

Adaptive Proportional-Integral Control Design for a Class of Continuous Stirred Tank Reactors with Uncertain Parameters

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ARTICLE INFO

Received: 30/04/2024
Revised: 28/07/2024
Accepted: 06/08/2024
Published: 28/12/2024

KEYWORDS

Chemical reactor;
Temperature regulation;
Control theory;
Lyapunov function;
Non-isothermal reactor.

ABSTRACT

Mathematical model of reaction systems contains experimental parameters such as reaction enthalpies, which may be inaccurate and, therefore, severely affect the computation as well as the implementation of feedback control laws. This paper aims to design an adaptive PI-like controller to regulate a chemical reaction system by means of the Lyapunov theory. More precisely, uncertain model parameters are updated online by solving a set of ordinary differential equations while the global asymptotic convergence of closed-loop system trajectories towards the desired equilibrium is ensured by using the proposed adaptive PI-like controller under the assumption of stability of isothermal conditions. The applicability of theoretical developments is illustrated with an irreversible first-order reaction system having multiple steady states and taking place in a non-isothermal continuous stirred tank reactor. Simulation results show that system trajectories initiated at different conditions are asymptotically stabilized at the desired values and the closed-loop system is robust against the uncertainty of heat exchange coefficient and dilution rate.

Doi: <https://doi.org/10.54644/jte.2024.1570>

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1. Introduction

From the viewpoint of mathematical modeling, the dynamics of continuous stirred tank reactors (CSTR), including material and energy balance equations, can be described by a set of ordinary differential equations (ODEs) [1], [2] and affected not only by reaction kinetics but also by transport phenomena with the presence of inlet and outlet streams, thereby giving rise to typical nonlinear behaviors such as input/output multiplicity, non-minimum phase behavior or limit cycle [3], [4]. In practice, these behaviors possibly cause the internal instability and restrict the nonlinear chemical processes themselves to achieve the desirable performance [5]-[7].

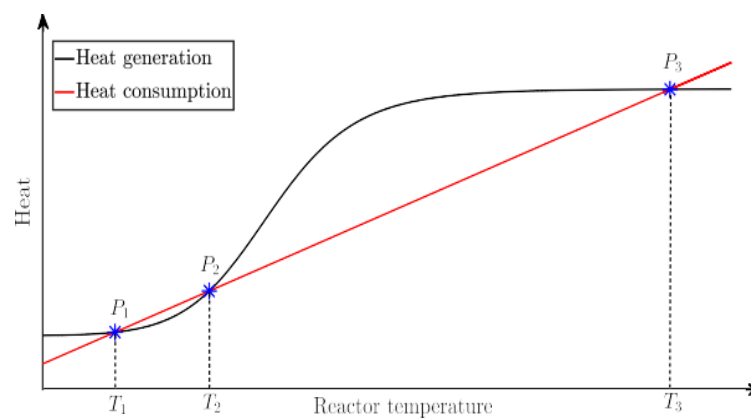


Figure 1. Van Heerden diagram of a first-order exothermic reaction system

For example, we consider an irreversible first-order exothermic reaction with the stoichiometry $A \rightarrow B$, occurring in a CSTR with one inlet stream and one outlet stream. The Van Heerden diagram that shows a graphical representation of heat generation and heat consumption with respect to reactor temperature at steady state [8] is given in Figure 1. Clearly, there are three intersections between these curves, namely P_1 , P_2 and P_3 , that corresponds to three steady states of the reaction system. Besides, P_1 and P_3 are locally stable, while P_2 is unstable because the reactor temperature changes to its new value T_1 (or T_3) corresponding to a temperature drop (or rise) from T_2 since the curve of heat consumption is above (or below) the one of heat generation. Although it is preferable to operate the reactor at P_2 to compromise both economic benefit and engineering constraints [6], [7], it is not possible to stabilize the reactor at this point without feedback control owing to the steady-state multiplicity behavior. To handle this challenging issue, numerous control methods such as passivity-based approach [4], [9], physics/energy-based method [3], [10], [11] and model predictive control [12] have been proposed for last few decades. However, these studies have only assumed to know a perfect model reactor, having no parameter uncertainties in the design of feedback laws. It is important to note that these uncertainties can cause inaccurate control actions that may affect the control performance. In this paper, we consider a parameter uncertainty, caused by reaction enthalpies¹, and aim to design an adaptive version of a proportional-integral-like control for regulating reactor temperature. It should be noted that from the thermodynamic viewpoint, reaction enthalpies, depending on reactor temperature, are computed from reference component molar enthalpies, which are determined from experiments and possibly the source of model uncertainties [13]. Interestingly, it will be shown that by constructing a suitable parameter update law, the global asymptotic stabilization of closed-loop system at the desired equilibrium point is guaranteed, which is the main contribution of this work.

The rest of this paper is organized as follows. Section 2 briefly reviews the CSTR model and positions the control objective. The main result, related to the development of an adaptive proportional-integral (PI) control with a parameter update law, is represented in Section 3. An irreversible first-order reaction system is utilized as a case study to illustrate the proposed control method in Section 4, while the conclusion is given in Section 5.

2. Dynamical model of non-isothermal chemical reactors

We consider here a reaction system, where R independent reactions with S components take place in a CSTR. The stoichiometry is given as follow:

$$\sum_{s=1}^S \nu_{rs} M_s = 0, \quad r = 1, 2, \dots, R,$$

where M_s is the molar mass of the s^{th} species and ν_{rs} is the suitably signed stoichiometric coefficient of the s^{th} component in the r^{th} reaction.

Remark 1

The coefficient ν_{rs} is positive, i.e. $\nu_{rs} > 0$, if the species is a reactant, and the coefficient ν_{rs} is negative, i.e. $\nu_{rs} < 0$, if the species is a product. Also, the coefficient ν_{rs} is equal to zero, i.e. $\nu_{rs} = 0$, for catalysis, solvent or inert.

For the purpose of modeling, the following assumptions, also used in [14], [15], is made throughout the paper.

Assumption 1

The reacting mixture is perfectly mixed, ideal and incompressible. On this basis, the concentrations of all species together with the reactor temperature are uniformly distributed throughout the reactor. Additionally, the reaction system occurs in the liquid phase and there is no friction caused by the mixing

process.

Assumption 2

All components are continuously fed to the reactor via only one inlet stream at a fixed inlet temperature and a fixed dilution rate, denoted by T_{in} and d , respectively. Also, the specific heat capacities of species, denoted by $c_{p,s}$ with $s = 1, 2, \dots, S$, are constant.

Assumption 3

The rate of heat flow from the jacket to the reacting mixture, denoted by $q_{ex}(t)$, can be modeled as follows:

$$q_{ex}(t) = \lambda(T_j(t) - T(t)) \quad (1)$$

where $T_j(t)$ and $T(t)$ are the jacket and reactor temperatures, respectively, and λ is the heat transfer coefficient.

Under the Assumptions 1–3, the mathematical model of the CSTR can be written in the following compact form [14], [15]:

$$\begin{cases} \dot{\mathbf{n}}(t) = \mathbf{N}^T \mathbf{r}_v(t) + d(\mathbf{n}_{in} - \mathbf{n}(t)), & \mathbf{n}(0) = \mathbf{n}_0, \\ \dot{H}(t) = q_{ex}(t) + d(H_{in} - H(t)), & H(0) = H_0, \end{cases} \quad (2)$$

where

- $\mathbf{n}(t)$ and \mathbf{n}_{in} are the S -dimensional vector of numbers of moles with the initial value \mathbf{n}_0 at time t and the one of the inlet stream, respectively,
- $\mathbf{r}_v(t) = [r_{v,1}(t) \ r_{v,2}(t) \ \dots \ r_{v,R}(t)]^T$ is the R -dimensional vector of reaction rates at time t ,
- $\mathbf{N} \in \mathbb{R}^{R \times S}$ is the stoichiometric coefficient matrix,
- $H(t)$ and H_{in} represent the enthalpy of the reaction system with the initial value H_0 at time t and the one of the inlet stream, respectively.

Remark 2

The enthalpy of reaction system $H(t)$ is computed by $H(t) = \mathbf{h}^T(t)\mathbf{n}(t)$, where $\mathbf{h}(t) = [h_1(t) \ h_2(t) \ \dots \ h_s(t)]^T$ is the S -dimensional vector of component molar enthalpies that is assumed to be represented as follows [13]:

$$\mathbf{h}(t) = \mathbf{h}_{ref} + \tilde{\mathbf{c}}_p (T(t) - T_{ref}). \quad (3)$$

In this equation, $\mathbf{h}_{ref} = [h_{ref,1} \ h_{ref,2} \ \dots \ h_{ref,S}]^T$ and $\tilde{\mathbf{c}}_p = [\tilde{c}_{p,1} \ \tilde{c}_{p,2} \ \dots \ \tilde{c}_{p,S}]^T$ are the constant S -dimensional vectors of component molar enthalpies evaluated at the reference temperature T_{ref} and of molar heat capacities of species, respectively.

Lemma 1

The dynamics of reactor temperature, i.e. $\dot{T}(t)$, can be expressed as follows:

$$\dot{T}(t) = \frac{\lambda(T_J(t) - T(t)) - \Delta\mathbf{H}^T(t)\mathbf{r}_v(t) + d(T_{in} - T(t))C_{p,in}}{C_p(t)} \quad (4)$$

With $\Delta\mathbf{H}(t) := \mathbf{N}\mathbf{h}(t)$, $C_{p,in} := \tilde{\mathbf{c}}_p^T \mathbf{n}_{in}$ and $C_p(t) := \tilde{\mathbf{c}}_p^T \mathbf{n}(t)$.

Proof. It can be seen from Eq. (3) that the derivative of $\mathbf{h}(t)$ is given by:

$$\dot{\mathbf{h}}(t) = \dot{T}(t)\tilde{\mathbf{c}}_p^T. \quad (5)$$

Furthermore, it is possible to obtain the derivative of $H(t)$ as follows:

$$\dot{H}(t) = \dot{\mathbf{h}}(t)^T \mathbf{n}(t) + \mathbf{h}^T(t) \dot{\mathbf{n}}(t)^T, \quad (6)$$

which is equivalent to the following equation:

$$\dot{H}(t) = \dot{T}(t)\tilde{\mathbf{c}}_p^T \mathbf{n}(t) + \mathbf{h}^T(t) \left[\mathbf{N}^T \mathbf{r}_v(t) + d(\mathbf{n}_{in} - \mathbf{n}(t)) \right], \quad (7)$$

by substituting Eq. (2) and Eq. (5) into $\dot{\mathbf{h}}(t)$ and $\dot{\mathbf{n}}(t)$, respectively. As a result, replacing $\dot{H}(t)$, given by Eq. (2), into Eq. (7) yields the following equation:

$$\dot{T}(t) = \frac{q_{ex}(t) + d(H_{in} - H(t)) - \mathbf{h}^T(t) \left[\mathbf{N}^T \mathbf{r}_v(t) + d(\mathbf{n}_{in} - \mathbf{n}(t)) \right]}{\tilde{\mathbf{c}}_p^T \mathbf{n}(t)}, \quad (8)$$

thereby immediately leading to Eq. (4). The latter completes the proof.

Remark 3

Noting that $\Delta\mathbf{H}(t)$ in Eq. (4), by definition, represents the R -dimensional vector of reaction enthalpies, which can be rewritten in the following form:

$$\Delta\mathbf{H}(t) = \Delta\mathbf{H}_{ref} + \mathbf{N}\tilde{\mathbf{c}}_p(t)(T(t) - T_{ref}), \quad (9)$$

where $\Delta\mathbf{H}_{ref} := \mathbf{N}\mathbf{h}_{ref}$ is defined as the constant R -dimensional vector of reaction enthalpies evaluated at the reference temperature. Moreover, $C_{p,in}$ and $C_p(t)$ denote the heat capacities of the inlet stream and the reacting mixture, respectively.

In this work, only $T_J(t)$ is considered as a manipulated variable to regulate the reactor dynamics (2). Therefore, we shall impose the following assumption, which was also used in [3], [4], [16], for the purpose of control design.

Assumption 4

Let consider the steady-state reactor temperature, denoted by T^* , that corresponds to the steady-state jacket temperature, denoted by T_J^* . Assume that at $T = T^*$, the system trajectory $\mathbf{n}(t)$, driven by the isothermal dynamics as follows:

$$\dot{\mathbf{n}}(t) = \mathbf{N}^T \mathbf{r}_v(\mathbf{n}, T^*) + d(\mathbf{n}_{in} - \mathbf{n}(t)) := f(\mathbf{n}, T^*), \quad (10)$$

has a single equilibrium point, denoted by \mathbf{n}^* , which is globally asymptotically stable (GAS).

Control objective: Let consider $\mathbf{x}^* := \begin{bmatrix} \mathbf{n}^* \\ T^* \end{bmatrix}$ be a desired equilibrium point of the reaction system. And,

under Assumption 4, we aim to design a controller to stabilize the reactor dynamics (2) at \mathbf{x}^* using only the manipulated variable $T_j(t)$ for two different scenarios as follows:

1. There is no model uncertainty,
2. There exists an uncertainty in the parameter \mathbf{h}_{ref} .

3. Main results

3.1. Stabilization of the reaction system without uncertain parameters

In this subsection, we shall deal with the first scenario, where the reactor model (2) is perfect, i.e. having no parameter uncertainty. On this basis, an ideal PI-like feedback law can be designed in the following proposition.

Proposition 1

Consider the control law $T_j(t)$ as follows:

$$T_j(t) = T(t) + \frac{C_p(t)}{\lambda} \left[u(t) - d(T(t) - T_{in}) \frac{C_{p,in}}{C_p(t)} + \frac{\Delta \mathbf{H}^T(t) \mathbf{r}_v(t)}{C_p(t)} \right], \quad (11)$$

where $u(t)$ is given by the following set of equations:

$$\begin{cases} \dot{x}_c(t) = \tilde{y}(t), \\ u(t) = -K_p \tilde{y}(t) - K_I x_c(t), \end{cases} \quad (12)$$

with the error state $\tilde{y}(t) := T - T^*$, the added state $x_c(t)$ and the tuning parameters K_p and K_I . Then, the dynamics of the reaction system (2) in closed-loop is globally asymptotically stabilized at the desired equilibrium point \mathbf{x}^* if K_p and K_I are chosen to be positive.

Proof. Let consider a quadratic function $V(t) = \frac{1}{2} \tilde{y}^2(t) + \frac{K_I}{2} x_c^2(t)$ as a Lyapunov function candidate. It can be verified that $V(t)$ is bounded from below by the origin, i.e. $V(t) \geq 0$, due to $K_I > 0$, and its time derivatives is obtained as follows:

$$\dot{V}(t) = \tilde{y}(t) \frac{\lambda(T_j(t) - T(t)) - \Delta \mathbf{H}^T(t) \mathbf{r}_v(t) + d(T_{in} - T(t)) C_{p,in}}{C_p(t)} + K_I x_c(t) \tilde{y}(t), \quad (13)$$

by using (4) and (12). Then, under the control law (11), Eq. (13) becomes:

$$\dot{V}(t) = -K_p \tilde{y}^2(t) \leq 0, \quad (14)$$

which is negative semidefinite. Therefore, it follows immediately that $\tilde{y}(t) \rightarrow 0$ as $t \rightarrow \infty$ and the trajectory $x_c(t)$ is bounded and converges to the largest invariant set contained within $\mathcal{I} = \{x_c^* \mid K_I x_c^* = 0\} = \{0\}$. As a result, the closed-loop reactor dynamics (2) is globally asymptotically stabilized at \mathbf{x}^* by invoking the LaSalle's invariant principle [17] and Assumption 4. The latter

completes the proof.

Remark 4

Clearly, the signal of $\Delta\mathbf{H}(t)$ explicitly depends on the parameter \mathbf{h}_{ref} , normally determined from experimental studies and therefore possibly having a large uncertainty [13], via Eq. (9). Hence, the design of the feedback law $T_J(t)$ in Proposition 1 just provides a non-adaptive version.

3.2. An adaptive PI-like controller via a parameter update law

In this subsection, we shall focus on investigating the second scenario, where the model parameter \mathbf{h}_{ref} is unknown. Therefore, we shall replace its true values in Eq. (12) by its estimate, which can be achieved in the following proposition.

Proposition 2

Consider the adaptive control law $T_J(t)$ as follows:

$$T_J(t) = T(t) + \frac{C_p(t)}{\lambda} \left[u(t) - d(T(t) - T_{in}) \frac{C_{p,in}}{C_p(t)} + \frac{[\hat{\mathbf{h}}_{ref}^T(t) + \tilde{\mathbf{c}}_p^T(t)(T(t) - T_{ref})] \mathbf{N}^T \mathbf{r}_v(t)}{C_p(t)} \right], \quad (15)$$

with $u(t)$ given by Eq. (12) and the time-varying control parameter $\hat{\mathbf{h}}_{ref}(t)$ updated by the following differential equation:

$$\dot{\hat{\mathbf{h}}}_{ref}(t) = -\frac{\tilde{y}(t)}{C_p(t)} \mathbf{N}^T \mathbf{r}_v(t). \quad (16)$$

Then, if K_p and K_I are chosen to be positive, the desired equilibrium point \mathbf{x}^* is GAS.

Proof. Let consider a quadratic function $W(t) = V(t) + \frac{1}{2} \hat{\mathbf{h}}_{ref}^T(t) \tilde{\mathbf{h}}_{ref}(t)$ as a Lyapunov function candidate. Clearly, $W(t)$ is positive definite due to $K_I > 0$, and its time derivatives is obtained as follows:

$$\begin{aligned} \dot{W}(t) = & \tilde{y}(t) \frac{\lambda(T_J(t) - T(t)) - \Delta\mathbf{H}^T(t) \mathbf{r}_v(t) + d(T_{in} - T(t)) C_{p,in}}{C_p(t)} \\ & + K_I x_c(t) \tilde{y}(t) + \hat{\mathbf{h}}_{ref}^T(t) \dot{\tilde{\mathbf{h}}}_{ref}(t), \end{aligned} \quad (17)$$

which is equivalent to

$$\begin{aligned} \dot{W}(t) = & \frac{\tilde{y}(t)}{C_p(t)} \left\{ \lambda(T_J(t) - T(t)) - [\hat{\mathbf{h}}_{ref}^T(t) + \tilde{\mathbf{c}}_p^T(t)(T(t) - T_{ref})] \mathbf{N}^T \mathbf{r}_v(t) + d(T_{in} - T(t)) C_{p,in} \right\} \\ & \left(\hat{\mathbf{h}}_{ref}^T(t) - \mathbf{h}_{ref}^T(t) \right) \left(\frac{\tilde{y}(t)}{C_p(t)} \mathbf{N}^T \mathbf{r}_v(t) + \dot{\hat{\mathbf{h}}}_{ref}(t) \right) + K_I x_c(t) \tilde{y}(t). \end{aligned} \quad (18)$$

By adopting the feedback law (15) and the update law (16), Eq. (18) becomes

$$\dot{W}(t) = -K_p \tilde{y}^2(t) \leq 0, \quad (19)$$

which, therefore, ensures $\lim_{t \rightarrow \infty} \tilde{y}(t) = 0$, that is, $T(t) \rightarrow T^*$ as $t \rightarrow \infty$ according to the Lyapunov theorem [17]. In addition, the system trajectories $x_c(t)$ and $\hat{\mathbf{h}}_{ref}(t)$, governed by Eq. (12) and Eq. (16), respectively, are bounded at $T = T^*$. Consequently, the desired equilibrium point \mathbf{x}^* is GAS by invoking Assumption 4. The latter completes the proof.

4. Case study

4.1. Model description

To illustrate the theoretical development, we consider here an irreversible first-order exothermic reaction of two species A and B with the stoichiometry is given by: $A(S_1) \xrightarrow{k_v} B(S_2)$ in a CSTR, where these species are dissolved together into the solvent $I(S_3)$. Besides, the stoichiometric matrix \mathbf{N} is given by $\mathbf{N} = [-1 \ 1 \ 0]$ and the reaction rate $r_v(t)$ is expressed by:

$$r_v(t) = k_0 \exp\left(\frac{-E_a}{RT(t)}\right) n_1(t), \quad (20)$$

where k_0 , E_a and R represent the kinetic constant, the activation energy and the ideal gas constant, respectively. Additionally, the values of physical and operating parameters, taken from [4], are listed in Table 1. These parameters, extracted from [4], are chosen to exhibit the multiplicity behavior of the considered first-order reaction system and to implement the designed adaptive PI-like controller.

Table 1. Physical and operating parameters of the first-order reaction system

Symbol	Quantity	Value	Unit
$h_{1,ref}$	Reference enthalpy of A	-2.7085×10^4	J.mol ⁻¹
$h_{2,ref}$	Reference enthalpy of B	-11.884×10^4	J.mol ⁻¹
$h_{3,ref}$	Reference enthalpy of I	-33	J.mol ⁻¹
$\tilde{c}_{P,1}$	Heat capacity of A	221.900	J.(K.mol) ⁻¹
$\tilde{c}_{P,2}$	Heat capacity of B	128.464	J.(K.mol) ⁻¹
$\tilde{c}_{P,3}$	Heat capacity of I	21.6940	J.(K.mol) ⁻¹
$n_{1,in}$	Mole number of A in the inlet stream	0.18	mol
$n_{2,in}$	Mole number of B in the inlet stream	0	mol
$n_{3,in}$	Mole number of I in the inlet stream	3.57	mol
E_a	Activation energy	73350	J.mol ⁻¹

k_0	Kinetic constant	2.58×10^9	s^{-1}
R	Ideal gas constant	8.314	J.(K.mol) ⁻¹
T_{ref}	Reference temperature	298.15	K
λ	Heat transfer coefficient	0.75	W/K
T_{in}	Temperature of the inlet stream	298	K
d	Dilution rate	0.007	s^{-1}
T_j	Jacket temperature	298	K

4.2. Simulation results

For sake of illustration, the reaction system is assumed to be initiated at two initial conditions as follows:

- (IC₁) $n_{1,0} = 0.04$ (mol), $n_{2,0} = 0.5$ (mol) and $T_0 = 310$ (K),
- (IC₂) $n_{1,0} = 0.06$ (mol), $n_{2,0} = 2.0$ (mol) and $T_0 = 340$ (K).

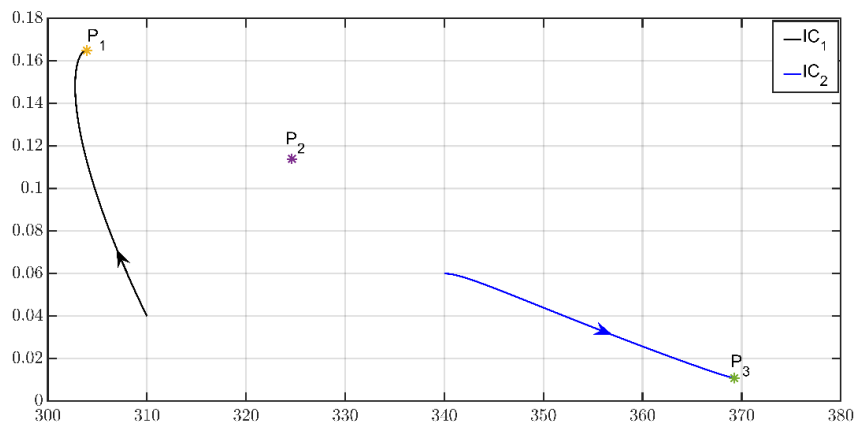


Figure 2. The representation of open-loop phase plane

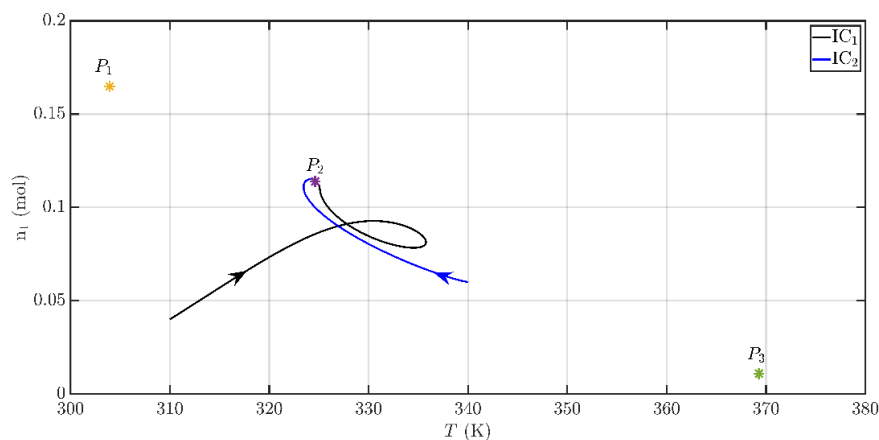


Figure 3. The representation of closed-loop phase plane

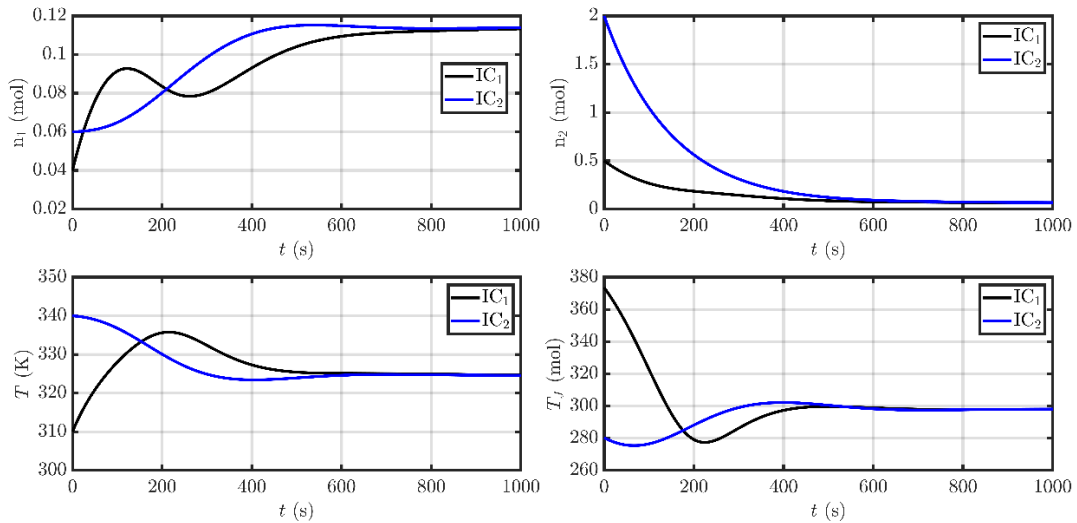


Figure 4. Transient responses of state variables and manipulated variable

It can be seen from Figure 2 that the considered reaction system has three steady states, denoted by $P_i = [n_{1,i}^* \ n_{2,i}^* \ T_i^*]$, $i = 1, 2$, whose values is given as follows: $P_1 = [0.165 \ 0.015 \ 303.93]$, $P_2 = [0.114 \ 0.066 \ 324.61]$ and $P_3 = [0.011 \ 0.169 \ 369.27]$. In addition, it can be verified that the points P_1 and P_3 are locally stable, while P_2 is an open-loop unstable equilibrium point. Next, we aim to stabilize the system at P_2 and simulate the closed-loop system in two scenarios.

Next, the tuning parameters K_p and K_I for the controller are chosen as follows: $K_p = 1.9$ and $K_I = 0.009$. Figure 3 shows the closed-loop phase plane, where the system trajectories starting at (IC_1) and (IC_2) converge to the desired equilibrium point, that is, the reaction system is globally asymptotically stabilized at P_2 under the feedback law (15) and the update law (16). Furthermore, the time responses of state variables, namely n_1, n_2 and T , and the representation of T_j are given in Figure 4. Clearly, the convergence of these state variables towards their desired values is assured despite the uncertainties on $h_{ref,1}$ and $h_{ref,2}$. Also, the control input T_j is physically admissible in terms of amplitude and variation rate.

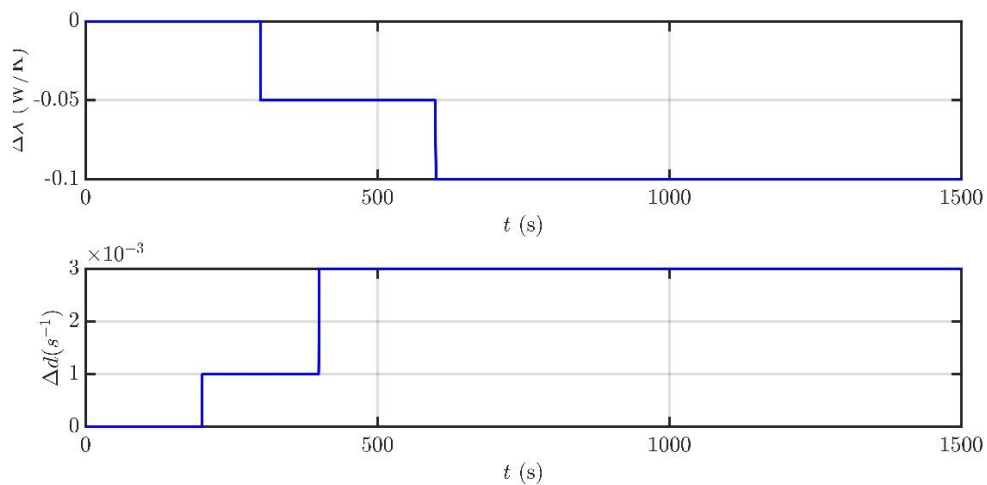


Figure 5. Step disturbance $\Delta\lambda$ and Δd

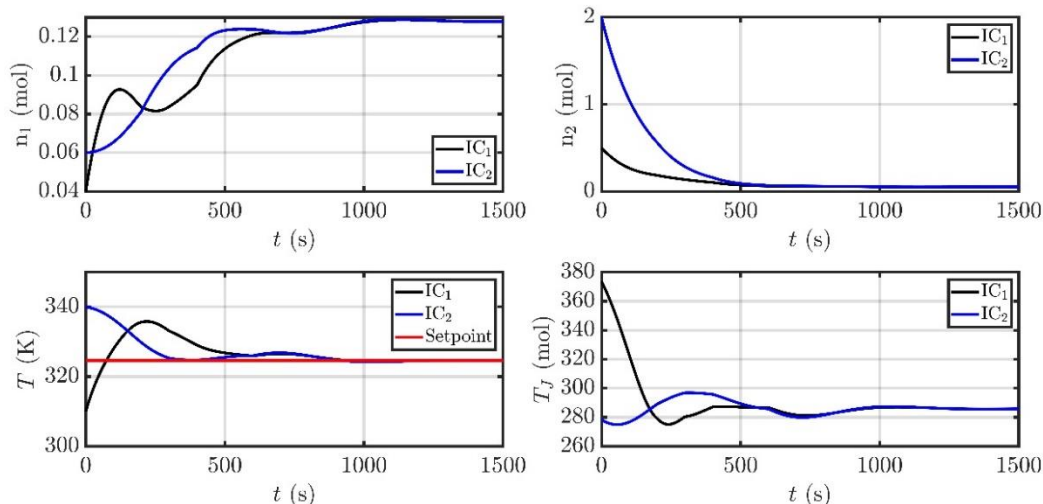


Figure 6. Transient responses of state variables and manipulated variable following step disturbance

In practice, the heat exchange coefficient λ can gradually decrease due to the increase in fouling resistance of the vessel jacket. And the dilution rate d can change with time due to effects of external disturbance. In this work, the robustness of the closed-loop system against the uncertainty of these model parameters can be tested with respect to the step variations on the nominal values of λ and d , denoted by $\Delta\lambda$ and Δd , as shown in Figure 5 (the considered range of these variations is about 10% for λ and 40% for d). It can be clearly seen from Figure 6 that the reactor temperature is stabilized at the set point despite the step disturbance in both λ and d , thereby ensuring the convergence of state variables n_1 and n_2 towards the desired steady states. Additionally, the amplitude and the time variations of the control input T_j are physically realizable.

5. Conclusions

This paper has designed an adaptive PI-like controller to regulate non-isothermal CSTRs using the Lyapunov theory. Concretely, once an online parameter update law is constructed, effective control actions can be computed. This allows driving closed-loop system trajectories to their desired values, that is, the global asymptotic stabilization of the closed-loop systems is ensured. Numerical simulations for an irreversible first-order reaction system in a CSTR having multiple steady states illustrate the effectiveness of the proposed adaptive control scheme. The robustness of the closed-loop system is tested in the presence of the uncertainty of other model parameters. It remains now to compare the proposed adaptive control approach with model predictive control (MPC) or other adaptive controllers in terms of control performance (such as rising time, amplitude and variation rate, etc.).

An extension of the proposed approach to non-isothermal batch and semi-batch reactors will be part of our future work.

Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

- [1] W. L. Luyben, *Process Modeling, Simulation, and Control for Chemical Engineers*, second ed. (Chemical Engineering Series). McGraw-Hill Higher Education, 1990.

- [2] B. W. Bequette, *Process dynamics: Modeling, analysis and simulation*, first ed. (Prentice Hall International Series in The Physical and Chemical Engineering Studies). New Jersey: Prentice Hall PTR, Upper Saddle River, 1998.
- [3] A. Favache and D. Dochain, "Power-shaping control of reaction systems: The CSTR case," *Automatica*, vol. 46, no. 11, pp. 1877-1883, 2010.
- [4] N. H. Hoang, F. Couenne, Y. Le Gorrec, C. L. Chen, and B. E. Ydstie, "Passivity-based nonlinear control of CSTR via asymptotic observers," *Annual Reviews in Control*, vol. 37, no. 2, pp. 278-288, 2013.
- [5] K. J. Astrom, "Limitations on control system performance," *European Journal of Control*, vol. 6, pp. 2-20, 2006.
- [6] D. D. Bruns and J. E. Bailey, "Process operation near an unstable steady state using nonlinear feedback control," *Chemical Engineering Science*, vol. 30, pp. 755-762, 1975.
- [7] A. Uppal and W. H. Ray, "On the dynamic behavior of continuous stirred tank reactors," *Chemical Engineering Science*, vol. 29, pp. 967-985, 1974.
- [8] C. Van Heerden, "Autothermic processes. Properties and reactor design," *Industrial & Engineering Chemistry Research*, vol. 45, no. 6, pp. 1242-1247, 1953.
- [9] N. T. Sang, H. N. M. Ha, and M. A. Hussain, "Feedback passivation plus tracking-error-based multivariable control for a class of free-radical polymerisation reactors," *International Journal of Control*, vol. 92, no. 9, pp. 1970-1984, 2019.
- [10] N. H. Hoang, F. Couenne, C. Jallut, and Y. Le Gorrec, "Lyapunov-based control of non isothermal continuous stirred tank reactors using irreversible thermodynamics," *Journal of Process Control*, vol. 22, no. 2, pp. 412-422, 2012.
- [11] N. H. Hoang, F. Couenne, C. Jallut, and Y. Le Gorrec, "Thermodynamics based stability analysis and its use for nonlinear stabilization of the CSTR," *Computers & Chemical Engineering*, vol. 58, pp. 156-177, 2013.
- [12] C. Panjapornpon, M. Soroush, and W. D. Seider, "Model-based controller design for unstable, non-minimum-phase, nonlinear processes," *Industrial & Engineering Chemistry Research*, vol. 45, pp. 2758-2768, 2006.
- [13] S. I. Sandler, *Chemical, biochemical, and engineering thermodynamics*. John Wiley & Sons, 2017.
- [14] T. S. Nguyen, "A port-Hamiltonian Framework for control of chemical reaction systems with variant and invariant states," Ph.D., Chemical Engineering, Universiti Malaya, Faculty of Engineering, 2023.
- [15] N. H. Hoang, D. Rodrigues, and D. Bonvin, "Revisiting the concept of extents for chemical reaction systems using an enthalpy balance," *Computers & Chemical Engineering*, vol. 136, p. 106652, 2020.
- [16] J. Alvarez, J. A. Ramirez, G. E. Perez, and A. Schaum, "Energy shaping plus damping injection control for a class of chemical reactors," *Chemical Engineering Science*, vol. 66, no. 23, pp. 6280-6286, 2011.
- [17] H. K. Khalil, *Nonlinear systems*, third ed. Prentice Hall, 2002.




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