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DISSIPATIVITY-BASED OBSERVER AND FEEDBACK CONTROL DESIGN FOR A CLASS OF CHEMICAL REACTORS

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Abstract: The problem of controlling exothermic continuous chemical reactors with non-monotonic reaction rate and temperature measurement is addressed within a dissipativity-passivity theoretical framework, yielding an output-feedback dynamic controller made of a nonlinear passive state-feedback controller combined with a nonlinear dissipative observer. The proposed approach is put in perspective with previous nonlinear controllers and is illustrated with a representative example through simulations.

Keywords: Chemical Reactor Models, Observer-Based Feedback Control, Nonlinear Observers, Dissipativity, Nonlinear Separation Principle

1. INTRODUCTION

Continuous reactors with non-monotonic kinetic rate play an important role in process engineering (Lapidus (1977); Elnashaie, et al. (1990)). These reactors may exhibit strongly nonlinear behavior, like steady-state multiplicity, limit cycling and parametric sensitivity. Due to the non-monotonicity of the reaction rate, the reactor lacks global observability. The operation at a steady-state with maximum reaction rate signifies that the concentration is not locally observable from a temperature measurement. From a local control design viewpoint, this lack of observability rises a problem: in spite of being able to control the temperature, it is not possible to know if the reactor concentration is in the isotonic or antitonic branch of the reaction rate. This phenomenon, known as indistinguishability, is well-known in nonlinear estimation theory (Hermann and Krener (1977)). The reactor problem has been tackled by choosing a nominal concentration sufficiently below the one of the maximum rate (Smets, et al. (2002)), so that the problem can be locally treated. Nevertheless, it can be shown that the system is detectable and so the system state can be detected after some time from the temperature measurement. This fact motivates the question addressed in the present work, on whether it is possible to non-locally (globally) control a continuous reactor with non-monotonic reaction rate about a prescribed open-loop unstable steady-state of maximum reaction rate. On the other hand, in a recent control study for an exothermic polymer reactor with monotonic reaction rates, the combination of feedforward, passivity and observability ideas yields an output feedback cascade controller (Gonzalez and Alvarez (2005)), but the monomer concentration was estimated with an open loop observer, resulting in

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an unduly slow convergence rate. This approach was applied to the present reactor control problem, with one difference: a reduced order-EKF was used to speed up the concentration reconstruction rate (Diaz (2006)). However, the study did not have a formal stability assessment, and, above all, lacked a theoretical back-up in terms of controllability and detectability properties. This considerations motivate the present study.

In this paper, the problem of designing a measurement driven control scheme that non-locally (globally) stabilizes the non-monotonic rate reactor about a (open-loop unstable and locally not observable) steady state of maximum reaction rate is addressed. The resulting controller has two parts that resemble industrial conventional control components: (i) a proportional passive controller that guarantees nominal stability, and (ii) a dissipativity-based state observer with a data assimilation mechanism based on a suitable compromise between reconstruction rate and robustness. The closed loop stability is established by verifying the fulfillment of a condition that enables the application of a nonlinear separation result. The proposed approach is tested with a representative case example through numerical simulations.

The paper is organized as follows. The problem is formulated in Section 2, the related nonlinear state-feedback (SF) is constructed in Section 3. Section 4 presents the design of the observer in open-loop as well as a discussion of some observability aspects. In Section 5 it is shown, that the combination of observer and control yields an assurance of (non-local) stability using a nonlinear separation principle. The control performance is illustrated in a simulation study. Finally the paper ends up with the Conclusions.

2. CONTROL PROBLEM

Consider a continuous chemical reactor with an exothermic non-monotonic reaction. The volume is kept constant with a level controller. Heat exchange is enabled via a cooling jacket, by manipulating the rate of heat exchange between the jacket and the surroundings. Since the secondary loop can be designed with existing techniques (Alvarez-Ramirez, et al. (2002); Gonzalez and Alvarez (2005)), here we will circumscribe ourselves to the primary temperature control component, in coordination with a composition controller. From standard conservation arguments the reactor model is given by (Lapidus (1977)):

$$\begin{aligned}\dot{T} &= \beta\rho(c,T,p) + \Theta(T_e - T) - \upsilon(T - T_j)\\ \dot{c} &= -\rho(c,T,p) + \Theta(c_e - c)\\ y &= T, z_c = c, z_T = T, d_T = T_e, d_c = c_e\end{aligned} \qquad (1)$$

$$\Omega = \left\{ (c,T) \mid \frac{\partial \rho(c,T,p)}{\partial c} \triangleq \rho_c(c,T,p) = 0 \right\} \qquad (2)$$

where c is the reactant dimensionless concentration, T is the reactor temperature, T_j is the jacket temperature, Θ is the dilution rate, υ is the heat transfer coefficient, and β is the adiabatic temperature rise. The *states* are the concentration c and the temperature T. The *control inputs* are the dilution rate Θ and the jacket temperature T_j. The *regulated outputs* (z_c and z_T) are the concentration c and the temperature T. The *measured output* (y) is the temperature T, meaning that only one of the two regulated outputs is known. The exogenous load disturbance inputs (d_T and d_c) are the measured feed temperature T_e and the unmeasured feed concentration c_e. The strictly positive scalar function $\rho(c,T,p)$ denotes the dependency of the non-monotonic kinetic rate on c, T and p (a parameter vector) and has a maximum in the curve Ω (2) signifying that, at a prescribed temperature $\bar{T}$, the pair $(\bar{T},p)$ uniquely determines a concentration value c^* where the reaction rate is maximum.

The reactor must operate about a (possibly open loop unstable) steady-state $\bar{x} = (\bar{c},\bar{T})^T$, according to the algebraic equation pair

$$\begin{aligned}0 &= \beta\rho(\bar{c},\bar{T},p) + \Theta(\bar{T}_e - \bar{T}) - \upsilon(\bar{T} - \bar{T}_j)\\ 0 &= -\rho(\bar{c},\bar{T},p) + \Theta(\bar{c}_e - \bar{c}), \quad \rho_c(\bar{c},\bar{T},p) = 0\end{aligned} \qquad (3)$$

In vector notation, reactor (1) is written as follows

$$\begin{aligned}\dot{x} &= f(x,d,u,p), \quad y = c_y x, \quad c_y = [1,0], \quad z = x,\\ x &= [T,c]^T, \quad d = [T_e,c_e]^T, \quad u = [\Theta,T_j]\end{aligned}$$

From standard arguments, it follows that: (i) at $\bar{x}$ the linear reactor approximation is controllable but not locally observable, (ii) when $x \neq \bar{x}$ the local approximation is controllable and observable, and (iii) except in the maximum argument, the reactor is nowhere globally instantaneously observable (Alvarez (2000)) because, given $(T,\dot{T},T_j,T_e)$, the equation $\rho(c,T,p) = [\dot{T} - \Theta(T_e - T) - \upsilon(T - T_j)]/\beta$ admits two concentration solutions (except in its only injective point: the maximum), and this in turn implies the existence of indistinguishable motions. This central point and its implications will be discussed in Section 4.

Technically speaking, *our problem* is: given a prescribed (possibly open-loop unstable) steady-state operation $\bar{x}$ (3) (with maximum production rate at $\bar{T}$, the prescribed nominal temperature), design an observer-based feedback controller that, driven by the measured output ($y = T$) and input (d_T), manipulates the dilution rate (Θ) and the jacket temperature (T_j) so that the related closed-loop system is stable.

3. STATE-FEEDBACK CONTROL

From standard arguments in passive nonlinear control, it follows that the reactor system (1) has relative degrees $RD = (1, 1)$ and the trivial zero-dynamics $\{\bar{x}\}$. Accordingly, the enforcement of the closed-loop linear noninteractive regulation error dynamics:

$$\dot{e}_T = -\kappa_T e_T, \quad \dot{e}_c = -\kappa_c e_c \qquad (4)$$
$$[e_t, e_c]^T \triangleq [T - \bar{T}, c - \bar{c}]^T$$

leads to the the nonlinear state-feedback *passive* controller

$$T_{jc} = \frac{1}{\nu}\left(-\kappa_T(T - \bar{T}) - \beta\rho(c, T, p) + \right. \qquad (5)$$
$$\left. + \nu T - \Theta_c(Te - T)\right)$$
$$\Theta_c = \frac{1}{c_e - c}\left(-\kappa_c e_c + \rho(c, T, p)\right). \qquad (6)$$

In a practical situation, c_e is sufficiently larger than c, meaning that the closed-loop dynamics are Lipschitz, and this in turn implies the nominal exponential stability of the closed-loop reactor about the prescribed critical point $e = 0$ $(x = \bar{x})$.

4. STATE ESTIMATION

4.1 Globally Convergent Observer

Next, a globally convergent observer for (1) is designed by imposing a dissipation property upon the observer error dynamics. For the purpose of hand, let us regard the representative non-monotonic (catalytic) kinetics adapted from (Baratti (1993))

$$\rho(c, T, p) = \frac{cke^{-\gamma/T}}{(1 + \sigma c)^2} \triangleq \psi(c)\Gamma(T), \; p = \{\gamma, k, \sigma\}.$$

Rewrite system (1) in the following form (compare Moreno (2005))

$$\dot{x} = Az + G\psi(c)\Gamma(T) + \varphi(y, \Theta, T_e, T_j)$$
$$y = Cx \quad c = Hx \qquad (7)$$

where

$$A \triangleq \begin{bmatrix} -\Theta & 0 \\ 0 & -\Theta \end{bmatrix}, \quad G \triangleq \begin{bmatrix} \beta \\ -1 \end{bmatrix},$$
$$\varphi \triangleq \begin{bmatrix} \Theta T_e - \nu(T - T_j) \\ \Theta c_e \end{bmatrix},$$
$$C \triangleq \begin{bmatrix} 1 & 0 \end{bmatrix}, \quad H \triangleq \begin{bmatrix} 0 & 1 \end{bmatrix},$$

recall that a corresponding observer is given by

$$\dot{\hat{z}} = A\hat{z} + G\psi(\hat{c} + N\tilde{T})\Gamma(T) + \varphi(y, \Theta, T_j) + L\tilde{T}$$
$$\hat{T} = C\hat{z}, \quad \hat{c} = H\hat{z}, \quad \tilde{T} \triangleq \hat{T} - T \qquad (8)$$
$$\tilde{x} = [\tilde{T}, \; \tilde{c}]^T \triangleq [\hat{T} - T, \; \hat{c} - c]^T,$$

where $L = [L_1, \; L_2]^T$ and N are adjustable gains and $\tilde{x}$ is the state observation error, and write the related error dynamics

$$\dot{\tilde{x}} = (A + LC)\tilde{x} + G[\psi(\hat{c} + N\tilde{T}) - \psi(c)]\Gamma(T).$$

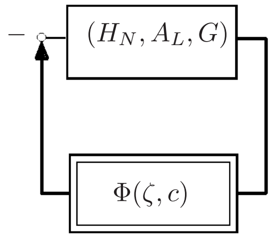

Fig. 1. Illustration of the structure of the observation error.

Next, the nonlinear function $\Phi(\zeta, c) \triangleq \psi(c) - \psi(c + \zeta)$ is introduced and $\zeta \triangleq H_N\tilde{x}$ is defined, so that the observation error dynamics acquires the form

$$\dot{\tilde{x}} = A_L\tilde{x} + G\Gamma(T)\omega$$
$$\omega = -\Phi(\zeta, c), \quad \zeta = H_N\tilde{x}, \qquad (9)$$
$$A_L = A + LC, \quad H_N = H + NC.$$

This system is diagrammatically depicted in Fig.1: a feedback connection of the linear subsystem (H_N, A_L, G) with the nonlinear negative output-feedback $\omega = -\Phi(\zeta, c)$. Figure 1 illustrates this interpretation in a block diagram. From an abstract energetic perspective, the linear part is supplied by the nonlinear function through the input $\omega = -\Phi(\zeta, c)$. On the other hand the nonlinear part $\Phi(\zeta, c)$ itself is supplied by the linear part through the output ζ. Thus, if the nonlinear part satisfies a dissipativity property and it can be assured that the linear part mets a dissipativity property that is compatible with it, in a suitable sense, then it can be concluded that the stored energy is dissipated until a point of minimal energy is reached. If this further holds uniformly and globally, then the global uniform asymptotic stability of $\tilde{x} = 0$ is ensured (see Willems (1972)). The enforcement of this coordinated dissipation feature upon the error system (9) (choosing the observer gains L_1, L_2 and N), determines a data assimilation scheme with a suitable tradeoff between robustness and reconstruction rate. It has to be mentioned, that this can be achieved, in principle, following various approaches. The approach presented here permits a direct energetic interpretation and thus offers a natural connection with classical dissipativity theory. The approach can be studied in more detail in (Moreno (2005)). Next, the global stability issue is addressed within the above mentioned dissipativity framework. For the purpose of hand, the time-strethcing coordinate transformation

$$d\tau = \Gamma(T)dt$$

is introduced. This yields, that (9) is taken into the form

$$\frac{d\,\tilde{x}}{d\tau} = \tilde{A}_L\tilde{x} + G\omega$$
$$\omega(\zeta, c) = -\Phi(\zeta, c), \quad \zeta = H_N\tilde{x}, \qquad (10)$$

with

$$\tilde{A}_L = \begin{bmatrix} \tilde{L}_1 & 0 \\ \tilde{L}_2 & -\tilde{\Theta} \end{bmatrix},$$

where $\tilde{L}_1 \triangleq \Gamma(T)^{-1}(L_1 - \Theta)$, $\tilde{L}_2 \triangleq \Gamma(T)^{-1}L_2$ and $\tilde{\Theta} \triangleq \Gamma(T)^{-1}\Theta$. The nonlinearity $\omega(\zeta, c)$ happens to be included in the sector $[K_1,\ K_2] = [-1, \frac{1}{27}]$ and thus satisfies a dissipativity property. This is known as (Q, S, R)-dissipativity ((Q, S, R)-D), with $(Q, S, R) = (-1, \frac{1}{2}(K_1 + K_2), -K_1K_2) = (-1, -\frac{13}{27}, \frac{1}{27})$. Note that this property can be expressed in the form of the quadratic supply rate (see Moreno (2005))

$$\mathcal{S}(\zeta, \Phi) = [\zeta\ \Phi] \begin{bmatrix} Q & S \\ S^T & R \end{bmatrix} \begin{bmatrix} \zeta \\ \Phi \end{bmatrix} \geq 0. \qquad (11)$$

An adequate property for the linear part is e.g. the $(-R, S, -Q)$-strictly state dissipativity (SSD) (see Moreno (2005)). The advantages of satisfying these properties lead to the fulfillment of the following

Proposition 1. Regard the observation error dynamics (10), where Φ is (Q, S, R)-D. There exist a positive definite symmetric matrix $P = P^T > 0$ and numbers $\epsilon > 0$, N as well as $L = [L_1,\ L_2]^T$, so that the nonlinear matrix inequality

$$\begin{bmatrix} A_L^T P + PA_L + \epsilon P + H_N^T R H_N & PG - H_N^T S \\ G^T P - SH_N & Q \end{bmatrix} \leq 0 \qquad (12)$$

is satisfied, or equivalently, the linear subsystem (H_N, A_L, G) in (10) is $(-R, S, -Q)$-SSD for all $\Theta \geq \delta > 0$ and the error $\tilde{x}$ converges to $\tilde{x} = 0$ in a global sense.

A proof of this proposition is given in (Moreno (2005)), ensuring the existence of the storage function $\mathcal{V}(\tilde{x}) = \tilde{x}^T P \tilde{x}$, and its decrease along all possible motions due to the presence of the correction terms with N and L. This enables us to identify the storage function with a Lyapunov function, and consequently the application of Lyapunov's second method to draw the stability result considering $\dot{\mathcal{V}} \leq -\epsilon\mathcal{V}$.

Without going into the derivation details a possible solution to (12) is presented. For example, consider

$$p_2 = \frac{\alpha R}{\delta}, \quad p_1 = \frac{(p_2 + S)^2}{p_2}, \quad p_3 = \frac{p_2 + S}{\beta}$$

ensuring the existence of $\epsilon = 2\Theta e^{-\gamma/T}/k - R > 0$ and $P = P^T > 0$ given by

$$P = \begin{bmatrix} p_1 & p_3 \\ p_3 & p_2 \end{bmatrix}, \qquad (13)$$

and the observer gains

$$\begin{aligned} N &= \frac{\beta p_1 - p_3}{S} \\ L_1 &= \Theta - \frac{\epsilon p_1 + 2L_2 k^{-1} e^{\gamma/T} p_3 - RN^2 - q}{2p_1} k e^{-\gamma/T} \\ L_2 &= e^{-\gamma/T} \left\{ \frac{p_3 p_1}{2p_1(p_2 p_1 - p_3)} \left(\epsilon p_1 - RN^2 - q\right) - \right. \\ &\quad \left. - \frac{p_1}{p_2 p_1 - p_3} \left(RN + (\epsilon - \Theta)p_3\right) \right\}. \end{aligned}$$

This solution guarantees the global stability of $\tilde{x} = 0$ for all $\Theta \geq \delta > 0$, which is a practically reasonable restriction for the control input (the dilution rate is sufficiently above a reasonably small value). Moreover, saturation bounds can be introduced to ensure the strict positivness of the calculated input signal $\tilde{\Theta}$.

4.2 Comments on motion indistinguishability

Given that the notion of nonlinear observability is behind what can be achieved by a globally convergent observer, some words on the observability of the regarded process are in order.
Two trajectories $x_1(\cdot),\ x_2(\cdot)$ of (1) are said to be *indistinguishable* if they produce the same output measurements, i.e. $T_1(\cdot)^{(n)} \equiv T_2(\cdot)^{(n)}$ for all $n \in \mathbb{N}$ representing the n-th derivative (Hermann and Krener (1977)). The analysis of this condition for $n = 1$ directly yields that all motions are pairwise indistinguishable with identical reaction rates $\rho(c_1, T_1, p) \equiv \rho(c_2, T_2, p)$. From the enfacement of the above equivalence condition one can analytically construct the so-called *bad Input functions* that produce indistinguishable motions, enabling the characterization of the reactor detectability property (Ibarra Rojas *et al.* (2004)). Such an analysis yields that: *all indistinguishable motions are detectable* (at least for a nominal load disturbance d). This rises the question on whether the existence of indistinguishable motions can effect the performance of the control scheme. The answer to this question is that it can, at least in an open-loop application, in the sense of wrong estimates (in the wrong reaction rate branch). On the other hand, it is assured, that after a certain time, determined by the plant's dynamics, the estimate converges near the actual concentration. Moreover the existence of indistinguishable motions does not allow the (at least formal) assignment of an arbitrary convergence rate of the observer. Thus it becomes clear, that – independently of the design method – using an output injection in the observer dynamics, there are a priori bounds for the convergence rate. For the closed loop application so far, by simulations in "realistic" situations no indistinguishable motions have been detected. Although, we do not have a formal assessment yet, a conjecture can be formulated here: the *bad inputs will be hardly present*, especially if the interlaced

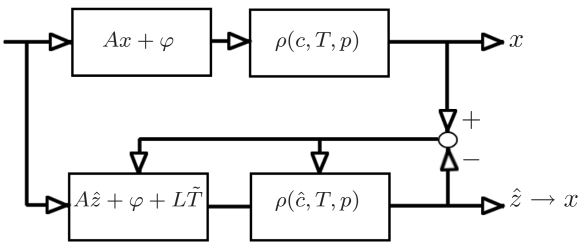

Fig. 2. Structure of the open-loop observer.

observer-controller design and implementation are appropriately performed.

4.3 Concluding remarks

The main features of the observer (8) are

1. The observer is of low dynamical order (two-states without augmented ones)
2. Structural features: Two measurement injection points (see Figure 2):
   a) The standard one (EKF or Luenberger) that corrects the rate of state prediction change.
   b) An additional one, that corrects the concentration argument of the reaction rate.
3. Global uniform convergence for all $\Theta \geq \delta > 0$.

5. OUTPUT-FEEDBACK CONTROL

5.1 Nonlinear Separation Principle

In general, the separation principle for linear systems does not hold for the nonlinear case. Nevertheless, results of different character have been recently reported (Angeli (2004); Moreno (2006)). According to these works a separation principle holds if the controller exponentially stabilizes the plant, yields a Lipschitz plant's dynamics, and the trajectories of the state estimation are assured to converge asymptotically and uniformly (i.e. for all admissible inputs). Notice that the first two conditions assure the Input-to-State-Stability (ISS) of the controlled plant with respect to the observation error (see e.g. Khalil (2002)). To show, that these conditions are satisfied, it suffices to put together the features associated with the different parts of the state-feedback observer-based control strategy:

(i) The observer error ϵ converges globally to $\epsilon = 0$, for all $\Theta \geq \delta > 0$.
(ii) The controlled plant is Lipschitz (at least for a range of estimation errors sufficiently wide for the practical application).
(iii) The designed controller stabilizes the control error exponentially.

From these properties the practical, uniform, asymptotic stability of the nominal closed-loop steady-state follows (Angeli (2004); Moreno (2006)).

The combination of the passive controller (5), (6) with the dissipative observer (8) yields the proposed robust dynamic output-feedback that globally stabilizes the chemical reactor at its locally unobservable prescribed steady-state with maximum reaction rate. Basically, this robustness-oriented observer-control design exploits the reactor nonlinear global structure (relative degrees and detectability) and, according to the celebrated Popov's solution to Lur'e's problem, can be interpreted as follows: the feedback correction and innovation mechanisms are tailored so that the model and estimation errors are efficiently lumped into conic nonlinearities over the first-third quadrant pair.

5.2 Controller Behavior

To test the nominal and global stabilizing control properties, the closed loop reactor was subjected to considerable initial state deviations, that are by far larger than the ones encountered in practical situations. The nominal behavior, without modeling error, is presented in Figure 3 (with gains $\kappa_T = \kappa_c = 3$ so that $\dot{V} \leq -\epsilon V$, $\epsilon \geq 0$), showing that, indeed, the closed loop motions converge to the prescribed steady-state. The behaviors with feed concentration, feed temperature, and feed concentration and temperature are presented in Figure 4, showing that: (i) in all cases the controller stabilizes the reactor with the same overall behavior of the nominal case (Figure 3), and (ii) as expected, the concentration is regulated with some (rather small) offsets, because of the proportional nature of the passive nonlinear controller. In principle, integral action can be added to improve behavior and reduce the concentration offset. It can be pointed out that the proposed observer has certain *a priori* robustness, due to the choice of the Lyapunov-function. The observer gains are determined in such a way, that it is assured that $\dot{V} \leq -\epsilon V$. Thus, for additive disturbances, at least ultimate and uniform boundedness of the solutions is assured.

6. CONCLUSIONS

A non locally stabilizing output-feedback controller for continuous chemical reactors with non-monotonic kinetics and temperature measurements has been presented. The reactor lacked local observability about its nominal steady-state with maximum reaction rate. An interlaced observer-control design was developed within a passivity-dissipativity framework, yielding a closed loop stability assessment. The theoretical findings

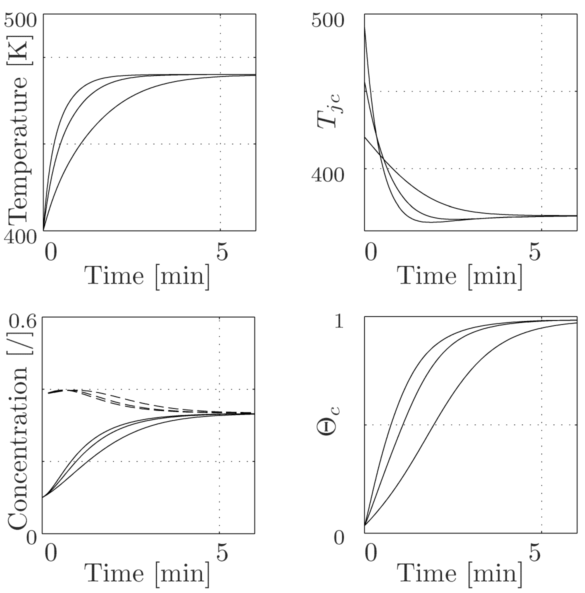

Fig. 3. Simulation results for the proposed control strategy for different $\kappa_T \in \{1, 2, 3\}$ and initial values $x_0 = [400, 0.1]^T$, $\hat{z}_0 = [450, 0.6]^T$.

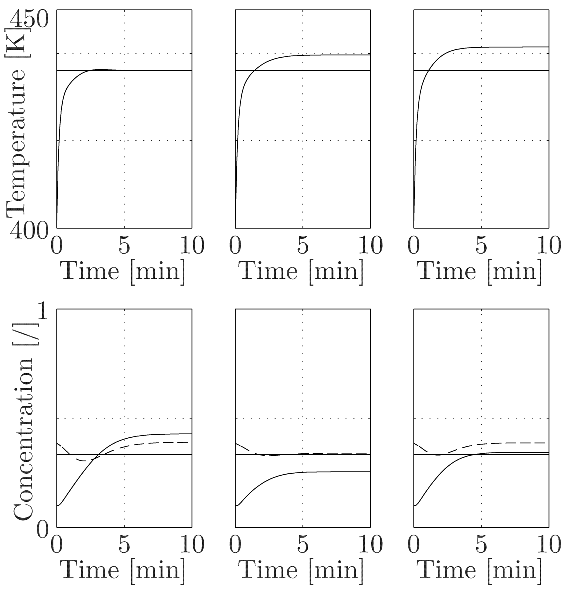

Fig. 4. Simulation results for different parameter uncertainties. Left: error in c_e of -5%, center: error in T_e of -5% and right: errors in c_e as well as T_e of -5%. Initial values $x_0 = [400, 0.1]^T$, $\hat{z}_0 = [450, 0.6]^T$. $\kappa_T = 3$, $\kappa_c = 1$. The set point values are $\bar{c} = 1/3$ and $\bar{T} = 436.02$.

and control behavior were illustrated and tested with a representative case example through simulations. Currently, work is underway to introduce integral action, with two purposes: (i) the overall improvement of the controller functioning, and (ii) the reduction of the concentration offset.

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