Adaptive Control of Axial Dispersion Non Isothermal Tubular Reactor: A Nonlinear Model

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Abstract—This paper propose a relatively simple adaptive control (in the presence of input constraints) for a class of nonlinear distributed parameter models with application to a nonisothermal exothermic chemical tubular reactor with axial dispersion. Our objective is to regulate the reaction temperature in a pre-specified neighborhood of a given reference temperature. We apply a λ-tracking controller, only little information on the systems is needed to show that the tracking error tends asymptotically to a ball centred at the reference temperature and of arbitrary prescribed radius λ > 0.

I. INTRODUCTION

For many years a considerable interest has developed in the dynamics and control of non isothermal tubular reactors. The dynamics of this processes are described by non linear coupled partial differential equation and hence by distributed parameter models (e.g. [2]). A large research has been dedicated to the analysis of the existence of state trajectories and to the analysis of the equilibrium profiles in tubular reactors ([6] and the references therein), more recently to the control design based on distributed parameter linearized models and to system theoretical properties of such models. The main obstacle lies in the nonlinearity of the reaction kinetics which are complex function of some variables of the process. Another difficulty is certainly due to the physical constraints which are inherent to the process input. In this paper we consider an input constrained adaptive output feedback controller for a nonlinear distributed parameter exothermic reaction models in tubular reactor. The main objective of this work is to regulate the reaction temperature in a pre-specified neighborhood of a given reference temperature. To achieve our objective we adopt an approach based on the modified λ-tracking controllers which is originally developed in finite dimensional context for similar problems [5] and adapt it to the class of systems considered in this paper. This control strategy was also applied to the linear infinite dimensional systems without input constraint by A. Ilchmann and coworkers [4], the output is not required to converge exactly to reference signal but to a ball of radius λ > 0.

The paper is organized as follows. In the second section we present the basic dynamical model, and use a new formulation of the problem within the framework of the semi-linear systems to transform the addressed boundary control problem to a semi-group formulation with distributed control action. Finally the main results on the λ-tracking are given and the theoretical result are illustrated via numerical simulation.

II. TUBULAR REACTOR MODEL

Let us consider a nonisothermal reactor with the following chemical reaction:

\[ A \rightarrow bB \]

where \( b > 0 \) denote the stoichiometric coefficient of the reaction. The dynamics of this process in an exothermic tubular reactor with axial dispersion are given, for all time \( t > 0 \) and for all \( z \in [0, L] \), by the following mass and energy balance equations:

\[
\frac{\partial T}{\partial t} = D_1 \frac{\partial^2 T}{\partial z^2} - v \frac{\partial T}{\partial z} + \alpha f(T, C) - k_0(T - T_c)
\]

\[
\frac{\partial C}{\partial t} = D_2 \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial z} - f(T, C)
\]

with the boundary conditions:

\[
-D_1 \frac{\partial T}{\partial z}(0, t) = v(T_{in}(t) - T(0, t))
\]

\[
-D_2 \frac{\partial C}{\partial z}(0, t) = v(C_{in}(t) - C(0, t))
\]

\[
\frac{\partial T}{\partial z}(L, t) = 0, \quad \frac{\partial C}{\partial z}(L, t) = 0
\]

where \( k_0 = \frac{4\sigma}{\rho C_p d} \)

so and where \( L \) is the reactor length.

In the above equations, \( T(t, z), C(t, z), D_1, D_2, v, \rho, C_p, \sigma, d, T_c, T_{in}, C_{in} \) hold for the temperature reactor, the reactant concentration, the energy and mass dispersion coefficients, the superficial fluid velocity, the density, the specific heat, the wall heat transfer coefficient, the reactor diameter, the coolant temperature, the inlet temperature, the inlet concentration, respectively and \( f(T, C) \) is a nonlinear locally Lipschitz function with \( f(T, C) \geq 0 \) for all \( T > 0 \) and \( C \geq 0 \) and models the reaction kinetics and \( \alpha \) is constant. The typical example of \( f \) is the first order kinetics with respect to the reactant concentration \( C \) and by Arrhenius-type dependence with respect to the temperature \( T, f(T, C) = k C_e x p(-\frac{E}{RT}) \) where \( k \) is the kinetic constant, \( E \) is the activation energy, and \( R \) is the ideal gas constant.
III. STATE SPACE FRAMEWORK

To regulate the temperature of the reactor in a prespecified neighborhood of a given reference temperature $T^*$, the inlet and coolant temperatures are considered as the control action. This implies that our problem is a non linear boundary control problem. An important prior step is to obtain a description of the model as an infinite-dimensional system in semi group formulation. For this reason, setting $T(t, z) = x_1(t)z$ and $C(t, z) = x_2(t)z$ with $x_1(.)$ and $x_2(.)$ in $H$, where $H = L^2(0, L)$ the usual Hilbert space of measurable square-integrable function endowed with the usual inner product and the usual order. We transform our system to a semi-linear system, for this setting we rewrite (1) and the boundary condition (3) in the context of Fattorini model of boundary control (see [3]) as follows:

\begin{align}
\dot{x}_1(t) &= A_1x_1(t) + \alpha f(x_1(t), x_2(t)) + u(t) \\
\dot{x}_2(t) &= -A_2(x_2^n(t) - x_2(t)) - f(x_1(t), x_2(t))
\end{align}

where $u = v\Delta_0 T_{in} + k_0 T_{ex}$, for physical reasons, we assume that $u$ is constrained so that $\underline{u} \leq u \leq \overline{u}$ where $\underline{u}, \overline{u}$ are as follows $0 < \underline{u} < \overline{u}$. $A_1$ is the linear operator defined on $D(A_1) = \{ x : x, \frac{dx}{dz} \in H, D_1\frac{dx}{dz}(0) - \nu(x) = 0, \frac{dx}{dz}(L) = 0 \}$ (where a.c means $x$ is absolutely continuous) by

\begin{equation}
A_1x = D_1\frac{d^2x}{dz^2} - \nu \frac{dx}{dz} - k_0x
\end{equation}

and $A_2$ is as follows:

\begin{equation}
A_2x = D_2\frac{d^2x}{dz^2} - \nu \frac{dx}{dz}
\end{equation}

$D(A_2) = \{ x : x, \frac{dx}{dz} \in H, D_2\frac{dx}{dz}(0) - \nu(x) = 0, \frac{dx}{dz}(L) = 0 \}$

The function $\Delta_h(.)$ is given by:

\begin{equation}
\Delta_h(z) = \begin{cases} 
\frac{1}{h} & 0 \leq z \leq h \\
0 & h < z \leq L
\end{cases}
\end{equation}

To achieve our control objective, we apply a simple adaptive controller of the form:

\begin{align}
e(t) &= x^* - x_1(t) \\
u(t) &= sat_{[\underline{u}, \overline{u}]}(\beta(t)e(t) + u^*) \\
\dot{\beta}(t) &= k_1 \begin{cases} 
\{ ||e(t)|| - \lambda \}^l & \text{if } ||e(t)|| > \lambda \\
0 & \text{if } ||e(t)|| \leq \lambda
\end{cases}
\end{align}

The constant $\lambda > 0$ is an upper bound for the asymptotic tracking error, $l \geq 1$, $k_1$, $\beta_0 > 0$ are chosen by the user, and $u^* \in (\underline{u}, \overline{u})$ is a constant offset.

The adaptive $\lambda$ tracker consists of a proportional error feedback with saturation and a time-varying proportional gain $\beta(.)$ determined adaptively by the measurement error only. The power $l$ in the gain adaptation influences the speed of adaptation, a similar effect can be achieved by varying $k_1$ or the initial gain $\beta_0$. The constant $u^*$ is an input reference. The following assumptions are made:

- $(H_1)$ the positif cone $H^+ \times H^+$ is positively invariant under (1-4) for all nonnegative control $u(.)$.
- $(H_2)$ For $x^* > 0$ there exist $0 < \underline{u} < \overline{u}$, such that

\begin{equation}
\begin{cases}
\underline{u} + \rho \leq k_0 x_1 - \alpha \nu(x_1, x_2) - Az^* \leq \overline{u} - \rho \\
D_1 \frac{d^2(z-x^*)}{dz^2} - \nu(\alpha(x_1, x_2) - Az^*) \leq 0
\end{cases}
\end{equation}

where $Az^* = D_1 \frac{d^2z^*}{dz^2} - \nu \frac{dz^*}{dz}$

- $(H_3)$ $0 \leq \lambda < \overline{u} - x^*$, $0 < \underline{u} < \overline{u} - x^*$

Remark 1: Assumption $(H_2)$ is natural for exothermic reactors. Indeed, the concentration and temperature should not become zero once they are positive, if the inlet temperature and the inlet concentration are strictly positive. Assumption $(H_2)$ guarantees the feasibility by relaxing the temperature set point $x^*$ and the positive input saturations $\underline{u}, \overline{u}$ to system data. Note that the first part of the assumption $H_2$ is similar to $A_1$ in [5].

The upper bound $\overline{u}$ depends not only on the feasibility condition $H_2$ but also on the physical limitations of the actuator when both conditions are compatible, i.e., the actuator limit is higher than the bound in $H_2$, $\underline{u}$ is chosen so that feasibility condition $H_2$ and saturation bound are checked. We assume without loss of generality that $L = 1$.

IV. ADAPTIVE $\lambda$ TRACKING

To achieve the main objective of this work, we present two feedback strategies that force the temperature into a $\lambda$-neighborhood of the given set point. The first is local, while the second one is global.

A. local tracking

In this part, we consider local $\lambda$- set-point control in the sense that the initial temperature $x_1(0)$ is constrained to be in the set $\Delta_1$ defined here below.

The main result of this section is the following theorem;

Theorem 1: Assume that $H_1$, $H_2$, and $H_3$ hold, and $(x_1(0), x_2(0)) \in \Delta_1 \times \Delta_2$ and suppose:

\begin{equation}
\beta(0) \geq \frac{u^* - \underline{u}}{\overline{u} - x^*}
\end{equation}

the closed loop system given by equations (6)-(7) and (10) has the following properties:

\begin{enumerate}
\item $x_1(.), x_2(.) \Rightarrow \Delta_1 \times \Delta_2 \times \mathbb{R}_{\geq 0}$
\item $\lim_{t \to +\infty} \beta(t)$ exists and is finite.
\item $\lim_{t \to +\infty} \frac{\|e(t)\|}{\lambda}$
\end{enumerate}
Where $\Delta_1$ and $\Delta_2$ are given by:

$$\begin{align*}
\Delta_1 &= \{x_1 \in H \text{ such that } 0 \leq x_1 < \pi\}, \\
\Delta_2 &= \{x_2 \in H \text{ such that } 0 \leq x_2 \leq x_2^n\}
\end{align*}$$

For the proof of this result we refer the reader to [8]. Note that the only information needed for the $\lambda$ tracker (10) to work is that the initial gain parameter $\beta(0)$ is sufficiently large as determined from knowledge of the upper feasibility bound $\pi$, reference signal $u^*$, the offset control $u^*$ and $\pi$.

The following example is quoted from [7] and illustrate our approach.

**example 1:** We consider the system (6-7) with reaction kinetics modelled by the Arrhenius law in temperature $f(x_1,x_2) = k x_2 e^{-E/R x_1}$. The objective is to regulate the temperature in a neighborhood of $x^* = 480$. The constraints for the input $U$ are chosen as follows:

$$u = 5179, \quad u^* = 5199, \quad \pi = 7800$$

It is easy to see that in this case the assumptions $H_1$, $H_2$, $H_3$ are satisfied if $\pi = 700[K], \quad \bar{\pi} = 400[K], \quad \rho = 0.2, \quad k_1 = 4, \quad l = 3, \quad x_2(0) = C_{in}[mol/l] = 0.2 \lambda = 2$ and the initial gain $\beta(0) = 40$.

The result of the simulations are shown in Figure (1-2), It can be observed that the temperature in the reactor tend asymptotically to the ball centred at the reference signal $x^* = 480[K]$ and of radius $\lambda > 0$ and the convergence of the adaption law.

**B. Global tracking**

The main result of the previous section, has the shortcoming in that it is local in the sense that the initial temperature must lie inside $(0, \pi)$. With such a control law, it may even be impossible to reduce the temperature of the reaction from such reference temperature by any type of control of the temperature alone. To overcome this problem, we borrow an idea from [5] to introduce an additional open loop control of the feedrate of reactant.

The overall model (6-7) is then replaced by

$$\begin{align*}
\dot{x}_1(t) &= A_1 x_1(t) + \alpha f(x_1(t),x_2(t)) + u(t) \\
\dot{x}_2(t) &= A_2 x_2 - f(x_1(t),x_2(t)) + v \Delta u V(t)
\end{align*}$$

(15)  \hspace{1cm} (16)

where $u = v \Delta u t_{in} + k_0 T_c$ and $V = C_{in}$, we assume that $u$ and $V$ are constrained so that:

$$u \leq u \leq \pi \quad 0 \leq V \leq c_{in} = x_{2}^n$$

where $c_{in}$ is the inlet reactant concentration supposed to be a positive constant.

The additional input $V$ is given as follows:

$$V(\beta e)(z) = \begin{cases} 0 & \text{if } \beta e(z) \in G_1 \\ g(\beta e(z)) & \text{if } \beta e(z) \in G_2 \\ c_{in} & \text{if } \beta e(z) \in G_3 \end{cases}$$

(17)

where $g(\beta e(z)) = (\beta e(z) - u + u^*) c_{in}/\delta$,

$\delta$ is sufficiently small positive constant and

$$G_1 = (-\infty, u - u^*), G_2 = (u - u^*, u - u^* + \delta)$$

$$G_3 = (u - u^* + \delta, +\infty)$$

In this global case, the assumption $(H_2)$ on the reaction kinetics must be strengthened to:

$$(H_1)$$ There exist a function $\hat{f}$ such that:

for all $0 \leq x_1$ and $0 \leq x_2 \leq c_{in} f(y_1,y_2) \leq \hat{f}(y_2)y_1$ for all $y_1 \geq 0$ and $0 \leq y_2 \leq x_2^n$ with $\lim_{y \rightarrow 0} f(y) = 0$

Our objective is to emphasize the asymptotic convergence of the temperature into a $\lambda$–neighborhood of a given temperature $x^*$.

The following theorem is the main result of this part.

**Theorem 2:** Assume that $H_1$, $H_2$, $H_3$, $H_4$ hold and

$$(A_1)^{-1} u(1) < \pi$$

Then the closed loop system has the following properties:

$$\begin{align*}
(1) & \quad x_1(.), x_2(.), \beta(.) : R_{\geq 1} \rightarrow X \\
& \quad (X = H^+ \times \{x_2 \in H : 0 < x_2 < c_{in}\} \times R_{\geq 0}) \\
(2) & \quad \lim_{t \rightarrow +\infty} \beta(t) \text{ exists and is finite.} \\
(3) & \quad \limsup_{t \rightarrow +\infty} \|c(t)\| \leq \lambda
\end{align*}$$

To fulfill hypotheses (18), we must calculate the inverse operator of $A_1$, however from Lemma 5.2 in [6] we can replace this hypothesis by:

$$u < k_0 \pi$$

(19)

**example 2:** We use some parameter of the previous section and

$$u = 5179, \quad \pi = 9100$$

the reference input $u^* = 5199$, $\bar{\pi} = 400$, $\rho = 0.22$, $w = 0.33$

the initial gain $\beta(0) = 40$, $\delta = 0.1$, $k_1 = 4 l = 3$, $\lambda = 1$ and the initial temperature $x_1(0) = 800[K]$.

Figure (3-4) shows that the obtained numerical results are in agreement with the theoretical results, $x_1$ tend asymptotically to a neighborhood of $x^* = 480$ and the gain $\beta(t) \approx 1400$ for all time $t > 1s$.

**V. Conclusion**

In the present paper we have developed a $\lambda$-tracking approach to the set-point control of the temperature for a nonlinear distributed parameter exothermic chemical reaction in tubular reactor with axial dispersion in presence of input constraint. The novelty of this work is the use of nonlinear distributed parameters model with boundary control. Under a simple a feasibility assumptions we have shown that the tracking objective is achievable.
Fig. 1. Temperature of the closed loop system for $x_1(0) = 600$

Fig. 2. Adaptation gain for $x_1(0) = 600$

Fig. 3. Temperature of the closed loop system

Fig. 4. Adaptation gain

Fig. 5. Temperature at several points along the reactor.

REFERENCES


