



Input constrained funnel control with applications to chemical reactor models

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Received 2 March 2004; received in revised form 21 May 2004; accepted 25 May 2004

Abstract

Error feedback control (in the presence of input constraints) is considered for a class of exothermic chemical reactor models. The primary control objective is regulation of a setpoint temperature T^* with prescribed accuracy: given $\lambda > 0$ (arbitrarily small), ensure that, for every admissible system and reference setpoint, the regulation error $e = T - T^*$ is ultimately smaller than λ (that is, $\|e(t)\| < \lambda$ for all t sufficiently large). The second objective is guaranteed transient performance: the evolution of the regulation error should be contained in a prescribed performance funnel F around the setpoint temperature T^* . A simple error feedback control with input constraints of the form $u(t) = \text{sat}_{[\underline{u}, \bar{u}]}(-k(t)[T(t) - T^*] + u^*)$, u^* an offset, is introduced which achieves the objective in the presence of disturbances corrupting the measurement. The gain $k(t)$ is a function of the error $e(t) = T(t) - T^*$ and its distance to the funnel boundary. The input constraints \underline{u}, \bar{u} have to satisfy certain feasibility assumptions in terms of the model data and the operating point T^* .

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Keywords: Adaptive control; Chemical reactions; Transient behaviour; Input saturation; Input constraints; Setpoint control

1. Introduction

In this note, error feedback control is considered for a class of nonlinear systems which arise as prototype models for controlled exothermic chemical reactions. The output T of the system is the reaction temperature, while the control u is the rate of change of reaction temperature. The primary control objective is regulation of a setpoint temperature T^* with prescribed accuracy: given $\lambda > 0$ (arbitrarily small), ensure that, for every admissible system and reference setpoint, the regulation error $e = T - T^*$ is ultimately smaller than λ (i.e., $\|e(t)\| < \lambda$ for all t sufficiently large). The second objective is guaranteed transient performance: the evolution of the regulation error should be contained in a prescribed performance funnel F around the setpoint temperature T^* . The control is objected to input constraints and the measurement is corrupted by disturbances. The controller is simple in its design: it is a time-varying proportional error feedback controller $u(t) = \text{sat}_{[\underline{u}, \bar{u}]}(-k(t)[T(t) - T^*] + u^*)$, where u^* denotes an offset. The gain $k(t)$ is a function of the error $e(t) = T(t) - T^*$ and its distance to the funnel boundary. The structural assumption on the system class (note that the system data need not be known explicitly) is a mild feasibility assumption in terms of the model data

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versus the input constraints \underline{u}, \bar{u} and the operating point T^* . Moreover, some chemically motivated assumptions have to be satisfied.

In chemical engineering, the analysis and control of exothermic continuous stirred tank reactors originates in the work [2]. They have subsequently been used extensively as models in several industries including continuous polymerization reactors, distillation columns, biochemical fermentation and biological processes. More recently, for the prototype class of chemical reaction models used in this note, various adaptive and non-adaptive control theory approaches have been developed for the setpoint control of temperature: In [10] a state feedback controller with observer was proposed for globally stabilizing the temperature of exothermic continuous stirred tank reactors. In [9] (adaptive) dynamic output PI-type controllers were derived, and similar stabilization results were obtained in [1], however they require exponentially stable zero dynamics. In [7] an adaptive controller, based on the concept of λ -tracking, see e.g. [5], which obeys input constraints has been introduced. However, this controller does not guarantee any transient behaviour and the time-varying gain of the proportional feedback is monotonically non-decreasing, albeit bounded. The controller of the present note circumvents these two drawbacks by adapting the two approaches of the “funnel controller”, as introduced in [6], and of the λ -tracking concept, as applied to chemical reactor models in [7]. Of particular interest is the interplay between the input constraints, the specific nature of the nonlinearities in chemical reaction models, and the setpoint to be tracked. It is shown that arbitrary prespecified transient behaviour is guaranteed in the presence of input constraints and noise corrupting the output measurement. As opposed to many existing control strategies, in our set-up the gain $t \mapsto k(t)$ is not monotone and may actually decrease.

In the following sub-sections we introduce and discuss the system class, the control objectives, the prespecified funnel, and the gain function. The main result, i.e. adaptive regulation within the prespecified funnel, is discussed and proved in Section 2. Finally, in Section 3, we illustrate the flexibility of the control mechanism by some simulations and discuss the different effects of the parameters in the control law.

1.1. System class

The following model of exothermic chemical reactions is considered (see also [10]):

$$\left. \begin{aligned} \dot{x}_1(t) &= C_1 r(x(t), T(t)) + d[x_1^{\text{in}} - x_1(t)], & x_1(0) &= x_1^0 \in \mathbb{R}_{\geq 0}^{n-m}, \\ \dot{x}_2(t) &= C_2 r(x(t), T(t)) + d[x_2^{\text{in}} - x_2(t)], & x_2(0) &= x_2^0 \in \mathbb{R}_{\geq 0}^m, \\ \dot{T}(t) &= b^T r(x(t), T(t)) - qT(t) + u(t), & T(0) &= T^0 \in \mathbb{R}_{> 0}, \\ x(t) &= (x_1(t)^T, x_2(t)^T)^T, \end{aligned} \right\} \quad (1)$$

In (1) it is assumed that $n, m \in \mathbb{N}$ with $0 < m < n$ and the variables and constants represent:

$x_1(t) \in \mathbb{R}_{\geq 0}^{n-m}$	concentrations of the $n-m$ chemical reactants at time $t \geq 0$
$x_2(t) \in \mathbb{R}_{\geq 0}^m$	concentrations of the m chemical products at time $t \geq 0$
$T(t) \in \mathbb{R}_{> 0}$	temperature of the reactor at time $t \geq 0$
$u(t) \in \mathbb{R}_{\geq 0}$	control of the temperature at time $t \geq 0$
$x^{\text{in}} = \begin{pmatrix} x_1^{\text{in}} \\ x_2^{\text{in}} \end{pmatrix} \in \mathbb{R}_{\geq 0}^{(n-m)+m}$	constant feed concentrations
$C = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \in \mathbb{R}^{n \times m}$	stoichiometric matrix with $C_2 \in \mathbb{R}^{m \times m}$ and
$C_1 \in \mathbb{R}_{\leq 0}^{(n-m) \times m}$	stoichiometric matrix of the reactants and therefore all entries are non-positive
$b \in \mathbb{R}_{\geq 0}^m$	coefficients of the exothermicity
$d > 0$	dilution rate
$q > 0$	heat transfer rate between heat exchanger and reactor
$r(\cdot, \cdot): \mathbb{R}_{\geq 0}^n \times \mathbb{R}_{> 0} \rightarrow \mathbb{R}_{\geq 0}^m$	model of the reaction kinetics.

The function $r(\cdot, \cdot)$ is assumed to be locally Lipschitz continuous and to satisfy

$$r(0, T) = 0 \quad \forall T > 0. \quad (2)$$

The condition (2) models the assumption that without any reactants or products a reaction cannot take place. In the context of chemical reactions, practical considerations lead to the assumption that the control input $u(\cdot)$ is constrained, i.e. there exists $\underline{u}, \bar{u} \in \mathbb{R}_{>0}$ so that

$$0 < \underline{u} < \bar{u} \quad \text{and} \quad \forall t \geq 0: \underline{u} \leq u(t) \leq \bar{u}. \quad (3)$$

Since (1) models exothermic reactions, the following assumptions may be justified for some given reference temperature $T^* > 0$ and \underline{u}, \bar{u} satisfying (3):

(A1) $\mathbb{R}_{\geq 0}^n \times \mathbb{R}_{>0}$ is positively invariant under (1) for any continuous $u: \mathbb{R}_{\geq 0} \rightarrow [\underline{u}, \bar{u}]$.

(A2) $\exists \gamma \in \mathbb{R}_{>0}^n \forall i \in \{1, \dots, m\}: \gamma^T c_i \leq 0$, where $[c_1, c_2, \dots, c_m] = C$.

(A3) $\exists \bar{T} > T^* \exists \rho_1, \rho_2 > 0$:

$$0 < \underline{u} + \rho_1 < qT - b^T r(x, T) < \bar{u} - \rho_2 \quad \forall (x, T) \in \Omega(\gamma, x^{\text{in}}) \times [T^*, \bar{T}],$$

where

$$\Omega(\gamma, x^{\text{in}}) := \{x \in \mathbb{R}_{\geq 0}^n \mid \gamma^T x < \gamma^T x^{\text{in}}\}.$$

Remark 1. (i) The assumption (A1) reflects the fact that concentrations of the reactants should not be negative and temperature should be positive.

Note that only continuous control inputs u with values between \underline{u} and \bar{u} are allowed, which is weaker than (A1) assumed in [7].

(ii) (A2) holds if (1) satisfies the law of conservation of mass, which means that there exists $\gamma \in \mathbb{R}_{>0}^n$ with $\gamma^T C = 0$. This can be found implicitly in [4], and it is also assumed in [10]. If C does not represent exactly the stoichiometric relationships between all species, then conservation of mass need not be satisfied. Nevertheless, the reaction model might still be relevant provided that all essential reactions are obeyed. This approach was adopted in [3,8]. In [8] a concept of non-cyclic process was developed and shown to ensure dissipativity of mass and hence that (A2) is satisfied.

(iii) (A3) is a feasibility assumption arising because of the saturation of the input u . It is a weaker assumption than (H2) in [10]. Similar to (A3') in [7], the values ρ_1, ρ_2 and \bar{T} are explicitly introduced, they are essential for the main results of this note.

Remark 2. The dynamics of the temperature as described by the third equation in (1) can directly be controlled by u , provided the concentrations remains in a bounded region and the input constraints are not “too tough”. More precisely, assumption (A3) ensures that if $x(t) \in \Omega(\gamma, x^{\text{in}})$ for some $t \geq 0$, then

$$[u(t) = \underline{u} \wedge T(t) \in [T^*, \bar{T}]] \Rightarrow \dot{T}(t) < -\rho_1, \quad (4)$$

$$[u(t) = \bar{u} \wedge T(t) \in [0, T^*]] \Rightarrow \dot{T}(t) > \rho_2. \quad (5)$$

This is seen as follows: If $u(t) = \underline{u}$ and $T(t) \in [T^*, \bar{T}]$, then (A3) yields,

$$\dot{T}(t) = b^T r(x(t), T(t)) - qT(t) + \underline{u} < -\rho_1.$$

Suppose $u(t) = \bar{u}$ and $T(t) \in [0, T^*]$. Note that $r_i(x, T) \geq 0 = r_i(0, T^*)$ for all $(x, T) \in \mathbb{R}_{\geq 0}^n \times \mathbb{R}_{>0}$ and all $i \in \{1, \dots, m\}$. Now $q > 0$, $b \in \mathbb{R}_{\geq 0}^m$ and (A3) gives

$$\dot{T}(t) = b^T r(x(t), T(t)) - qT(t) + \bar{u} \geq b^T r(0, T^*) - qT^* + \bar{u} > \rho_2.$$

1.2. Control objective

For every solution $T : [0, \omega) \rightarrow \mathbb{R}_{>0}$ of (1) with $\omega > 0$ define the (measured) error as

$$e : [0, \omega) \rightarrow \mathbb{R}, \quad t \mapsto e(t) := T(t) - T^* + \zeta(t), \tag{6}$$

where $\zeta : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$ represent a disturbance signal satisfying certain bounds in terms of the funnel as specified in (11).

The control objective is, that the temperature evolves within a prespecified neighbourhood of a setpoint (that will be the funnel F described in Section 1.3), which should be achieved by saturated proportional error feedback

$$u(t) = \text{sat}_{[\underline{u}, \bar{u}]}(-k(t)e(t) + u^*), \tag{7}$$

where $k(\cdot)$ is a time-varying gain function, $u^* \in [\underline{u}, \bar{u}]$ is a constant offset and

$$\text{sat}_{[\underline{u}, \bar{u}]}(s) := \begin{cases} \underline{u} & \text{if } s < \underline{u}, \\ s & \text{if } s \in [\underline{u}, \bar{u}], \\ \bar{u} & \text{if } s > \bar{u}. \end{cases}$$

Remark 3. Remark 6 in [7] shows that the closed-loop system (1), (7) satisfying (A1) and (A2) with any continuous $k : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ has, for every $(x^0, T^0) \in \mathbb{R}_{\geq 0}^n \times \mathbb{R}_{>0}$, a unique solution $(x, T) : [0, \omega) \rightarrow \mathbb{R}_{\geq 0}^n \times \mathbb{R}_{>0}$ for some $\omega \in (0, \infty]$, and ω may be maximally extended. Furthermore, it is shown that $\Omega(\gamma, x^{\text{in}}) \times \mathbb{R}_{>0}$ is positively invariant under (1) and (7).

1.3. The prespecified funnel F

Define

$$\Phi := \{ \phi \in C(\mathbb{R}_{\geq 0}, \mathbb{R}_{\geq 0}) \mid \phi \text{ is Lipschitz continuous, bounded and } \inf_{t \geq 0} \phi(t) > 0 \}.$$

For \bar{T}, T^* as in (A3), let $\phi_1, \phi_2 \in \Phi$. Then, the funnel F is defined as (see Fig. 1)

$$F := \{ (t, e) \in \mathbb{R}_{\geq 0} \times \mathbb{R} \mid e \in (-\phi_2(t), \phi_1(t)) \} \tag{8}$$

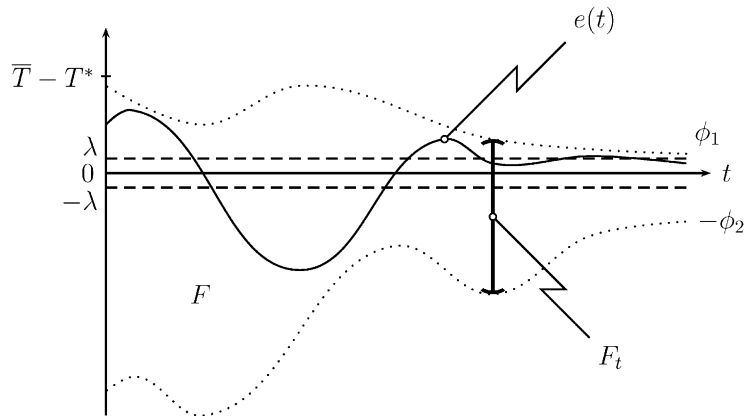


Fig. 1. The funnel F .

and

$$F_t := \{e \in \mathbb{R} \mid (t, e) \in F\} = (-\phi_2(t), \phi_1(t)) \quad \forall t \geq 0.$$

Let

$$\left. \begin{aligned} \lambda &:= \min \left\{ \inf_{t \geq 0} \phi_1(t), \inf_{t \geq 0} \phi_2(t) \right\} > 0, \\ L_i &> 0 \text{ a Lipschitz constant of } \phi_i, \quad i = 1, 2, \\ \underline{L}_i &< 0 \text{ a lower Lipschitz constant of } \phi_i, \quad i = 1, 2.^1 \end{aligned} \right\} \quad (9)$$

1.4. The gain function $k(\cdot)$

Let

$$K_F : F \rightarrow \mathbb{R}_{\geq 0}, \quad (t, e) \mapsto K_F(t, e)$$

be a locally Lipschitz continuous function satisfying

Property 1. $\forall K \geq 0 \exists \varepsilon > 0 \forall (t, e) \in F : [\text{dist}(e, \partial F_t) \leq \varepsilon \Rightarrow K_F(t, e) \geq K]$.

Property 2. $\forall \varepsilon > 0 \exists K \geq 0 \forall (t, e) \in F : [\text{dist}(e, \partial F_t) \geq \varepsilon \Rightarrow K_F(t, e) \leq K]$,
where ‘dist’ denotes the usual distance function

$$\text{dist}(e, M) := \inf\{|e - m| : m \in M\} \quad \text{for } M \subset \mathbb{R}^n \text{ and } e \in \mathbb{R}^n.$$

For the closed-loop system (1), (7) and the error $e(\cdot)$ as in (6), the gain $k(\cdot)$ is set to

$$k(t) = K_F(t, e(t)) \quad \forall t \in [0, \omega). \quad (10)$$

The Properties 1 and 2 are essential: first, to relate the distance between the error and the funnel boundary to the size of the gain, and secondly to allow for a great flexibility in the design of the gain. Property 1 prevents that $e(\cdot)$ leaves the funnel: If $e(t)$ is “close” to ∂F_t , then $k(t)$ is large and so the input saturates. Property 2 ensures that the gain $k(t)$ is not unnecessarily large if $e(t)$ is away from the funnel boundary.

A simple example for K_F is $K_F(t, e) = 1/\text{dist}(e, \partial F_t)$, and so for $\phi_1 = \phi_2 = \phi \in \Phi$ a feasible error feedback is

$$u(t) = \text{sat}_{[\underline{u}, \bar{u}]} \left(\frac{-e(t)}{\phi(t) - |e(t)|} + u^* \right).$$

2. Main result

We are now in a position to state the main result of this note. The proof is delegated to Section 4.

Theorem 4. *Suppose the exothermic chemical reaction model (1) satisfies, for some constants $\underline{u}, \bar{u}, \rho_1, \rho_2, T^*, \bar{T}$, the assumptions (A1)–(A3). Let a funnel F , as defined in (8), be given by some $\phi_1, \phi_2 \in \Phi$ and assume that a locally Lipschitz continuous function $K_F : F \rightarrow \mathbb{R}_{\geq 0}$ satisfies Properties 1 and 2. Suppose*

¹A constant $L \leq 0$ is deemed a lower Lipschitz constant of a function $f : \mathbb{R} \rightarrow \mathbb{R}$, if and only if, $f(t) - f(s) \geq L(t - s)$ for all $s, t \in \mathbb{R}$ and all $t \geq s$.

further, that a disturbance $\xi: \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$ of the temperature measurement is differentiable and satisfies, in terms of the funnel constants defined in (9), the inequalities

$$\|\xi\|_{\infty} \leq \lambda/2, \quad -(\underline{L}_2 + \rho_2) < \dot{\xi}(t) < \underline{L}_1 + \rho_1 \quad \text{and} \quad \xi(t) \geq \phi_1(t) - (\bar{T} - T^*) \quad \forall t \geq 0. \quad (11)$$

Then for every initial data (x^0, T^0) with $(x^0, T^0 - T^* + \xi(0)) \in \Omega(\gamma, x^{\text{in}}) \times F_0$, $T^0 > 0$, the output error feedback (7) with some constant offset $u^* \in (\underline{u}, \bar{u})$ and gain (10) applied to (1) yields the closed-loop system

$$\left. \begin{aligned} \dot{x}(t) &= Cr(x(t), T(t)) + d[x^{\text{in}} - x(t)], \\ \dot{T}(t) &= b^T r(x(t), T(t)) - qT(t) + \text{sat}_{[\underline{u}, \bar{u}]}(-K_F(t, e(t))e(t) + u^*), \\ e(t) &= T(t) - T^* + \xi(t), \\ x(0) &= x^0, \quad T(0) = T^0, \end{aligned} \right\} \quad (12)$$

which has a unique solution $(x, T, e): \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^{n+2}$ and this solution satisfies:

- (i) $\forall t \geq 0: (x(t), T(t)) \in \Omega(\gamma, x^{\text{in}}) \times \mathbb{R}_{\geq 0}$;
- (ii) $\forall t \geq 0: e(t) \in F_t$;
- (iii) $\exists \varepsilon > 0 \forall t \geq 0: \text{dist}(e(t), \partial F_t) \geq \varepsilon$;
- (iv) $\exists k_{\max} > 0 \forall t \geq 0: k(t) = K_F(t, e(t)) \leq k_{\max}$.

Remark 5. If the temperature measurement is not corrupted by any disturbance, i.e. $\xi \equiv 0$, then the inequalities in (11) simplify to

$$\underline{L}_1 > -\rho_1, \quad -\underline{L}_2 < \rho_2 \quad \text{and} \quad \phi_1(t) \leq \bar{T} - T^* \quad \forall t \geq 0.$$

The first two inequalities ensure that the change of the funnel boundaries ϕ_1, ϕ_2 , which is bounded by the Lipschitz constants, is not faster than the change of the error e by saturated input u as specified in (4) and (5).

Remark 6. The control in Theorem 4 is local in the sense that the initial temperature T^0 is constrained in the interval $(0, \bar{T})$. If this constrained is waved or the feasibility assumption does not hold for \bar{T} , then the controller (7) does, in general, not work (see the thermal runaway in the simulations of [7]).

To overcome this problem, [7,10] have introduced an additional input action which has a cooling effect if the temperature is too large. The overall model (1) is then replaced by

$$\begin{aligned} \dot{x}_1(t) &= C_1 r(x(t), T(t)) + d[v(t) - x_1(t)], \\ \dot{x}_2(t) &= C_2 r(x(t), T(t)) + d[x_2^{\text{in}} - x_2(t)], \\ \dot{T}(t) &= b^T r(x(t), T(t)) - qT(t) + u(t). \end{aligned} \quad (13)$$

In [10] the additional input v is

$$v(t) = \begin{cases} x_1^{\text{in}} & \text{if } T(t) \in (0, \bar{T}), \\ 0 & \text{if } T(t) \in [\bar{T}, \infty), \end{cases}$$

and in [7] v is chosen as a piecewise linear and continuous control

$$v(t) = \begin{cases} 0 & \text{if } \beta(t)e(t) \in (-\infty, \underline{u} - u^*], \\ [\beta(t)e(t) + u^* - \underline{u}]x_1^{\text{in}}/\delta & \text{if } \beta(t)e(t) \in (\underline{u} - u^*, \underline{u} - u^* + \delta), \\ x_1^{\text{in}} & \text{if } \beta(t)e(t) \in [\underline{u} - u^* + \delta, \infty), \end{cases}$$

for some $\delta > 0$ and β is determined adaptively.

However, if the model is (13), then the cooling action $v \equiv 0$ gives only

$$\dot{x}_1(t) = C_1 r(x(t), T(t)) - dx_1(t)$$

and there is no way to speed up the decrease of x_1 . One may use an adaptive or non-adaptive cooling action as suggested in [7,10], resp., and once $e(t)$ is within the funnel the controller of the present note can take over to ensure transient behaviour.

3. Simulations

We consider a prototype model for a single exothermic chemical reaction as suggested by Viel et al. [10]. Specifically the reaction kinetics of (1) with $n=2$, $m=1$ are modelled by the Arrhenius law $r(x, T) = k_0 e^{-k_1/T} x_1$. As in [10] and [7] (where in the latter contribution λ -tracking has been considered in the presence of input constraints, but not obeying any transient behaviour), the system parameters are set to

$$C_1 = -1, \quad C_2 = 1, \quad k_0 = e^{25}, \quad k_1 = 8700 \text{ K}, \quad d = 1.1 \text{ min}^{-1},$$

$$q = 1.25 \text{ min}^{-1}, \quad x_1^{\text{in}} = 1 \text{ mol/l}, \quad x_2^{\text{in}} = 0, \quad b = 209.2 \text{ K/mol}.$$

As observed by Viel et al. [10], system (1) has, with the above parameters, exactly three open-loop steady states: two of which are locally stable and the unstable one is approximately $(T^{\text{un}}, x_1^{\text{un}}, x_2^{\text{un}}) \approx (337.1, 0.71, 0.29)$ with constant input $u^{\text{un}} \approx 355.1$.

The objective is to regulate the temperature—within a prespecified funnel—to a neighbourhood of $T^* = T^{\text{un}} = 337.1$ K, corresponding to the temperature of the unstable steady state. The input constraints are chosen to be

$$\underline{u} = 295 \quad \text{and} \quad \bar{u} = 505.$$

It is easy to see that in this case the assumptions (A1)–(A3) are satisfied for

$$\gamma = (1, 1)^T, \quad \bar{T} = 340 \text{ K}, \quad \rho_1 = 10.1, \quad \rho_2 = 80.1.$$

The neighbourhood of T^* is prespecified to be an interval of length 2λ , $\lambda = 1.5$. If the temperature measurement is not corrupted by noise, i.e. $\xi \equiv 0$, then the assumptions in Theorem 4 are fulfilled for the initial values $(x_1^0, x_2^0, T^0) = (0.02, 0.9, 270)$. As constant offset u^* we choose, as in [7] where λ -tracking is treated for the same model, $u^* = 330$.

Note that the general result in Theorem 4 allows for a great flexibility in the design parameters. In the following simulations, we compare the effect of different funnels and gain functions in (7).

Simulations for noise-corrupted measurement is omitted due to space limitation. Our simulations have shown that noise is tolerated as proved in Theorem 4, but does not show any more interesting features.

3.1. Non-smooth funnel and nominal gain

As prespecified (non-smooth) funnels choose

$$\phi_1(t) = \max\{\bar{T} - T^* - 10t, \lambda\}, \quad \phi_2(t) = \max\{T^* - 250 - 80t, \lambda\},$$

the (nominal) gain function k is set, as in Section 1.4 suggested to

$$k(t) = K_F(t, e(t)) = \frac{1}{\text{dist}(e(t), \partial F_t)} = 1/\min\{\phi_1(t) - e(t), \phi_2(t) + e(t)\} \quad (14)$$

and the feedback is

$$u(t) = \text{sat}_{[295, 505]}(-k(t)[T(t) - 337.1] + 330).$$

For the set of simulations in this sub-section, we have chosen extreme parameters to illustrate the limitation of the adaptation mechanism. Although the controller still shows a satisfactory behaviour in the sense of the

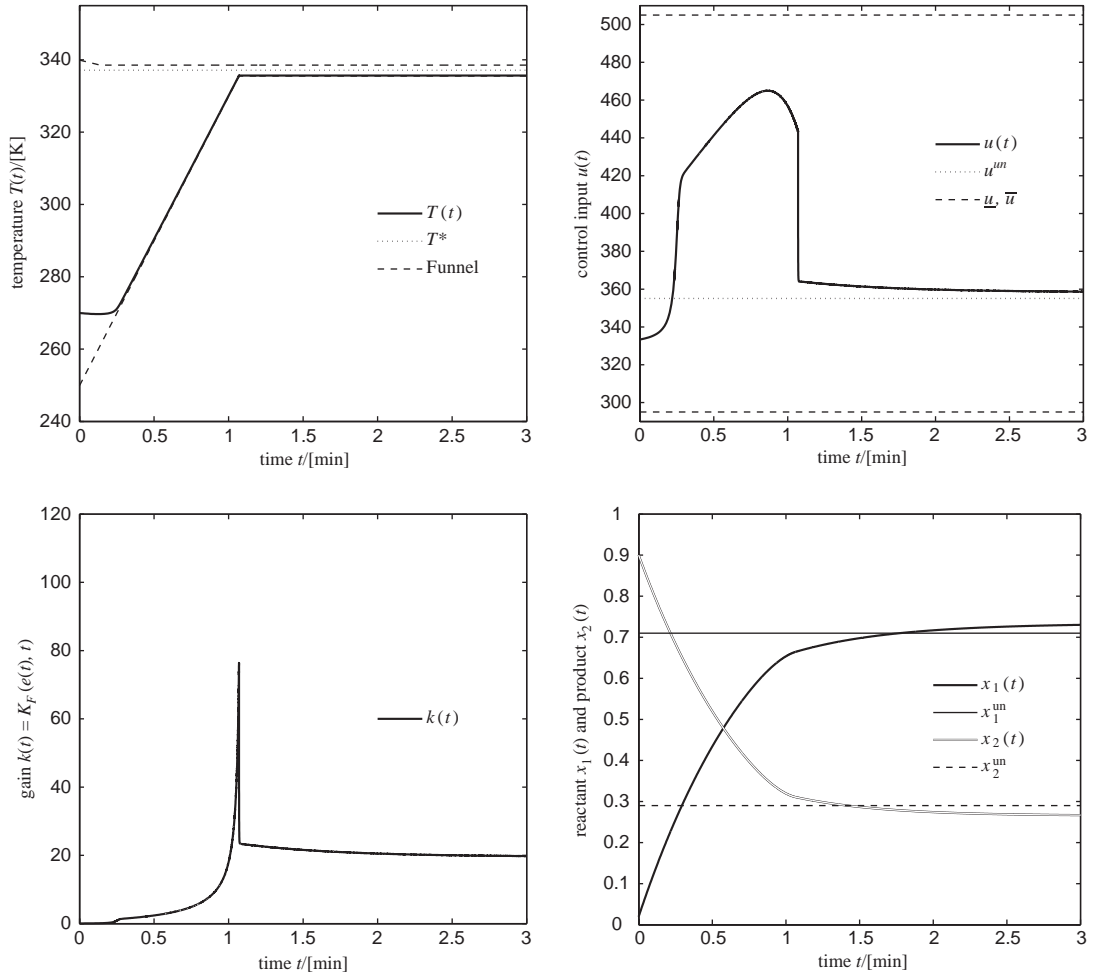


Fig. 2. Evolution of temperature $T(t)$, control input $u(t)$, gain $k(t) = 1/\text{dist}(e(t), \partial F(t))$ and concentrations of reactant $x_1(t)$, product $x_2(t)$ in presence of non-smooth funnel boundaries.

general result of Theorem 4, i.e. the temperature remains within the funnel and the reactant and the product tend to a neighbourhood of the unstable steady state (see Fig. 2), there is a significant steepness of $u(t)$ and $k(t)$ at $t \approx 0.25$ and at $t \approx 1.07$. The increase at $t \approx 0.25$ is due to the fact that the error is approaching the funnel boundary horizontally, and detecting it vertically too late. From then on until $t \approx 1$ the temperature is close to the funnel boundary and gets closer to the boundary while t increases; which yields the increase of $k(t)$. At $t \approx 1.07$ the funnel boundary is set to a constant so that the large $u(t)$ yields an overshoot of $T(t)$ (but within the funnel), resulting in a steep decrease of $k(t)$ and $u(t)$. Finally, $u(t)$ settles close to the component of the unstable steady state, whence all other variables settle, too.

Although the gain k is not actually implemented, but u is, a high k results in a high amplification of measurement noise. Note that $t \mapsto k(t)$ is not monotone and actually decreases to a fairly low value $k(t) \approx 20$. We evaluated by simulations that $\bar{k} \approx 28$ is sufficient to ensure that $T(t)$ stays within the non-smooth funnel when $u(t) = \text{sat}_{[295, 505]}(-\bar{k}[T(t) - 337.1] + 330)$ is applied. These results compare favourably with the λ -tracker introduced in [7]: for the identical set-up, the monotonically non-decreasing gain of the λ -tracker tends to $k(t) \approx 650$.

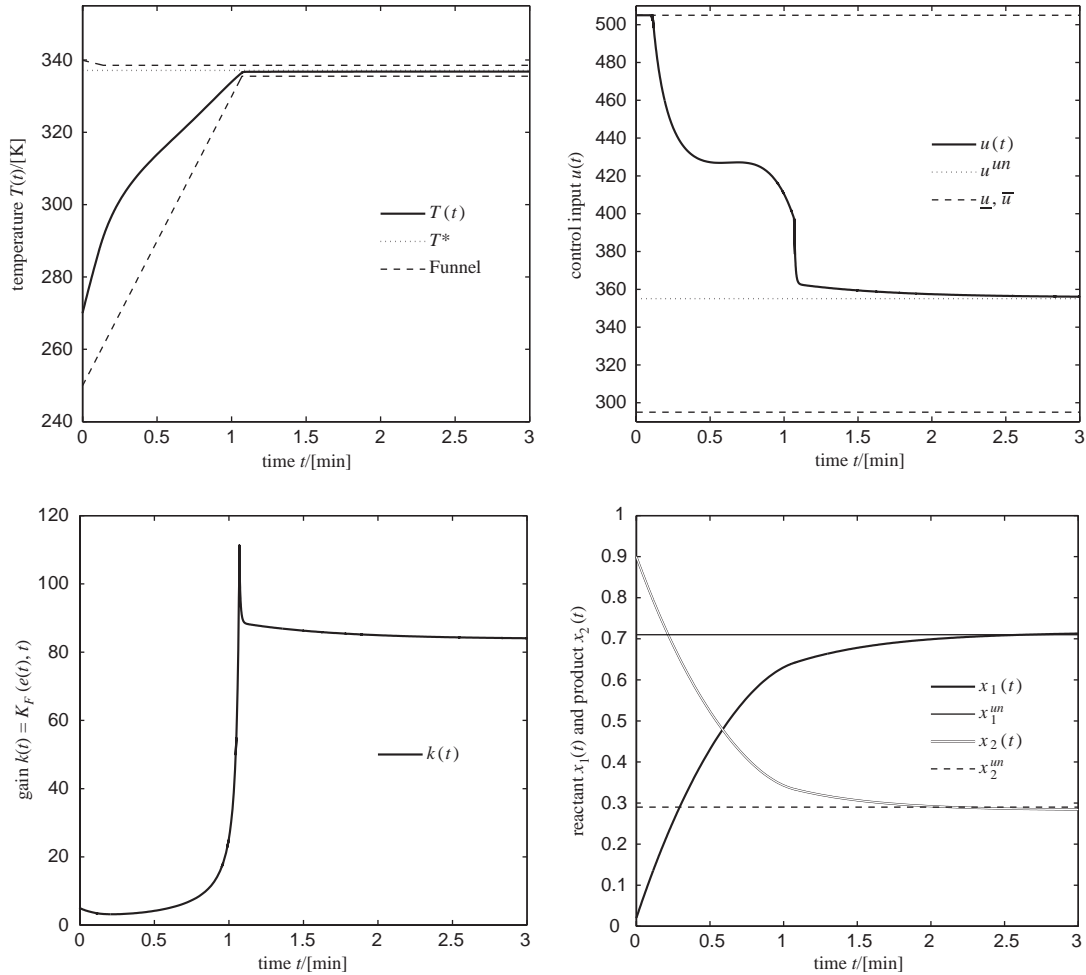


Fig. 3. Evolution of temperature $T(t)$, control input $u(t)$, scaled gain $k(t) = 100/\text{dist}(e(t), \partial F(t))$, and concentrations of reactant $x_1(t)$, product $x_2(t)$ for non-smooth funnel boundaries.

3.2. Non-smooth funnel and scaled gain

In this sub-section, the gain function is chosen more sensitively by multiplying the reciprocal of the distance by 100:

$$k(t) = 100 \frac{1}{\text{dist}(e(t), \partial F_t)}.$$

The error $e(t)$ is big over the initial interval $[0, 0.2]$ and therefore the product $k(t)e(t)$ is large, which results in a saturation of the input u (see Fig. 3). The control input u is less steeper, however there is still a steep increase of $k(t)$ and decrease of $u(t)$ at $t \approx 1.07$. This is due to the effect that the funnel boundary at $t = 1$ has an edge and the distance suddenly becomes very small. The steepness of $u(\cdot)$ is unsatisfactory. In future research, we will show that the unsatisfactory problem of steepness of $u(\cdot)$ and $k(\cdot)$ can be resolved by measuring the distance to the boundary of the funnel not only vertically but allows for future values.

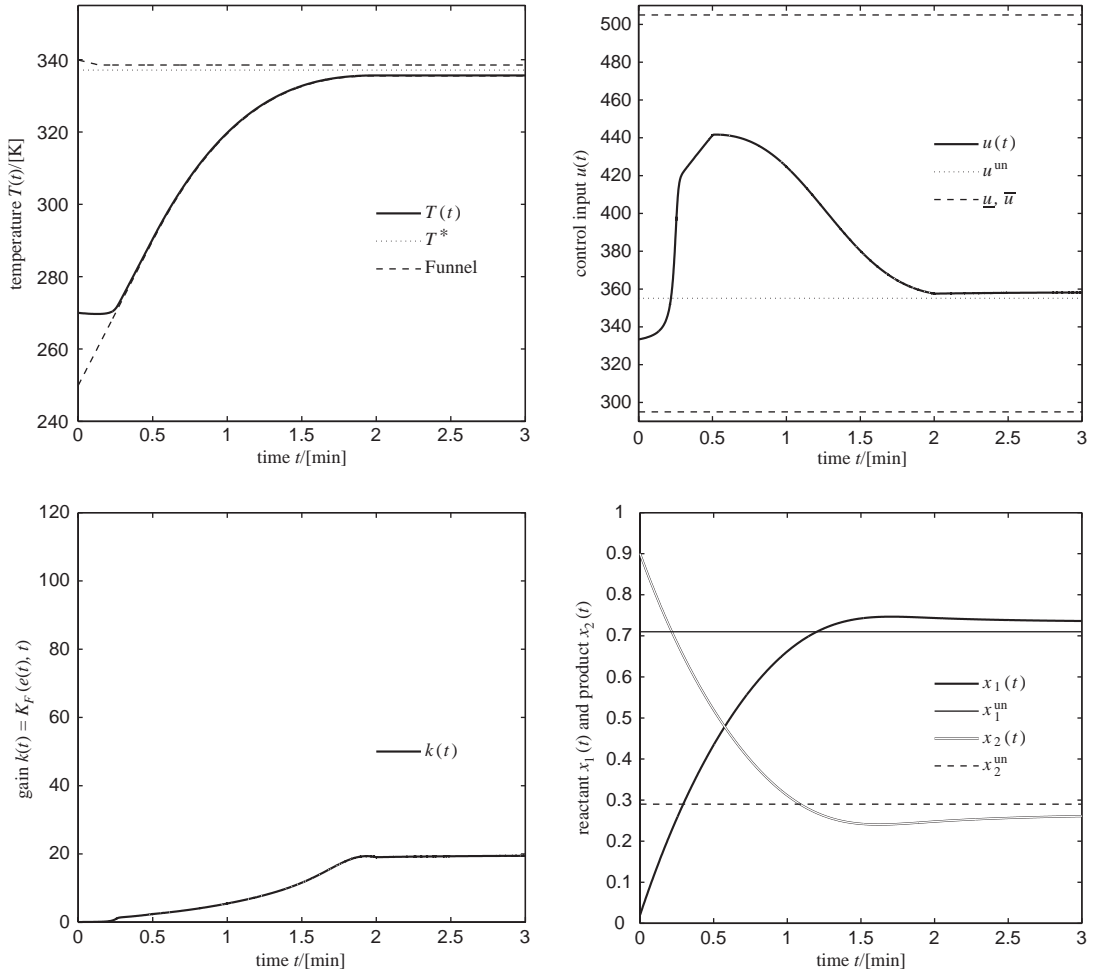


Fig. 4. Evolution of temperature $T(t)$, control input $u(t)$, gain $k(t) = 1/\text{dist}(e(t), \partial F(t))$ and concentrations of reactant $x_1(t)$, product $x_2(t)$ in presence of a smooth funnel boundary.

3.3. Smooth funnel and nominal gain

In this sub-section, we keep the nominal gain (14) but alter the lower funnel boundary to become a C^1 -function

$$\phi_1(t) = \max\{\bar{T} - T^* - 10t, \lambda\}, \quad \phi_2(t) = \begin{cases} T^* - 250 - 80t, & t \in [0, 0.5], \\ p(t), & t \in (0.5, 2), \\ \lambda, & t \geq 2, \end{cases}$$

where $p(\cdot)$ is a real polynomial with degree 3 which interpolates two linear functions (same value and derivative at the boundary points). As depicted in Fig. 4, the temperature T follows the lower funnel boundary while the nominal gain k stays on a low level and has no peaks. The input function u is effected by the C^1 -function choice of funnel: see $t = 0.5$.

It is worth noting that the gain is moderate compared to the simulations in Sections 3.1 and 3.2.

4. Proof of Theorem 4

Step 1: We show existence and uniqueness of the solution $(x, T, e) : [0, \omega) \rightarrow \Omega(\gamma, x^{\text{in}}) \times \mathbb{R}_{>0} \times \mathbb{R}$ of (12) on a maximally extended interval $[0, \omega)$, $\omega \in (0, \infty]$. Note that existence yields especially $(t, e(t)) \in F$, i.e. $e(t) \in F_t$, for all $t \in [0, \omega)$.

Introducing the artifact $z(t) = t$ and $e(t) = T(t) - T^* + \zeta(t)$, the closed-loop system (12) can be written as

$$\left. \begin{aligned} \dot{x} &= f_1(x, z, e), \\ \dot{z} &= 1, \\ \dot{e} &= f_2(x, z, e), \\ x(0) &= x^0 \in \Omega(\gamma, x^{\text{in}}), \quad e(0) = e^0 := T^0 - T^* + \zeta(0) \in F_0, \quad z(0) = 0, \end{aligned} \right\} \quad (15)$$

where

$$f_1 : \mathbb{R}_{\geq 0}^n \times \mathbb{R}_{\geq 0} \times \mathbb{R} \rightarrow \mathbb{R}^n, \quad (x, z, e) \mapsto Cr(x, e + T^* - \zeta(z)) + d[x^{\text{in}} - x]$$

and

$$f_2 : \mathbb{R}_{\geq 0}^n \times F \rightarrow \mathbb{R}, \quad (x, (z, e)) \mapsto b^T r(x, e + T^* - \zeta(z)) - q(e + T^* - \zeta(z)) + \text{sat}_{[u, \bar{u}]}(K_F(z, e)e + u^*) - \dot{\zeta}(z).$$

Introducing

$$f : \Omega(\gamma, x^{\text{in}}) \times F \rightarrow \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}, \quad (x, (z, e)) \mapsto (f_1(x, e)^T, 1, f_2(x, z, e)^T)^T,$$

the initial value problem (15) can be written as

$$\dot{X} = f(X), \quad X(0) = ((x^0)^T, 0, (e^0)^T)^T. \quad (16)$$

Since f is locally Lipschitz continuous, the theory of ordinary differential equations ensures that (16) has a unique solution

$$X : [0, \omega) \rightarrow \Omega(\gamma, x^{\text{in}}) \times F, \quad t \mapsto X(t) = (x(t)^T, t, e(t)^T)^T$$

for some $\omega \in (0, \infty]$, and ω can be maximally extended. This proves the claim.

Step 2: We show: If $\omega < \infty$, then $\lim_{t \rightarrow \omega} \text{dist}(e(t), \partial F_t) = 0$.

Introduce, for notational convenience,

$$d : [0, \omega) \rightarrow \mathbb{R}_{>0}, \quad t \mapsto \text{dist}(e(t), \partial F_t).$$

Note that

$$\text{dist}(e(t), \partial F_t) = \min\{\phi_1(t) - e(t), \phi_2(t) + e(t)\} \quad (17)$$

and therefore $d(\cdot)$ is continuous. Since $\phi_1(\cdot)$, $\phi_2(\cdot)$ are Lipschitz and $\dot{e}(\cdot)$ is, by (15), bounded on $[0, \omega)$, the function $d(\cdot)$ is even Lipschitz continuous.

Step 2a: We show: If $\omega < \infty$, then $\liminf_{t \rightarrow \omega} \text{dist}((t, e(t)), \partial F) = 0$.

The supposition $\omega < \infty$ implies, by invoking (16),

$$\liminf_{t \rightarrow \omega} \text{dist}((x(t), t, e(t)), \partial(\Omega(\lambda, x^{\text{in}}) \times F)) = 0.$$

By Remark 3 and $x(0) \in \Omega(\lambda, x^{\text{in}})$, the inequality $\inf_{t \in [0, \omega)} \text{dist}(x(t), \partial\Omega(\lambda, x^{\text{in}})) > 0$ holds true for $\omega < \infty$ and therefore

$$\liminf_{t \rightarrow \omega} \text{dist}((t, e(t)), \partial F) = 0.$$

Step 2b: We show: If $\omega < \infty$, then $\liminf_{t \rightarrow \omega} d(t) = 0$.

In passing by, we note that, for all $t \in [0, \omega)$,

$$\text{dist}((t, e(t)), \partial F) = \min \left\{ \inf_{\tau \geq t} \|(\tau, \phi_1(\tau)) - (t, e(t))\|, \inf_{\tau \geq t} \|(\tau, -\phi_2(\tau)) - (t, e(t))\| \right\}. \tag{18}$$

Seeking a contradiction, suppose that $\liminf_{t \rightarrow \omega} d(t) =: \underline{d} > 0$.

Since $\liminf_{t \rightarrow \omega} \text{dist}((t, e(t)), \partial F) = 0$, either there exists, by (18), a sequence $(t_n^1) \in [0, \omega)^\mathbb{N}$ with $t_n^1 \rightarrow \omega$ as $n \rightarrow \infty$ and

$$\inf_{\tau \geq t} \|(\tau, \phi_1(\tau)) - (t_n^1, e(t_n^1))\| = \inf_{\tau \geq t} \sqrt{(\tau - t_n^1)^2 + (\phi_1(\tau) - e(t_n^1))^2} < \frac{1}{n} \quad \forall n \in \mathbb{N},$$

or there exists a sequence $(t_n^2) \in (0, \omega)^\mathbb{N}$ with $t_n^2 \rightarrow \omega$ as $n \rightarrow \infty$ and

$$\inf_{\tau \geq t} \|(\tau, -\phi_2(\tau)) - (t_n^2, e(t_n^2))\| = \inf_{\tau \geq t} \sqrt{(\tau - t_n^2)^2 + (\phi_2(\tau) + e(t_n^2))^2} < \frac{1}{n} \quad \forall n \in \mathbb{N}.$$

Choose $i \in \{1, 2\}$ such that the inequality with respect to the sequence (t_n^i) is true, then there exists a sequence $(\tau_n) \in [0, \omega)^\mathbb{N}$ such that

$$|\tau_n - t_n^i| < \frac{1}{n} \quad \text{and} \quad |\phi_i(\tau_n) \mp e(t_n^i)| < \frac{1}{n} \quad \forall n \in \mathbb{N}_{>0}.$$

We may choose $N \in \mathbb{N}$ sufficiently large such that $|\tau_N - t_N^i| < \underline{d}/(2L_i)$, $|\phi_i(\tau_N) \mp e(t_N^i)| < \underline{d}/2$ and $d(t_N^i) > \underline{d}$. Then we arrive at the contradiction

$$\begin{aligned} \underline{d} &< d(t_N^i) \stackrel{(17)}{\leq} |\phi_i(t_N^i) \mp e(t_N^i)| \\ &\leq |\phi_i(t_N^i) - \phi_i(\tau_N)| + |\phi_i(\tau_N) \mp e(t_N^i)| \\ &\stackrel{(9)}{\leq} L_i |t_N^i - \tau_N| + |\phi_i(\tau_N) \mp e(t_N^i)| < \underline{d}/2 + \underline{d}/2 = \underline{d}. \end{aligned}$$

Therefore

$$\liminf_{t \rightarrow \omega} d(t) = 0 \tag{19}$$

holds true.

Step 2c: Finally, we show: If $\omega < \infty$, then $\lim_{t \rightarrow \omega} d(t) = 0$.

Seeking a contradiction suppose that there exists $\varepsilon > 0$ and $(t_n) \in [0, \omega)^\mathbb{N}$ with $t_n \rightarrow \omega$ and $d(t_n) > \varepsilon$. By (19) there exists $(s_n) \in [0, \omega)^\mathbb{N}$ with $s_n \rightarrow \omega$ and $d(s_n) < \varepsilon/2$. Since, $\omega < \infty$ we may assume, without restriction of generality, that $|t_n - s_n| < 1/n$ for all $n \in \mathbb{N}$. Since $d(\cdot)$ is Lipschitz continuous with Lipschitz constant $L > 0$ we arrive at the contradiction:

$$\varepsilon/2 < d(t_n) - d(s_n) < L|t_n - s_n| < L/n \quad \forall n \in \mathbb{N}.$$

This completes the proof of Step 2.

Step 3: We show $\omega = \infty$ and Assertion (i) and (ii).

Seeking a contradiction, suppose $\omega < \infty$. Then, by Step 2, $\lim_{t \rightarrow \omega} \text{dist}(e(t), \partial F_t) = 0$, and since $\text{diam}(F_t) = \phi_1(t) + \phi_2(t) \geq 2\lambda > 0$ for all $t \geq 0$ we have

$$\text{either } \lim_{t \rightarrow \omega} (\phi_1(t) - e(t)) = 0 \quad \text{or} \quad \lim_{t \rightarrow \omega} (\phi_2(t) + e(t)) = 0.$$

Case A: We show that $\lim_{t \rightarrow \omega} (\phi_1(t) - e(t)) = 0$ is not possible.

Choose $t_0 \in [0, \omega)$ such that $\phi_1(t) - e(t) < \lambda/2 \ \forall t \in [t_0, \omega)$. Then $e(t) > \lambda/2$ for all $t \in [t_0, \omega)$. Set $K_1 := (u^* - \underline{u})/(\lambda/2)$. Then by Property 1 in Section 1.4, there exists $\varepsilon_1 > 0$ such that for all $(t, e) \in F$ with $\text{dist}(e, \partial F_t) \leq \varepsilon_1$ we have $K_F(t, e) \geq K_1$. Choose now $t_1 \in [t_0, \omega)$ such that

$$\text{dist}(e(t), \partial F_t) = \phi_1(t) - e(t) \leq \varepsilon_1 \quad \forall t \in [t_1, \omega),$$

then

$$k(t) = K_F(t, e(t)) \geq K_1 \quad \text{and} \quad -k(t)e(t) + u^* < -K_1 \frac{\lambda}{2} + u^* = \underline{u} \quad \forall t \in [t_1, \omega).$$

Therefore,

$$u(t) = \text{sat}_{[\underline{u}, \bar{u}]}(-k(t)e(t) + u^*) = \underline{u} \quad \forall t \in [t_1, \omega).$$

Since $e(t) \in (\lambda/2, \phi_1(t))$ for all $t \in [t_1, \omega)$, we conclude

$$T(t) = T^* + e(t) - \zeta(t) \in [T^* + \lambda/2 - \zeta(t), T^* + \phi_1(t) - \zeta(t)]$$

$$\stackrel{(11)}{\subseteq} [T^*, \bar{T}] \quad \forall t \in [t_1, \omega),$$

and so (4) together with Remark 3 yields $\dot{T}(t) < -\rho_1$ for all $t \in [t_1, \omega)$. Since $\lim_{t \rightarrow \omega} (\phi_1(t) - e(t)) = 0$ and $\phi_1(t) - e(t) > 0$ for all $t \in [0, \omega)$, we may choose $s \in (t_1, \omega)$ such that

$$0 < \phi_1(s) - e(s) < \phi_1(t_1) - e(t_1),$$

then, for some $\hat{s} \in [t_1, s]$,

$$0 < \phi_1(t_1) - \phi_1(s) - (e(t_1) - e(s)) \leq -\underline{L}_1(s - t_1) - \dot{e}(\hat{s})(t_1 - s).$$

Since

$$\dot{e}(\hat{s}) = \dot{T}(\hat{s}) + \dot{\zeta}(\hat{s}) < -\rho_1 + \dot{\zeta}(\hat{s})$$

and, by (11) (ii), $\dot{\zeta}(\hat{s}) < \underline{L}_1 + \rho_1$, we arrive at the contradiction

$$0 < -\underline{L}_1(s - t_1) + \dot{e}(\hat{s})(s - t_1) < (-\underline{L}_1 + \dot{\zeta}(\hat{s}) - \rho_1)(s - t_1) < 0.$$

Therefore, the case $\lim_{t \rightarrow \omega} (\phi_1(t) - e(t)) = 0$ is not possible.

Case B: We show that $\lim_{t \rightarrow \omega} (\phi_2(t) + e(t)) = 0$ is not possible.

As in the first case there exists t_0 such that $\phi_2(t) + e(t) < \lambda/2$ for all $t \in [t_0, \omega)$ and therefore $e(t) < -\lambda/2$ for all $t \in [t_0, \omega)$ and furthermore, we may choose $t_2 \in [t_0, \omega)$ and $\varepsilon_2 > 0$ such that

$$u(t) = \bar{u} \quad \forall t \in [t_2, \omega).$$

Since

$$T(t) = T^* + e(t) - \zeta(t) < T^* - \lambda/2 - \zeta(t) \stackrel{(11)}{\leq} T^*,$$

the implication (5) yields $\dot{T}(t) > \rho_2$ for all $t \in [t_2, \omega)$. Choose $s \in (t_2, \omega)$ such that

$$0 < \phi_2(s) + e(s) < \phi_2(t_2) + e(t_2);$$

then, as in Case A, there exists $\hat{s} \in [t_2, s]$ and

$$0 < \phi_2(t_2) - \phi_2(s) + (e(t_2) - e(s)) \leq -\underline{L}_2(s - t_2) + \dot{e}(\hat{s})(t_2 - s) < (-\underline{L}_2 - \rho_2 - \dot{\zeta}(\hat{s}))(s - t_2).$$

This is a contradiction, because by (11) the inequality $-\underline{L}_2 - \rho_2 - \dot{\zeta}(\hat{s}) < 0$ holds true.

Summarizing, Cases A and B yield $\omega = \infty$, and hence Assertion (i) and (ii) follow from Step 1 and Remark 1.

Step 4: We show (iii).

Set

$$K := \max \left\{ \frac{\bar{u} - u^*}{\lambda/2}, \frac{u^* - \underline{u}}{\lambda/2} \right\},$$

choose $\hat{\varepsilon} > 0$ such that the implication in Property 1 is fulfilled for K , and let

$$\varepsilon := \min\{\lambda/2, \hat{\varepsilon}, \text{dist}(e(0), \partial F_0)\}.$$

If $\text{dist}(e(t), \partial F_t) \leq \varepsilon \leq \lambda/2$, then, by definition of λ in (9),

$$e(t) > \lambda/2, \quad \text{if } e(t) > 0 \quad \text{and} \quad e(t) < -\lambda/2 \quad \text{if } e(t) < 0,$$

and hence, by invoking the definition of K ,

$$-k(t)e(t) + u^* < \underline{u}, \quad \text{if } e(t) > 0 \quad \text{and} \quad -k(t)e(t) + u^* > \bar{u} \quad \text{if } e(t) < 0$$

This shows, that for all $t \geq 0$ we have

$$\text{dist}(e(t), \partial F_t) \leq \varepsilon \Rightarrow \begin{cases} u(t) = \underline{u} & \text{if } e(t) > 0, \\ u(t) = \bar{u} & \text{if } e(t) < 0. \end{cases} \quad (20)$$

It remains to show

$$\text{dist}(e(t), \partial F_t) \geq \varepsilon \quad \forall t \geq 0. \quad (21)$$

Seeking a contradiction to (21), suppose there exists $t_1 > 0$ such that $\text{dist}(e(t_1), \partial F_{t_1}) < \varepsilon$, and set

$$t_0 := \max\{t \in [0, t_1] \mid \text{dist}(e(t), \partial F_t) = \varepsilon\}.$$

Note that $t_0 \geq 0$ is well defined, since $\text{dist}(e(0), \partial F_0) \geq \varepsilon$ and $t \mapsto \text{dist}(e(t), \partial F_t)$ is continuous, and furthermore, $\text{dist}(e(t), \partial F_t) \leq \varepsilon$ for all $t \in [t_0, t_1]$ and therefore (20) yields $u(t) = \underline{u}$ for all $t \in [t_0, t_1]$ or $u(t) = \bar{u}$ for all $t \in [t_0, t_1]$. With

$$\text{dist}(e(t_0), \partial F_{t_0}) - \text{dist}(e(t_1), \partial F_{t_1}) = \begin{cases} \phi_1(t_0) - e(t_0) - (\phi_1(t_1) - e(t_1)) & \text{if } e(t_1) > 0, \\ \phi_2(t_0) + e(t_0) - (\phi_2(t_1) + e(t_1)) & \text{if } e(t_1) < 0, \end{cases}$$

and similar as in Step 3 together with (4) and (5) we arrive, for some $\hat{t} \in [t_0, t_1]$, either at the contradiction

$$0 < \text{dist}(e(t_0), \partial F_{t_0}) - \text{dist}(e(t_1), \partial F_{t_1}) \leq -\underline{L}_1(t_1 - t_0) - \dot{e}(\hat{t})(t_0 - t_1) < (-\underline{L}_1 + \dot{\xi}(\hat{t}) - \rho_1)(t_1 - t_0) < 0$$

or at the contradiction

$$0 < \text{dist}(e(t_0), \partial F_{t_0}) - \text{dist}(e(t_1), \partial F_{t_1}) \leq -\underline{L}_2(t_1 - t_0) + \dot{e}(\hat{t})(t_0 - t_1) < (-\underline{L}_2 - \rho_2 - \dot{\xi}(\hat{t}))(t_1 - t_0) < 0.$$

Therefore $\text{dist}(t, e(t)) \geq \varepsilon \quad \forall t \geq 0$.

Step 5: We show (iv).

Assertion (iii) applied to property 2 in Section 1.4 shows that there exists some $k_{\max} > 0$ so that Assertion (iv) holds. \square

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