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NONLINEAR PREDICTIVE CONTROL OF A BENCHMARK CSTR

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Keywords: Benchmark problem, reactor control, nonlinear control, nonlinear model predictive control

Abstract

The intention of this paper is twofold: First, we want to propose a benchmark problem for nonlinear control system design. This problem involves control of a highly nonlinear chemical reactor that exhibits interesting properties, like a change of steady state gain at the main operating point. Secondly, we give a "reference" solution to this benchmark problem based on a nonlinear model predictive control scheme. Despite the difficulty of the problem this controller achieves stability and good performance to setpoint changes and disturbances in a robust way.

1 Introduction

For economic and chemical engineering reasons, it is often desirable to operate chemical reactors such that the production of a wanted product is maximized. For this, a reactor is considered at an operating point where optimal yield with respect to a desired product is achieved. However, operation at this point can considerably complicate the design of control system, and is then the motivation to propose a benchmark problem for nonlinear control system design, which is based on a specific continuous stirred tank reactor (CSTR) that is described in [1, 4]. The benchmark problem that will be described in Sections 2 and 3 is characterized by a number of interesting features:

- The steady state gain changes its sign at the operating point. Thus, linear controllers (with integral action) will not be able to stabilize this reactor and accomplish satisfying performance [6].
- The zero dynamics changes its stability property at this operating point. Therefore, the qualitative behavior of the CSTR differs considerably for different setpoints and disturbances.
- The problem has a "real world" background.
- A complete set of performance objectives including an uncertainty description is given.

A more detailed discussion on the reasons and implications of the first two points can be found in [5].

Furthermore, we propose a solution to the control of this benchmark problem based on on-line optimization in a receding horizon manner. Such control schemes are usually termed nonlinear model predictive controllers [9].

The paper is structured as follows: In Section 2 a complete description of the reactor is given including the mathematical model with parameters. Section 3 briefly describes the specific operating point and the control problem. We suggest a multi-input and a single-input control problem. Finally, we propose a "reference" solution to those control problems in Section 4 where we explain the structure and parameters of the controller used.

2 Description of the CSTR [4]

The reactor under consideration is a continuous stirred tank reactor with a cooling jacket in which cyclopentenol is produced from cyclopentadiene by acid-catalyzed electrophylic hydration in aqueous solution. This reactor was first described in [4] and is adopted unchanged in this paper. The reaction scheme and parameters are derived by theoretical modeling based on physical properties described in the literature for a real process. Details on the derivation of the chemical parameters and the physico-chemical background can also be found in [4].

Fig. 1 shows a schematic diagram of the reactor. The main reaction is given by the transformation of cyclopentadiene (substance A) to the product cyclopentenol (substance B). The initial reactant cyclopentadiene also reacts in an unwanted parallel reaction to the by-product dicyclopentadiene (substance D). Furthermore, cyclopentanediol (substance C) is formed in an unwanted consecutive reaction from the product cyclopentenol. This, so-called *van der Vusse* reaction, is described by the following reaction scheme:

$$\begin{array}{ccccc} A & \xrightarrow{k_1} & B & \xrightarrow{k_2} & C \\ 2A & \xrightarrow{k_3} & D\ . & & \end{array} \qquad (1)$$

The flow $\dot{V}$ fed to the reactor contains only cyclopentadiene (substance A) with concentration c_{A0} and temper-

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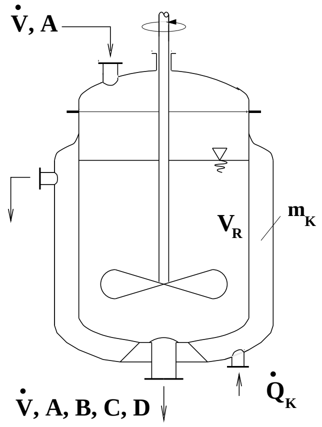

Figure 1: Schematic representation of the CSTR

ature ϑ_0. The heat removal $\dot{Q}_K$ can be withdrawn from the coolant by an external heat exchanger.

The dynamics of the reactor can be described by the following nonlinear differential equations that are derived from component balances for substances A and B and from energy balances for the reactor and cooling jacket:

$$
\begin{aligned}
\dot{c}_A &= \frac{\dot{V}}{V_R}(c_{A0} - c_A) - k_1(\vartheta)c_A - k_3(\vartheta){c_A}^2 && \text{(2a)}\\
\dot{c}_B &= -\frac{\dot{V}}{V_R}c_B + k_1(\vartheta)\, c_A - k_2(\vartheta)c_B && \text{(2b)}\\
\dot{\vartheta} &= \frac{\dot{V}}{V_R}(\vartheta_0 - \vartheta) - \frac{1}{\rho C_p}\Big(k_1(\vartheta)c_A\Delta H_{R_{AB}} \\
&\quad + k_2(\vartheta)c_B\Delta H_{R_{BC}} + k_3(\vartheta){c_A}^2\Delta H_{R_{AD}}\Big) \\
&\quad + \frac{k_w A_R}{\rho C_p V_R}(\vartheta_K - \vartheta) && \text{(2c)}\\
\dot{\vartheta}_K &= \frac{1}{m_K C_{PK}}\Big(\dot{Q}_K + k_w A_R(\vartheta - \vartheta_K)\Big)\,, && \text{(2d)}\\
& \qquad c_A \geq 0,\; c_B \geq 0\,.
\end{aligned}
$$

The concentrations of substances A and B are c_A and c_B respectively. The temperature in the reactor is denoted by ϑ, while the temperature in the cooling jacket is given by ϑ_K. The reaction velocities k_i are assumed to depend on the temperature via the Arrhenius law

$$
k_i(\vartheta) \;=\; k_{i0}\cdot\exp\left(\frac{E_i}{\vartheta/^oC + 273.15}\right),\; i = 1, 2, 3\,. \quad \text{(2e)}
$$

Values for the physical and chemical parameters in equations (2a)–(2e) are given in Table 1. It should be noted that most parameters are only known within bounds.

3 Control problem at the point of optimal yield

The reactor is operated at a point where optimal yield with respect to the product B is achieved (within a tolerance of $0.02\frac{mol}{l}$). The yield Φ of product B is defined as the ratio between product concentration c_B and concentration of initial reactant c_{A0} in the feed[1]

$$
\Phi = \frac{c_B|_S}{c_{A0}}\,, \tag{3}
$$

and is a measure for the effectiveness of the production. This optimal operating point is found by optimization of the steady state yield with respect to the design variables steady state feed flow $\frac{\dot{V}}{V_R}|_S$, steady state heat removal $\dot{Q}_K|_S$ and feed temperature $\vartheta_0|_S$. It is described by the following values:

$$
\begin{aligned}
c_{A0}|_S &= 5.10\,\frac{mol}{l} & c_A|_S &= 2.14\,\frac{mol}{l} \\
\vartheta_0|_S &= 104.9\,^oC & c_B|_S &= 1.09\,\frac{mol}{l} \\
\left.\frac{\dot{V}}{V_R}\right|_S &= 14.19\,h^{-1} & \vartheta|_S &= 114.2\,^oC \\
\left.\dot{Q}_K\right|_S &= -1113.5\,\frac{kJ}{h} & \vartheta_K|_S &= 112.9\,^oC\,.
\end{aligned} \tag{4}
$$

The operating point considered here is different from the one suggested in [4]: The yield is increased by about 20%; the selectivity[2] with respect to initial reactant A is also increased by more than 50%; and in addition, the energy consumption is considerably reduced. Thus, this operating point of optimal yield is very desirable for economic reasons.

By use of control we want to guarantee the production of cyclopentenol with desired purity $c_{B\,|s}$ despite variations in the feed temperature ϑ_0. We distinguish two control problems: A multi-input problem and a (more demanding) single-input problem.

3.1 Multi-input control problem

For the multi-input control problem we suggest that the flow rate normalized by the reactor volume $\frac{\dot{V}}{V_R}$ and the heat removal $\dot{Q}_K$ are used as manipulated variables. We assume that the product concentration c_B and the reactor temperature ϑ can be measured. However, only the concentration c_B is of interest to be controlled. We want to be able to produce substance B with concentration c_B in the following range (setpoint):

$$
0.8\,\frac{mol}{l} \quad\leq\quad c_{B\,|s} \quad\leq\quad 1.09\,\frac{mol}{l}\,.
$$

The feed of the reactor is assumed to come from an upstream unit. Therefore, the feed temperature ϑ_0 is assumed to vary between

$$
100\,^oC \quad\leq\quad \vartheta_0 \quad\leq\quad 115\,^oC
$$

and is considered as unmeasurable disturbance.

[1] By $|_S$ we denote the steady state value of a variable.
[2] The selectivity S is defined as $S = \frac{c_B}{c_{A0} - c_A}$.

Table 1: Physico-chemical parameters for the CSTR

Name of parameter	Symbol	Value of parameter
collision factor for reaction k_1	k_{10}	$(1.287 \pm 0.04) \cdot 10^{12}\ h^{-1}$
collision factor for reaction k_2	k_{20}	$(1.287 \pm 0.04) \cdot 10^{12}\ h^{-1}$
collision factor for reaction k_3	k_{30}	$(9.043 \pm 0.27) \cdot 10^{9}\ \frac{1}{mol\,A \cdot h}$
activation energy for reaction k_1	E_1	$-9758.3K$
activation energy for reaction k_2	E_2	$-9758.3K$
activation energy for reaction k_3	E_3	$-8560K$
enthalpies of reaction k_1	$\Delta H_{R_{AB}}$	$(4.2 \pm 2.36)\ \frac{kJ}{mol\,A}$
enthalpies of reaction k_2	$\Delta H_{R_{BC}}$	$-(11.0 \pm 1.92)\ \frac{kJ}{mol\,B}$
enthalpies of reaction k_3	$\Delta H_{R_{AD}}$	$-(41.85 \pm 1.41)\ \frac{kJ}{mol\,A}$
density	ρ	$(0.9342 \pm 4.0 \cdot 10^{-4})\ \frac{kg}{l}$
heat capacity	C_p	$(3.01 \pm 0.04)\ \frac{kJ}{kg \cdot K}$
heat transfer coefficient for cooling jacket	k_w	$(4032 \pm 120)\ \frac{kJ}{h \cdot m^2 \cdot K}$
surface of cooling jacket	A_R	$0.215\ m^2$
reactor volume	V_R	$0.01\ m^3$
coolant mass	m_K	$5.0\,kg$
heat capacity of coolant	C_{PK}	$(2.0 \pm 0.05)\ \frac{kJ}{kg \cdot K}$

Table 2: Two extreme cases for parameter uncertainty

Parameter	Case 1	Case 2
$k_{10}\ [h^{-1}]$	$1.327 \cdot 10^{12}$	$1.247 \cdot 10^{12}$
$k_{20}\ [h^{-1}]$	$1.327 \cdot 10^{12}$	$1.247 \cdot 10^{12}$
$k_{30}\ [\frac{1}{mol\,A \cdot h}]$	$8.773 \cdot 10^{9}$	$9.313 \cdot 10^{9}$
$\Delta H_{R_{AB}}\ [\frac{kJ}{mol\,B}]$	6.56	1.84
$\Delta H_{R_{BC}}\ [\frac{kJ}{mol\,A}]$	-9.08	-12.92
$\Delta H_{R_{AD}}\ [\frac{kJ}{mol\,A}]$	-40.44	-43.26

The controller has to compensate the effects of changes in the setpoint value $c_{B\,|s}$ and of disturbance in ϑ_0 simultaneously. The manipulated variables are constrained by

$$
\begin{aligned}
3\,h^{-1} \quad &\leq \quad \frac{\dot{V}}{V_R} \quad \leq \quad 35\,h^{-1} \\
-9000\,\frac{kJ}{h} \quad &\leq \quad \dot{Q}_K \quad \leq \quad 0\,\frac{kJ}{h}\,.
\end{aligned}
$$

In order to test the performance of the controller, we suggest step changes in the setpoint and feed temperature from their maximal value to the minimal value and back. The maximal steady state offset should not exceed $0.02\frac{mol}{l}$ (control tolerance). Robustness can be tested by considering the two parameter sets given in Table 2. Parameters not listed in Table 2 are assumed to have their nominal value. Those sets are related to two extreme cases chosen by physical considerations, that represent a kind of worst-case deviation from the nominal values.

3.2 Single-input control problem

The second control problem of interest involves derivation of a single-input controller. Here, only the flow rate $\frac{\dot{V}}{V_R}$ is available as manipulated variable. Heat removal $\dot{Q}_K$ is held constant at the steady state value given by (4). We consider the same disturbances and constraints in the manipulated variable $\frac{\dot{V}}{V_R}$ as in the multi-input case. Only the range of setpoint values is reduced to

$$
0.95\,\frac{mol}{l} \quad \leq \quad c_{B\,|s} \quad \leq \quad 1.09\,\frac{mol}{l}\,.
$$

Again the same test signals and uncertainty sets can be chosen for testing the controllers.

4 Nonlinear predictive control of the CSTR

4.1 Model predictive control

Model predictive control (MPC) has become an attractive feedback strategy, especially for linear or nonlinear plants subject to input and state constraints. During the last decade, many formulations have been developed for linear and nonlinear, stable and unstable, and non-minimum-phase plants (e.g. [2, 8, 9]). This method has been successfully applied also in the process industry (e.g. [10]). In MPC the controller predicts the behavior of a plant over a prediction horizon using the plant model and measurement, and determines a manipulated variable sequence that optimizes some open-loop performance objective over the prediction horizon. This manipulated variable sequence is implemented until the next measurement becomes available. Then, the optimization problem is solved again.

The general formulation for nonlinear model predictive control (NMPC) may be stated (by some abuse of notation) as

$$\min_{\boldsymbol{u}^{N_c}} J\left(\boldsymbol{u}^{N_c}, \boldsymbol{x}(t), \boldsymbol{y}(t)\right) \tag{5a}$$

subject to

$$\begin{aligned} \dot{\boldsymbol{x}}(t) &= \boldsymbol{f}\left(\boldsymbol{x}(t), \boldsymbol{u}^{N_c}\right), \quad t \in (t_k, t_{k+N_p}] && \text{(5b)} \\ \boldsymbol{y}(t) &= \boldsymbol{g}\left(\boldsymbol{x}(t), \boldsymbol{u}^{N_c}\right) && \text{(5c)} \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{h}_1\left(\boldsymbol{x}(t), \boldsymbol{u}^{N_c}\right) &= 0 && \text{(5d)} \\ \boldsymbol{h}_2\left(\boldsymbol{x}(t), \boldsymbol{u}^{N_c}\right) &\geq 0 && \text{(5e)} \end{aligned}$$

with initial condition

$$\boldsymbol{x}(t_k) = \boldsymbol{x}_k, \tag{5f}$$

where $\boldsymbol{x}$ is the state vector, $\boldsymbol{y}$ is the vector of controlled variables, N_p and N_c are the length of the prediction and control horizon respectively corresponding to sampling period ΔT, satisfying $N_p \geq N_c$. The scalar function J is the performance objective, equations (5b) and (5c) represent the plant dynamics and output function, equations (5d) and (5e) describe equality and inequality constraints which have to be satisfied in practical application (for example, actuator saturation). The sequence

$$\boldsymbol{u}^{N_c} = [\boldsymbol{u}_k, \boldsymbol{u}_{k+1}, \cdots, \boldsymbol{u}_{k+N_c-1}]^T \tag{5g}$$

is the discrete manipulated variable vector, with $\boldsymbol{u}_{k+i} = \boldsymbol{u}(t_k + i\Delta T), i = 0, 1, \cdots, N_c - 1$. The manipulated variables are considered in a discretized way, because it is in general unrealistic to solve optimization problem (5) analytically over the prediction horizon N_p with continuous manipulated variables.

In this formulation it is assumed that the full state measurement is available at time t_k, *i.e.*, $\boldsymbol{x}_k$ in initial condition (5f) is known. However, in most applications, not all of the states can be measured directly. In this case the initial condition can merely be set equal to the states predicted at the previous sampling time. Of course, model-plant mismatch and unmeasurable disturbances will then lead to poor performance or even instability. Thus, a state estimator is needed in the case of output feedback. Here, we use a continuous-discrete extended Kalman filter (EKF) [3], which is an extension of the linear Kalman filter to the more general case of nonlinear system with discrete output measurements

$$\begin{aligned} \dot{\boldsymbol{x}}(t) &= \boldsymbol{f}\left(\boldsymbol{x}(t)\right) + \boldsymbol{w}(t) && \text{(6a)} \\ \boldsymbol{y}_k &= \boldsymbol{g}\left(\boldsymbol{x}(t_k)\right) + \boldsymbol{v}_k, && \text{(6b)} \end{aligned}$$

where $\boldsymbol{w}(t)$ and $\{\boldsymbol{v}_k\}$ are random variables that represent noise. For details see for example [3].

For a more detailed description of NMPC we refer for example to [2, 7, 9].

4.2 Simulation results

In this section we present a "reference" solution to the benchmark problem described in Sections 2 and 3. The objective function for NMPC is taken as the integral square error of the controlled variable from its setpoint:

$$J = \int_{t_k}^{t_{k+N_p}} \left(c_B(t) - c_{B\,|s}(t)\right)^2 dt. \tag{7}$$

It is very time consuming to solve the on-line optimization problem posed. The complexity depends mainly on the number of independent variables in $\boldsymbol{u}^{N_c}$. In order to reduce the number of independent variables, a technique called "blocking" is used [7]. The idea is not to allow the manipulated variables to vary at every future sampling time but to require them to be constant over several sampling periods. In addition, we also set the control horizon N_c smaller than the prediction horizon N_p, and let the manipulated variables be constant after the control horizon. In physical terms, a manipulated variable sequence of only N_c steps *cannot* make the system follow the setpoint *exactly* over all N_p steps, when $N_c < N_p$ [7]. Therefore, only the setpoint change in the control horizon is considered for each optimization.

With the EKF not only the four states $(c_A, c_B, \vartheta, \vartheta_K)$ but also the unmeasurable disturbance (feed temperature ϑ_0) are estimated. In order to estimate the disturbance it is assumed that the disturbance is constant but unknown, thus, satisfying the differential equation

$$\dot{\vartheta}_0(t) = 0. \tag{8}$$

Here, the reactor temperature ϑ is used as secondary measurement to enhance the estimation performance.

4.2.1 Controller tuning

The NMPC controller with EKF has a number of tuning parameters (among others the prediction horizon N_p, the control horizon N_c, and the parameters for the EKF). There are no general criteria to achieve stability and robustness for nonlinear model predictive control. In particular, for NMPC with EKF no separation principle is known to hold. Hence, we choose the parameters for the EKF in such a way that it has a good estimation performance. It is known that for linear non-minimum-phase systems the closed-loop system can become unstable if the control action is too aggressive (*i.e.* the prediction horizon is too "short" or the control horizon is too "long") [7]. This happens also in the nonlinear case, especially when the operating point is at the point of optimal yield as in the case of the CSTR considered. Here, we choose the prediction horizon to be $N_p = 200$, the control horizon to be $N_c = 3$ with a sampling period of 20 seconds. And we also make the manipulated variables to maintain constant over two sampling periods.

4.2.2 Setpoint tracking

Fig. 2 shows the closed-loop response of the CSTR to step changes in the setpoint $c_{B\,|s}$ from maximum to minimum and back to maximum value without disturbance. During

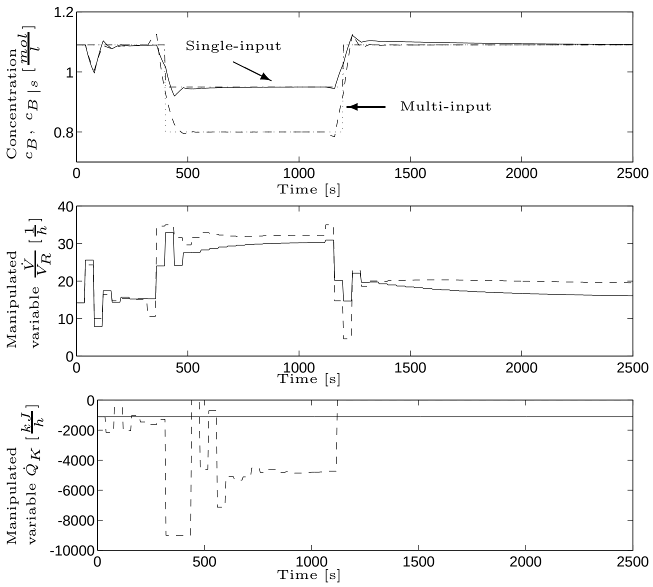

Figure 2: Setpoint tracking of the CSTR controlled with NMPC (— single-input; – – multi-input; – · – setpoint for the single-input case; · · · setpoint for the multi-input case).

the first 400 seconds the controller deals with the initial estimation error. The true and estimated initial states and disturbance ($\boldsymbol{x}_k, \vartheta_{0k}$ and $\hat{\boldsymbol{x}}_k, \hat{\vartheta}_{0k}$) are

$$\begin{bmatrix} \boldsymbol{x}_k \\ \vartheta_{0k} \end{bmatrix} = [2.14 \quad 1.09 \quad 114.2 \quad 112.9 \quad 104.9]^T \,,$$

$$\begin{bmatrix} \hat{\boldsymbol{x}}_k \\ \hat{\vartheta}_{0k} \end{bmatrix} = [2.50 \quad 1.09 \quad 114.2 \quad 114.0 \quad 110.0]^T \,.$$

Thus, a rather large initial error was assumed.

It can be seen from Fig. 2 that both in the multi-input and single-input case only three steps are needed to bring the concentration of product B into the required control tolerance ($\pm 0.02\frac{mol}{l}$) of the setpoint without large overshoot.

It is shown in Fig. 3 that the EKF quickly recovers from the initial estimation error and gives very good estimates

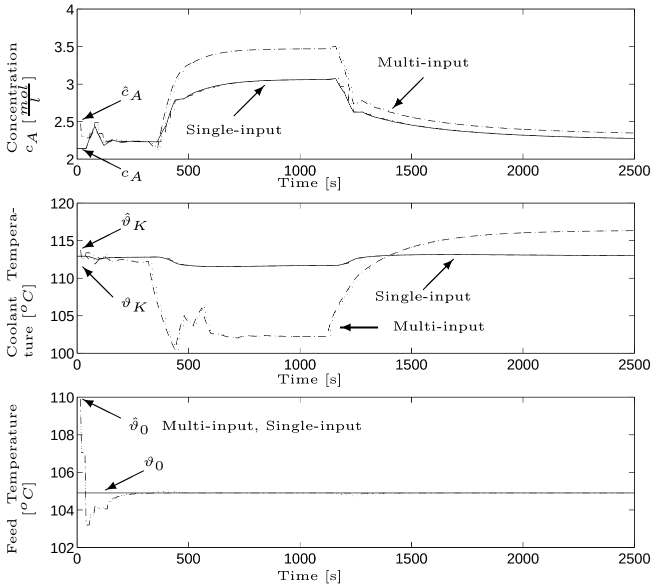

Figure 3: State and disturbance estimation for setpoint tracking (—, – · – true and estimated variable in the single-input case; – –, · · · true and estimated variable in the multi-input case).

of the states and the disturbance for both the multi-input and single-input case.

In the Sections 4.2.3 and 4.2.4 we assume that there is no estimation error in the initial states, but the initial estimated disturbance $\hat{\vartheta}_0$ takes the nominal value in (4).

4.2.3 Disturbance rejection

Because the operating point is at optimal yield, it is very difficult to maintain this operating point especially when the feed temperature ϑ_0 is decreased to 100^oC. Fig. 4 shows the closed-loop response of the CSTR to step disturbances in the feed temperature. At time $t = 0s$ the feed temperature changes abruptly from the "steady state" value $\vartheta_0 = 104.9^oC$ to 115^oC and then at time $t = 1500s$ down to 100^oC, while the setpoint remains constant at the optimal value. The system is stable and only a steady state offset of $-0.008\frac{mol}{l}$ (single-input), which is smaller than the required control tolerance, can be observed. In principle, the NMPC controller is designed for zero offset, but the maximally achievable concentration c_B in steady state is of course lower than the optimal value of $c_B = 1.09\frac{mol}{l}$ when the feed temperature is reduced to $\vartheta_0 = 100^oC$, ($\frac{\dot{V}}{V_R}$ and $\dot{Q}_K$ being free within their constraints and the other parameters being not changed). It is clear that the manipulated variable sequence is not totally stationary at the last optimization step, because the controller always tries to overcome the offset. Altogether, the controller achieves a very good disturbance attenuation.

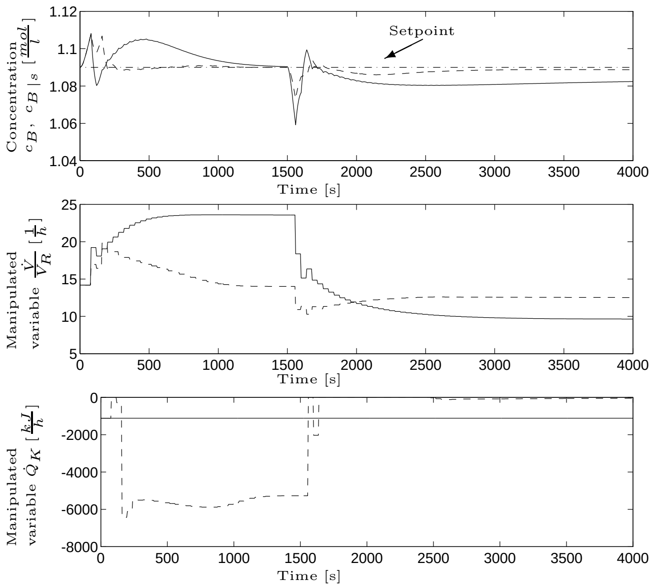

Figure 4: Disturbance attenuation of the CSTR controlled with NMPC (— single-input; −− multi-input).

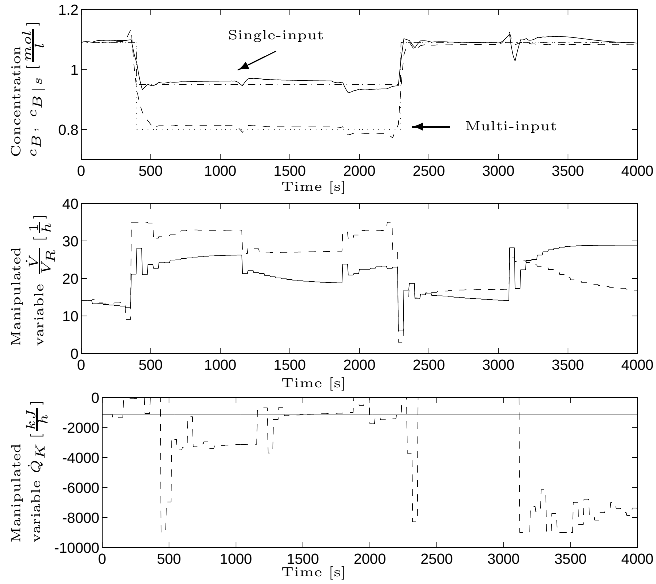

Figure 5: Robustness to parameter uncertainties (— single-input; −− multi-input).

4.2.4 Robustness to parameter uncertainties

The physico-chemical parameters of the benchmark problem are only known within bounds. To study the robustness of the NMPC controller with EKF, two extreme cases of model-plant mismatch as described in Section 3 will be discussed.

Fig. 5 shows how the NMPC controller with EKF tries to make the system track setpoint changes at time $t = 400s$ and $t = 2300s$, against model-plant mismatch and disturbances: There is model-plant mismatch in the first 1800 seconds according to Case 1 and after that according to Case 2 of Table 2; At time $t = 1100s$ and $t = 3000s$ the feed temperature ϑ_0 changes from 104.9^oC down to 100.0^oC and from 100.0^oC up to 115.0^oC respectively. Because of the uncertainties a stationary error in the state and disturbance estimation is observed and the setpoints cannot be held exactly. But the controlled variable remains within the required tolerance of $\pm 0.02\frac{mol}{l}$ for both sets of uncertainties and for both the multi-input and single-input case.

5 Conclusions

In this paper we proposed a benchmark problem for nonlinear control system design. The system to be controlled is a realistic chemical reactor, that is operated at the point of optimal yield. This operating point is especially desirable for economic reasons. Due to the operation at this highly nonlinear operating point, the control problem is very challenging. It can for example be shown that in the single-input case *no* linear controller with integral action can robustly stabilize the reactor.

In the second part of the paper we gave a particular solution to this benchmark problem based on a nonlinear model predictive control scheme. Despite the difficulty of the problem very satisfying control performance in both setpoint tracking and disturbance attenuation is robustly achieved with the controller proposed.

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