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Regional Stabilization of Exothermal Plug-Flow Tubular (Bio) Reactors

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Abstract This paper presents a regional stabilization of an exothermal (bio)chemical process around a specified steady-state temperature and concentration profiles. These desired profiles provide a constant temperature equilibrium that has lead to a closed-loop steady-state behavior which is close to that of an isothermal process. To achieve the regional stability a nonlinear state estimator based on the component temperature measurements is included into a state feedback system so that there is no need for measuring the process component concentration. Performance issues are illustrated in a simulation study.

Keywords: *(bio)chemical process, compensator design, feedback stabilization, distributed parameter systems, nonlinear systems, tubular (bio)reactors*

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1. Introduction

System theory properties for distributed parameter systems have been the object of active research over the last decades. In this direction, a large research activity has been dedicated, mainly to the analysis and to the control design of distributed parameter tubular (bio)reactors (see [1,2,3] and the references quoted therein). However, a number of important questions remained unsolved so far, in particular, the stability of unstable equilibrium points of non-isothermal tubular (bio)processes and, papers in this topic are scattered in the literature [4,5,6]. In [4], the authors provide a discontinuous feedback stabilization which globally and regionally asymptotically stabilizes non-isothermal chemical tubular reactors around desired steady-states.

In this direction, this paper proposes an exponentially feedback stabilization with a region of attraction around an unstable profile in steady-state of an exothermal plug-flow (bio)chemical reactor, corresponding to an optimal coolant temperature, this desired profile provides a constant temperature equilibrium, that forces the (bio)process to have a closed-loop steady-state behavior which is close to that of an isothermal reactor. To achieve the regional stability around the desired region of attraction, a component concentration estimator is constructed and included into a closed-loop system based on the component temperature measurements without need of component concentration measurement which is normally unavailable in practice.

The dynamics of the (bio)process are given, for all time $t \geq 0$ and for all $z \in [0,1]$, by mass balance equations (see [4]):

$$\frac{\partial x_1}{\partial t} = -\upsilon \frac{\partial x_1}{\partial z} - \beta(x_1 - x_{in}) + \delta k_0 (1 - x_2) r(x_1), \qquad (1)$$

$$\frac{\partial x_2}{\partial t} = -\upsilon \frac{\partial x_2}{\partial z} + k_0 (1 - x_2) r(x_1) \qquad (2)$$

with the boundary and the initial conditions:

$$x_1(z=0,t) = 0, \quad x_1(z,t=0) = x_1^0, \qquad (3)$$

$$x_2(z=0,t) = 0, \quad x_2(z,t=0) = x_2^0 \qquad (4)$$

where $x_1(z,t), x_2(z,t), x_{in}(z,t), \upsilon$ and r are the temperature and the reactant concentration, the influent reactant concentration (mol/l), the fluid superficial velocity (m/s), and the reactant rate $(mol/l\,s)$. We assume that the kinetics depend only on the temperature x_1 and we consider a reaction rate model of the form $r(x_1) = \exp(\frac{\mu x_1}{1+x_1})$, where k_0 is the kinetic constant (s^{-1}). x_1^0, x_2^0 are the initial states.

The real constants β, μ are strictly positive, whereas the constant δ is strictly positive for of exothermic reaction and strictly negative for the endothermic reaction. In this paper, we investigate the case of exothermic reaction.

2. Notations and Preliminaries

Throughout the sequel, we assume $H = L^2[0,L]\times L^2[0,L]$, the Hilbert space with the usual inner product $\langle z_1, z_2\rangle = \langle x_1, x_2\rangle_{L^2} + \langle y_1, y_2\rangle_{L^2}$, for all $z_1 = (x_1, y_1)^T$ and $z_2 = (x_2, y_2)^T$ in H, and the induced norm defined by $\left\|(x_1, x_2)^T\right\| = \sqrt{\|x_1\|_{L^2}^2 + \|x_2\|_{L^2}^2}$ for all $(x_1, x_2)^T \in H$.

Clearly the Hilbert space H is a real Banach Lattice (for more details, see [7]) where,

$$x \le y \Leftrightarrow (\ x_1 \le y_1\ ,\ x_2 \le y_2\ )$$

for almost all $z \in [0,1]$
for all given

$$x = (x_1, x_2)^T \in H,\quad y = (y_1, y_2)^T \in H,$$

In the (bio)chemical process (1)-(4), x_{in} is considered as the control law. In order to facilitate our study we write the dynamic model (1)-(4) in terms of a nonlinear differential equation on H, viz., for all positive t and all initial condition $x_0 := (x_1^0, x_2^0)^T$ in H, on its abstract form as

$$\begin{cases} \dot{x}(t) = Ax(t) + N(x(t)) + Bu(t) \\ x(0) = x_0 \end{cases}$$

where, $\dot{x}$ stands for the time derivative of the state $x(t) = (x_1(.,t), x_2(.,t))^T$, and the linear operator A is defined by (see [1] for more details),

$$Ax(t) := \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \begin{pmatrix} -\upsilon\dfrac{d\cdot}{dz} - \beta & 0 \\ 0 & -\upsilon\dfrac{d\cdot}{dz} \end{pmatrix}\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$$

on its domain

$$D(A) = \left\{ \begin{array}{l} x := (x_1(t), x_2(t))^T \in H : x \ \ is \ \ absolutely. \\ continuous, \ \ \dfrac{dx}{dz} \in H, \ \ x_{i=1,2}(0) = 0 \end{array} \right\}$$

Remark 2.1 The linear operator A is non-positive definite on its domain $D(A)$, for all $x = (x_1, x_2)^T \in D(A)$,

$$\begin{aligned} < A_1x_1, x_1 > &= \int_0^L (-\upsilon\frac{dx_1(z)}{dz} - \beta x_1(z))x_1(z)dz \\ &= -\frac{1}{2}\upsilon\left[x_1^{\,2}(z)\right]_0^L - \beta\int_0^L x_1^{\,2}(z)dz \\ &\le 0 \end{aligned}$$

and

$$\begin{aligned} < A_2x_2, x_2 > &= \int_0^L -\upsilon\frac{dx_2(z)}{dz}x_2(z)dz \\ &= -\frac{1}{2}\upsilon\left[x_1^{\,2}(z)\right]_0^L \le 0 \end{aligned}$$

The control operator B is a bounded linear operator from IR^2 to H, which is defined by $B = \begin{pmatrix} \beta I \\ 0 \end{pmatrix}$. The control law $u(t) = x_{in}(t)$.

The nonlinear operator N is defined on

$$D := \left\{ \begin{array}{l} x = (x_1, x_2)^T \in H, \ \ 0 \le x_1(z) \ \ and \ \ 0 \le x_2(t) \le 1, \\ for \ \ almost \ \ all \ \ z \in [0,1] \end{array} \right\}$$

for all $x = (x_1, x_2)^T$ in D,

$$N(x) = \begin{pmatrix} N_1(x) \\ N_2(x) \end{pmatrix} := \begin{pmatrix} k_0\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} \\ k_0(1-x_2)e^{\frac{\mu x_1}{1+x_1}} \end{pmatrix} \qquad (5)$$

From physical point of view, it is expected that in the case of exothermic reaction, for all $(z,t) \in [0,1]\times[0,+\infty)$

$$-1 \le x_1(z,t) \le x_{1,\max}, -1 \le x_2(z,t) \le 1$$

where $x_{1,\max}$ could possibly be equal to $+\infty$ (see e.g. [4,8] and the references within)

Lemma 2.2 The nonlinear operator N given by (5) is l_N - Lipschitz on D, where

$$l_N := k_0e^{\mu}(1+\mu)(1+|\delta|).$$

Proof: Let $x = (x_1, x_2)^T$ and $y = (y_1, y_2)^T$ be in D then,

$$\|N(x) - N(y)\| = \max(\|N_1(x) - N_1(y)\|_{L^2}, \|N_2(x) - N_2(x)\|_{L^2})$$

Observe that $N_1 = \delta N_2$, therefore it is sufficient to prove that N_2 is a Lipschitz operator on D. Now for all

$$x = (x_1, x_2)^T \text{ and } y = (y_1, y_2)^T \text{ in } D,$$

$$\begin{aligned} &\|N_2(x) - N_2(y)\|_{L^2} \\ &= k_0\left\|(1-x_2)\exp(\frac{\mu x_1}{1+x_1}) - (1-y_2)\exp(\frac{\mu y_1}{1+y_1})\right\|_{L^2} \\ &\le k_0e^{\mu}\|x_2 - y_2\|_{L^2} + k_0\left\|\exp(\frac{\mu x_1}{1+x_1}) - \exp(\frac{\mu y_1}{1+y_2})\right\|_{L^2} \\ &\le k_0e^{\mu}(\|x_2 - y_2\|_{L^2} + \mu\|x_1 - y_1\|_{L^2}) \\ &\le k_0e^{\mu}(1+\mu)(\|x_2 - y_2\|_{L^2} + \|x_1 - y_1\|_{L^2}) \end{aligned}$$

Thus,

$$\|N_2(x) - N_2(y)\|_{L^2} \le k_0e^{\mu}(1+\mu)\|x - y\|_{L^2}$$

Whence N_2 is a Lipschitz operator on D. Thus we can take $l_N := k_0e^{\mu}(1+\mu)(1+|\delta|)$ as a Lipschitz constant of N.

3. Feedback Stabilization

The problem that arises is how to stabilize the nonlinear system (1)-(4) around a desired profile

$x_e = \left(x_e^1, x_e^2\right)^T$ solution of the following steady-state equation:

$$Ax_e + N(x_e) + Bv^* = 0 \tag{6}$$

under a prescribed control v^* that ensures the (optimal) profile x_d in the steady state.

In [5] temperature equilibrium profiles are studied that minimize different kinds of performance criterion. The following deals with the case where the performance criterion represents the energy consumption along the reactor. In [8] the author gives an unstable equilibrium profile that minimizes the energy consumption by

$$x_e(.) = \begin{pmatrix} 0 \\ 1-\exp(-\alpha_e .) \end{pmatrix}, \qquad x_{c,e}(.) = -\frac{k_0\delta}{\beta}\exp(-\alpha_e .)$$

Where,

$$\alpha_e = \frac{k_0}{\upsilon}\exp(-\frac{E}{RT_{in}})$$

with E, R, T_{in} are respectively the activation energy, the ideal gas constant, and the inlet temperature.

We aim in this paper to achieve a temperature feedback stabilization around this optimal profile.

3.1. State Observer Design

Hereafter we consider, as in [4], that the temperature $x_1(z,t)$ is the only available measurement on the system. In this case, as in [4], a simple component state observer for the dynamical system (1)-(4) is constructed as:

$$\frac{\partial \hat{x}_1}{\partial t} = -\upsilon\frac{\partial \hat{x}_1}{\partial z} - \beta(\hat{x}_1 - x_{in}) + \delta k_0(1-\hat{x}_2)r(x_1) \tag{7}$$

$$\frac{\partial \hat{x}_2}{\partial t} = -\upsilon\frac{\partial \hat{x}_2}{\partial z} + k_0(1-\hat{x}_2)r(x_1) \tag{8}$$

with the boundary and the initial conditions:

$$\hat{x}_1(z=0,t) = 0, \quad \hat{x}_1(z,t=0) = \hat{x}_1^0, \tag{9}$$

$$\hat{x}_2(z=0,t) = 0, \qquad \hat{x}_2(z,t=0) = \hat{x}_2^0 \tag{10}$$

The reconstruction error $e_2(z,t) = x_2(z,t) - \hat{x}_2(z,t)$ is shown to converge to zero.

Theorem 3.1: Consider the observer dynamics (7)-(10) for the controlled system (1)-(4). Let for all $z \in [0,1]$, $\hat{x}_1(z,0) = x_1(z,0)$, then the reconstruction error $e_2(z,t)$ has the property that $\|e_2(.,t)\|_{L^2} \le l\exp(-\mu t)$ for all initial error $e_2(.,0)$ satisfying the condition $\|e_2(.,0)\|_{L^2} \le l$ with a positive constant l.

Proof: Representing the observer dynamics (7)-(8) in terms of the reconstruction error $e_2(z,t)$ and differentiating the functional

$$V_2(t) = \|e_2(t)\|_{L^2}{}^2 \ (:= \int_0^L e_2^2(z,t)dz)$$

along the trajectories of the resulting error system, we obtain for all $t \ge 0$

$$\begin{aligned} \dot{V}_2(t) &= 2 < \dot{e}_2(t), e_2(t) >_2 \\ &= 2 < A_2 e_2(t), e_2(t) >_2 \\ &\quad - 2k_0 < r(x_1(t))e_2(t), e_2(t) >_2 \end{aligned}$$

by applying Remark 2.1, we have

$$\begin{aligned} \dot{V}_2(t) &\le -2k_0\int_0^L r(x_1(z,t))e_2^2(z,t)dz \\ &\le -2k_0 r_{\min} V_2(t). \end{aligned}$$

Thus,

$$V_2(t) \le V_2(0)\exp(-2k_0 r_{\min} t),$$

and that ensures the exponential stability of the error system, thereby yielding that

$$\|e_2(.,t)\|_{L^2} \le l\exp(-2k_0 r_{\min} t)$$

for all initial error $e_2(.,0)$ satisfying the condition $\|e_2(.,0)\|_{L^2} \le l$. The proof of the Theorem 3.1 is thus completed.

3.2. Temperature Feedback Stabilization

The aim of this section is to involve the system observer into a closed-loop system to achieve feedback stabilization of the temperature of (1)-(4), with the region of attraction containing a prescribed set of the form

$$\begin{aligned} &R_l(e_1, e_2) \\ &= \left\{ x_1(z), x_2(z) : \ \sqrt{\|x_1 - e_1\|_{L_2}^2 + \|x_2 - e_2\|_{L_2}^2} \le l \right\} \end{aligned}$$

In the sequel, such a stabilization is referred to as a regional stabilization.

The following control law is shown to regionally stabilize system (1)-(4) around the desired steady state:

$$\begin{aligned} x_{in}(t) = v^* &- \frac{k_0\delta l_N(\hat{x}_1(t) - x_e^1(t))}{\beta\left\|\hat{x}_1(t) - x_e^1(t)\right\|_{L^2}}\left\|\hat{x}(t) - x_e(t)\right\| \\ &+ \gamma(\hat{x}_1(t) - x_e^1(t)) \end{aligned} \tag{11}$$

where $\hat{x}(t) = \left(\hat{x}_1(t), \hat{x}_2(t)\right)^T$ is the output of the concentration observer (7)-(10) and g is a positive number .

Theorem 3.2: Let consider the dynamic temperature feedback controller (7)-(10) and (11) such that $\gamma > 0$. Then, the (bio)chemical process (1)-(4) is regionally exponentially stable around the optimal steady-state profile (6).

Proof: Let us represent the feedback controller (7)-(10) and (11) in term of the reconstruction error

$$\begin{aligned} \bar{e}(t) (:= (\bar{e}_1(t), \bar{e}_2(t)))^T \\ = \left(\hat{x}_1(t) - x_e^1, \hat{x}_2(t) - x_e^2\right)^T \end{aligned}$$

by

$$\begin{aligned} \frac{\partial \bar{e}_1}{\partial t} = &-\upsilon\frac{\partial \bar{e}_1}{\partial z} - \beta\bar{e}_1 - \frac{k_0 l_N \delta\|\bar{e}\|}{\|\bar{e}_1\|_{L^2}}\bar{e}_1 - \beta\gamma\bar{e}_1 \\ &+ k_0\delta((1-\hat{x}_2)r(x_1) - (1-x_e^2)r(x_e^1)), \end{aligned} \tag{12}$$

$$\frac{\partial \bar{e}_2}{\partial t} = -\upsilon \frac{\partial \bar{e}_2}{\partial z} + k_0((1-\hat{x}_2)r(x_1) - (1-x_e^2)r(x_e^1)) \quad (13)$$

$$\bar{e}_1(z=0,t)=0, \quad \bar{e}_1(z,t=0)=\bar{e}_1^0, \quad (14)$$

$$\bar{e}_2(z=0,t)=0, \quad \bar{e}_2(z,t=0)=\bar{e}_2^0, \quad (15)$$

Let now differentiating the functionals

$$\bar{V}_1(t) = \|\bar{e}_1(t)\|_{L^2}{}^2, \qquad \bar{V}_2(t) = \|\bar{e}_2(t)\|_{L^2}{}^2$$

along the trajectory (12)- (15), yields

$$\begin{aligned}\dot{\bar{V}}_1(t) &= 2 < \dot{\bar{e}}_1(t), \bar{e}_1(t) >_2 \\ &= 2 < A_1\bar{e}_1(t), \bar{e}_1(t) >_2 - 2\frac{k_0\delta l_N \|\bar{e}(t)\|}{\|\bar{e}_1(t)\|_{L^2}} < \bar{e}_1(t), \bar{e}_1(t) >_2 \\ &- 2\beta\gamma < \bar{e}_1(t), \bar{e}_1(t) >_2 \\ &+ 2k_0\delta < N_1(x_1(t), \hat{x}_2(t)) - N_1(x_e^1(t), x_e^2(t)), \bar{e}_1(t) >_2\end{aligned}$$

From Remark 2.1 and Lemma 2.2, we obtain for all $t \geq 0$

$$\begin{aligned}\dot{\bar{V}}_1(t) &\leq -2k_0\delta l_N \|\bar{e}(t)\|\|\bar{e}_1(t)\|_{L^2} - 2\beta\gamma\|\bar{e}_1(t)\|_{L^2}^2 \\ &+ 2k_0\delta l_N \|\bar{e}(t)\|\|\bar{e}(t)\|_{L^2} \\ &\leq -2\beta\gamma\bar{V}_1(t)\end{aligned}$$

Thus,

$$\bar{V}_1(t) \leq \bar{V}_1(0)\exp(-2\beta\gamma t),$$

Suppose $g > 0$, that ensures the exponential stability of the temperature error, yielding that

$$\|\bar{e}_1(.,t)\| \leq l\exp(-2\beta\gamma t)$$

for all initial error $e_1(.,0)$ satisfying the condition $\|\bar{e}_1(.,0)\| \leq l$, with a positive constant l.

Then, there exists a time $\bar{t}$ such that for all $t \geq \bar{t}$ the reconstruction error $\bar{e}_1(t)$ is maintained within the manifold

$$\bar{e}_1(t) = 0 \quad (16)$$

It follows that for all $t \geq \bar{t}$ the system motion along the manifold (16) is governed by

$$\frac{\partial \bar{e}_2}{\partial t} = -\upsilon \frac{\partial \bar{e}_2}{\partial z} + k_0((1-\hat{x}_2)r(x_e^1) - (1-x_e^2)r(x_e^1)) \quad (17)$$

with the conditions (13)-(14).

The derivative of the functional $\bar{V}_2(t) = \|\bar{e}_2(t)\|_{L^2}{}^2$ yields from Remark 2.1, for all $t \geq \bar{t}$

$$\begin{aligned}\dot{\bar{V}}_2(t) &= 2 < \dot{\bar{e}}_2(t), \bar{e}_2(t) >_2 \\ &= 2 < A_2\bar{e}_2(t), \bar{e}_2(t) >_2 \\ &+ < N_2(x_e^1, \hat{x}_2) - N_2(x_e^1, x_e^2), \bar{e}_2(t) >_2 \\ &\leq -2k_0 r_{\min} < \bar{e}_2(t), \bar{e}_2(t) >_2 \\ &\leq -2k_0 r_{\min} V_2(t)\end{aligned}$$

Thus,

$$\bar{V}_2(t) \leq \bar{V}_2(0)\exp(-2k_0 r_{\min} t)$$

More precisely, for all $t \geq \bar{t}$

$$\begin{aligned}\left\|x_1(t) - x_e^1\right\| &\leq l\exp(-2\beta\gamma t) \\ \left\|x_2(t) - x_e^2\right\| &\leq \left\|x_2(t) - \hat{x}_2(t)\right\| + \left\|\hat{x}_2(t) - x_e^2\right\| \\ &\leq 2l(\exp(-2k_0 r_{\min} t)\end{aligned}$$

Now, if $g > 0$, then the reconstruction errors $x_1 - x_e^1$ and $x_2 - x_e^2$ are exponential stability. The proof of the Theorem 3.2 is thus completed.

4. Simulation Results

In order to test the performance of the proposed observers, numerical simulations will be given with the following set of parameter values (see [4,5,8]):

$$\delta = 0.5 \qquad \upsilon = 0.025 m/s, \qquad L = 1m,$$
$$k_0 = 10^6 s^{-1}, \quad \beta = 0.05 s^{-1}, \quad T_{in} = 340K$$
$$E = 11.250 cal.mol^{-1}, \quad R = 1.986 cal.mol^{-1}.L^{-1},$$

The process model has been arbitrary initialized with the constant profiles $x_1(0,z) = 1, x_2(0,z) = 0, \hat{x}_1(0,z) = 0$, and $\hat{x}_2(0,z) = 1$. In order to response to the assumption of the Theorem 3.2 we set $\gamma = 1/\beta$ for the compensator design parameter.

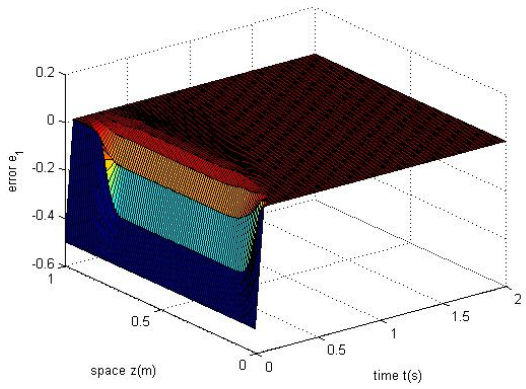

Figure 1. Evolution of the component temperature error $e_1 = x_1 - x_e^1$

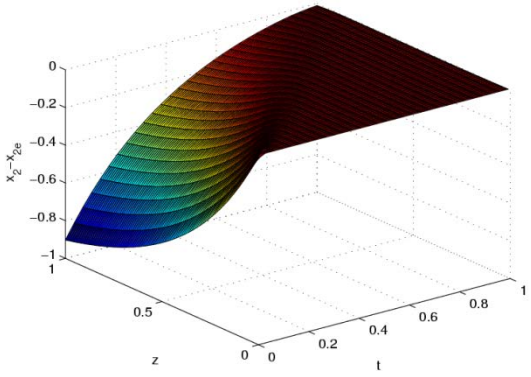

Figure 2. Evolution of the component concentration error $e_2 = x_2 - x_e^2$

Figure 1 and Figure 2 show respectively the time evolution in time and space of the temperature and concentration errors $x_1 - x_e^1$ and $x_2 - x_e^2$, it can be observed that the optimal equilibrium x_e is exponentially stable and, more precisely, the temperature converges exponentially to the constant temperature equilibrium.

It is proved as expected in the theoretical study that the error between the component state (1)-(4) and the optimal steady-state (6) converges exponentially to zero.

5. Conclusions

The exothermic reactors represent an interesting class of systems that may exhibit multiple steady states, either stable or unstable. In this paper, we present a conception of a regional exponentially feedback stabilization around an optimal unstable profile in steady-state when the temperature is the only available measurement on the system. This desired profile provides a constant temperature equilibrium, that has lead to a closed-loop steady-state behavior which is close to that of an isothermal reactor model. It is shown in the simulations that the given regional compensator is effective and satisfactory since it answers to difficulties of the reactant concentration measurements for a wide range of (bio)-chemical reactors.

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