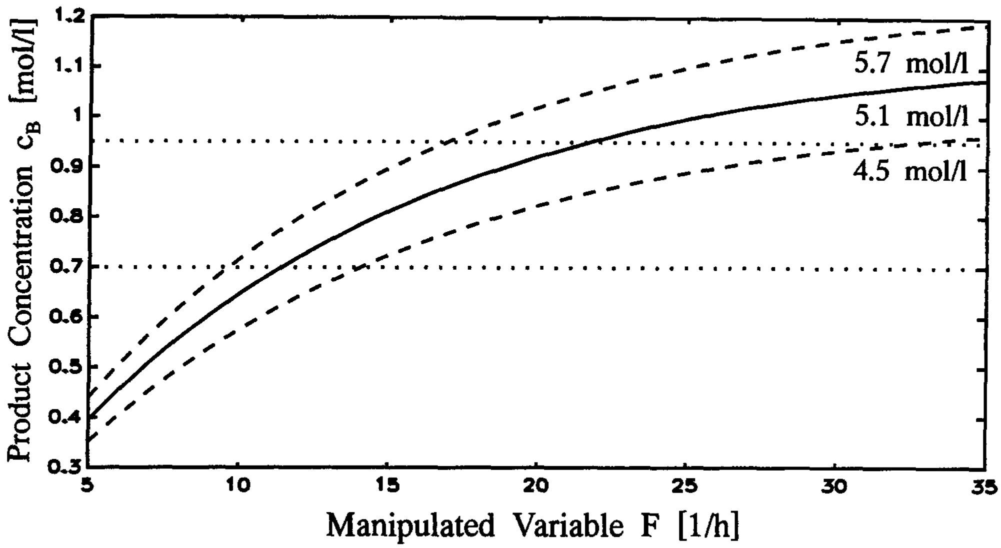

Fig. 3. Steady-state behaviour of the system for $\vartheta=134.14$°C.

and the eigenvalue of its linearization gives the value of the transfer function zero. Within the range of operation considered here, the system is restricted to the non-minimum-phase region i.e. its zero dynamics is unstable and the singular point cannot be attained.

4.3. Concentration control

The unstable zero dynamics of the process makes standard input/output linearization or GLC impossible. Wright and Kravaris (1992) propose an extension of the standard GLC scheme for non-minimum-phase processes which is based on the on-line prediction of a statically equivalent minimum phase output. This auxiliary output then is controlled by standard GLC. However, the choice of the auxiliary output is arbitrary and the performance characteristics strongly depend on this choice. We therefore generate the nominal trajectory by exact input/state linearization. Following the exposition in Schlacher and Kugi (1993) the smooth coordinate transformation

$$z=\begin{bmatrix}\lambda(x)\\ L_f\lambda(x)\end{bmatrix} \tag{27}$$

with

$$\lambda(x)=\frac{c_B}{c_{A0}-c_A} \tag{28}$$

transforms the reduced system to

$$\begin{aligned}\dot{z}_1&=z_2\\ \dot{z}_2&=L_f^2\lambda(x)+L_gL_f\lambda(x)\cdot u,\end{aligned} \tag{29}$$

where $u=F$. The nonlinear state feedback

$$\tilde{F}=\frac{v-L_f^2\lambda(x)-c_0\lambda(x)-c_1L_f\lambda(x)}{L_gL_f\lambda(x)} \tag{30}$$

yields the system

$$\begin{bmatrix}\dot{z}_1\\ \dot{z}_2\end{bmatrix}=\begin{bmatrix}0 & 1\\ -c_0 & -c_1\end{bmatrix}\begin{bmatrix}z_1\\ z_2\end{bmatrix}+\begin{bmatrix}0\\ 1\end{bmatrix}v \tag{31}$$

with linear dynamics from the auxiliary input v to the transformed state z. To achieve convergence of the output c_B to a specified set point value w_B, the auxiliary input v must be

$$v=\frac{c_0w_B}{c_{A0}-\dfrac{k_1+\sqrt{k_1^2c_{A0}^2-4k_1c_{A0}w_B(k_1+k_3w_B)}}{2(k_1+k_3w_B)}}. \tag{32}$$

Considering the non-minimum-phase behaviour of the process and the manipulated variable constraints, which restrict the attainable bandwidth of the closed-loop system, the free parameters are chosen as $c_0=3125$ and $c_1=100$ placing the eigenvalues of (31) at $\mu_{1,2}=-50\pm25j$. For the nominal case this gives a transient response to set point changes of the concentration control loop which converges sufficiently fast to w_B. The on-line simulation of the reduced model is used as an open-loop observer to calculate the unmeasured state $\tilde{c}_A$ and the process output $\tilde{c}_B$ along the nominal trajectory which are necessary to compute $\tilde{F}$ from (30):

$$\begin{aligned}\dot{\tilde{c}}_A&=\tilde{F}(c_{A0}-\tilde{c}_A)-k_1\tilde{c}_A-k_3\tilde{c}_A^2\\ \dot{\tilde{c}}_B&=-\tilde{F}\tilde{c}_B+k_1\tilde{c}_A-k_2\tilde{c}_B,\end{aligned} \tag{33}$$

where the model parameters and the inflow concentration are at their nominal values. Note that only the relation of v and z is exactly linearized but the dynamics from the reference input w_B to the output c_B is still nonlinear and contains the unstable zero dynamics of the process which must not be cancelled in order to preserve internal stability of the control loop.

To achieve robustness against model uncertainties and inflow disturbances and convergence to the nominal trajectory, the gain-scheduling reference controller is computed by linearizing the reduced process model of (25) around the nominal trajectory $(\tilde{x}, \tilde{u})$ generated by the nominal nonlinear control scheme. The linear approximation of (25) results in a parametrized linear transfer function

$$G_P(s) = \frac{\tilde{c}_B(n-s)}{(s+p_1)(s+p_2)}, \qquad (34)$$

where

$$p_1 = \tilde{F} + k_1,\; p_2 = \tilde{F} + k_1 + 2k_3\tilde{c}_A,$$

$$n = \frac{k_1}{\tilde{c}_B}(c_{A0} - \tilde{c}_A - \tilde{c}_B) - \tilde{F} - 2k_3\tilde{c}_A.$$

A parametrized linear PI-controller is designed such that the tracking error $e = \tilde{c}_B - c_B$ converges to zero with specified dynamics for the linear approximation around the nominal trajectory:

$$\Delta\dot{x}_R = K_I(\alpha)\Delta e \qquad (35)$$
$$\Delta F_\delta = \Delta x_R + K_P(\alpha)\Delta e.$$

As the zero dynamics of the system is unstable, the zero in (34) is in the right half-plane. This right half-plane zero limits the attainable bandwidth of the linearized reference control loop to one third of the value of the zero, which varies considerably within the operational range. If one tries to make the bandwidth larger, the sensitivity of the closed-loop system will be very high for certain frequencies, and robustness can no longer be assured (Engell, 1988). It is therefore advantageous if the reference controller provides a variable bandwidth depending on the value of the right half-plane (rhp) zero and hence the actual state of the process.

We used a frequency-domain design method for non-minimum-phase plants from Engell *et al.* (1982). Starting from time domain specifications such as overshoot, undershoot and rise time, certain critical parameters of the open-loop frequency response are determined, and this frequency response then is shaped such that these values are achieved. In the non-minimum-phase situation, the transient behaviour can be shaped best by controlling the phase of the open-loop system at the frequency where the gain equals -3dB. We first compensated the slower pole $-p_1$ and then determined the controller gain for a set of extremal trajectories such that the phase at gain crossover was not below $-145°$. Interpolating these values by a first order polynomial yielded

$$K_P(\alpha) = 0.9\alpha + 12,\; K_I(\alpha) = (k_1 + \alpha)K_P,$$

where $\alpha = \tilde{F}$. Because $e = 0$ and $x_R = 0$ on the nominal trajectory,

$$\beta(t) = \tilde{F}(t) + x_R(t)$$

can be chosen as the scheduling variable. This results in the overall nonlinear gain-scheduling reference controller

$$\dot{x}_R = (k_1 + \tilde{F} + x_R)(0.9(\tilde{F} + x_R) + 12)e \qquad (36)$$
$$F_\delta = x_R + (0.9(\tilde{F} + x_R) + 12)e,$$

The linearization of (36) at an arbitrary point of the nominal trajectory yields the respective desired linear controller. The actual value of the manipulated variable $F(t)$ is the sum of the output of the nominal nonlinear feedback controller and the gain-scheduling reference controller according to (18): $F(t) = \tilde{F}(t) + F_\delta(t)$. The simulation results shown below illustrate the excellent performance of the resulting concentration control scheme.

4.4. *Simulation results*

The control structure (fast linear temperature control and GSTC to control the product concentration c_B) was tested by simulating sequences of step changes of the set point starting from the main operating point $w_B = 0.9$ mol/l to the extremal values of the operating range $w_B = 0.7$ mol/l and $w_B = 0.95$ mol/l. Fig. 4 shows the response of the product concentration c_B to the set point step sequence in the nominal case (nominal model parameters and inflow concentration) where the performance is compared to those of the standard gain-scheduling controller and the linear controller from Engell and Klatt (1993a). The standard gain-scheduling controller was based on a family of constant operating points and the linear controller was designed for the main operating point. In all cases the same frequency-domain design method was applied to compute the linear controllers. The output c_B of the GSTC loop (solid line) exactly tracks the desired nominal trajectory which is generated by the nominal nonlinear controller and the output of the gain-scheduling reference controller F_δ is zero here.

An analysis of the model dynamics and uncertainties revealed that the inflow variations have a major influence on the process dynamics. Fig. 5 shows the response of the product concentration c_B for extremal values of the inflow concentration c_{A0} compared with the nominal case. The output of the gain-scheduling reference controller F_δ rejects the disturbance and leads to good tracking of the nominal trajectory. The temperature variations of the controlled reactor are very small irrespective of setpoint changes and disturbances which justifies the assumption of approximately constant temperature.

The uncertainties of the model parameters within the bounds given in Table 1 lead to relatively small deviations from the nominal trajectory in all cases. However, the uncertainty of E_A, which is not explicitly given in the problem formulation, may strongly influence the dynamical behaviour of the process. For example, a deviation $\Delta E_{1,2} = 2\%$ from its nominal value increases the rate coefficients $k_{1,2}$ by about 40%, thus leading to a significant change of the process dynamics. Fig. 6 shows that also in this extreme case, the GSTC structure results in stable concentration control with a performance which is again superior to that of standard gain-scheduling or linear control.

5. Conclusions

We have presented the application of gain-scheduling trajectory control to the control of a continuous stirred

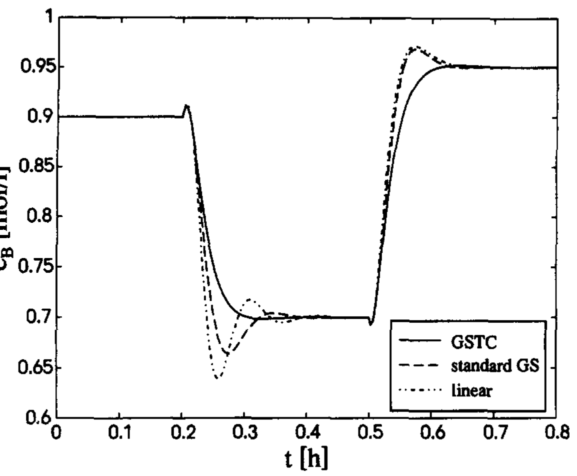

Fig. 4. Set point step sequence (nominal case).

tank reactor with non-minimum-phase dynamics. An exact state linearizing controller is combined with a simulation of the nonlinear process model to generate a desired nominal trajectory and to ensure overall stability and performance in the case of no model mismatch and disturbances. The gain-scheduling reference controller is used to achieve robustness of the overall nonlinear control structure against model uncertainties and disturbances. It only acts for non-vanishing reference error and forces the process output to track the desired nominal trajectory if the controller is properly initialized and the specified nominal dynamics are sufficiently slow compared to the dynamics of the reference control loop. Gain-scheduling trajectory control is a local design approach. However, the transient dynamics are correctly represented in the gain-scheduling controller design, which is a considerable advantage compared to common gain-scheduling. Although global stability cannot be proven a priori, the proposed design approach makes it possible for the designer to consider stability and robustness issues using methods from linear control theory in the design of the gain-scheduling controller.

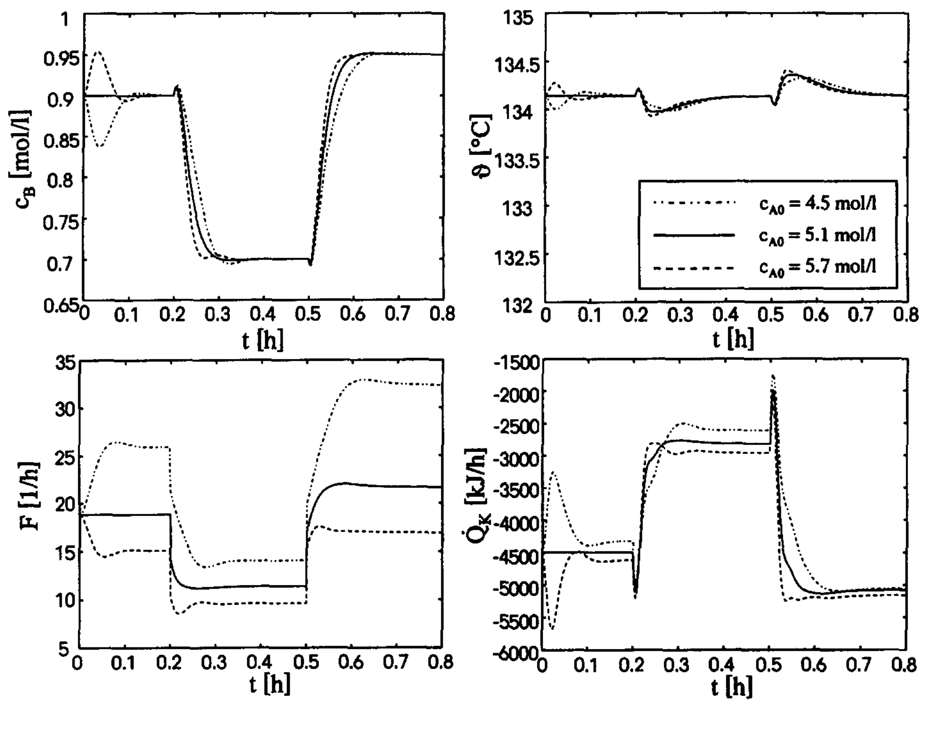

Fig. 5. Set point step sequence for different values of the inflow concentration c_{A0} (GSTC).

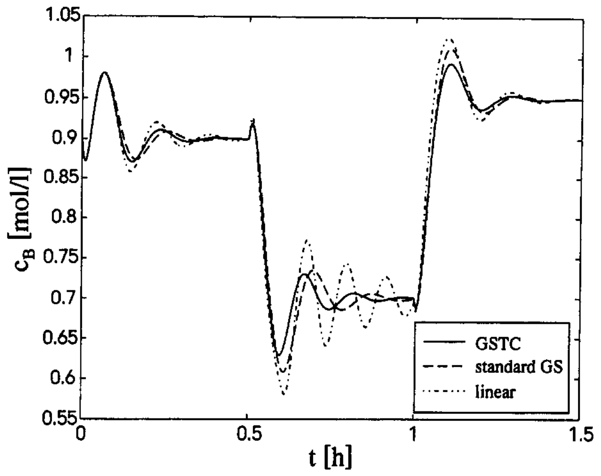

Fig. 6. Set point step sequence, $\Delta E_{A_{1,2}}=+2\%$.

The resulting control structure has some similarities with asymptotically exact linearization (Gilles *et al.*, 1994) and adaptive feedback linearization (Kabuli and Kosut, 1992) but here a gain-scheduling controller is used to compensate for model mismatch and disturbances. The extension of the presented approach to multivariable systems is straightforward because both exact feedback linearization and gain-scheduling can be applied to multivariable systems (Wang and Rugh, 1987; Isidori, 1989). Moreover, alternative techniques to generate the nominal trajectory such as nonlinear optimization are possible for systems where exact feedback linearization is difficult to apply or not successful.

For the CSTR control problem the proposed control scheme achieves good set point tracking and disturbance rejection in the presented large parameter uncertainties. The GSTC scheme performs significantly better than a standard gain-scheduling controller or a linear controller. Of course, other model-based nonlinear control approaches could also be used and may lead to comparable or better results. The use of standard GLC control is not possible here because of the unstable zero-dynamics of the process. The design of a state feedback linearizing controller that employs integral action with some kind of anti-reset windup compensation also does not seem promising. This is due to the fact, that only the relation between the auxiliary input v and the transformed state z can be linearized and an error term for the transformed state z due to modelling errors and/or disturbances can neither be established nor be measured. The simple addition of a integral term to the state linearizing feedback was reported in Schlacher and Kugi (1993) for the same process. This resulted in a severe performance deterioration compared to the specified nominal dynamics. The GLC structure with non-minimum-phase compensation could be an interesting alternative for the design problem at hand. Wright and Kravaris (1992) also illustrated their results for a van de Vusse reaction scheme, but their reaction rates are rather different so that their results cannot directly be compared with those shown here. It is plausible that the fact that in GSTC, in contrast to GLC, the integral part only acts on the error between the real trajectory and the reference trajectory is an advantage. This however remains to be explored in detail.

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