

ADAPTIVE EXTREMUM SEEKING CONTROL OF NONISOTHERMAL CONTINUOUS STIRRED TANK REACTORS ¹

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Abstract: In this paper, we present an adaptive extremum seeking control scheme for non-isothermal continuous stirred tank reactors. We assume limited knowledge of the reaction kinetics. An adaptive learning technique is introduced to construct an optimum seeking algorithm that drives the system states to optimal equilibrium concentrations of the reaction mixture. Lyapunov's stability theorem is used in the design of the extremum seeking controller structure and the development of the parameter learning laws. Under mild assumptions, the resulting controller is an output-feedback controller. The performance of the technique is demonstrated with the van de Vusse reaction.

Keywords: Extremum seeking, Lyapunov function, adaptive learning, persistence of excitation

1. INTRODUCTION

The task of extremum seeking is to find the operating set-points that maximize or minimize an objective function. Since the early research work on extremum control in the 1920's (Leblanc 1922), many successful applications of extremum control approaches have been reported (e.g., (Vasu 1957), (Astrom and Wittenmark 1995), (Sternby 1980) and (Drkunov *et al.* 1995)). Recently, Krstic *et al.* ((Krstic 2000), (Krstic and Deng 1998)) presented several extremum control schemes and stability analysis for extremum-seeking of linear unknown systems and a class of general nonlinear systems ((Krstic 2000) and

(Krstic and Deng 1998)). An alternative Lyapunov-based adaptive extremum-seeking technique is developed in (Guay and Zhang 2002) in which the function to be optimized is not available for measurement.

In this study, we investigate an alternative extremum seeking scheme for nonisothermal continuous stirred tank reactors. Only limited knowledge of the reaction kinetics are assumed. A Lyapunov-based adaptive learning control technique is used to approximate the unknown kinetics and to steer the system to its unknown extremum. The technique ensures convergence of the system to an adjustable neighbourhood of its unknown optimum that depends on the approximation error. We also show that a certain level of persistence of excitation (PE) condition is necessary to guarantee the convergence of the extremum-seeking mechanism. The paper is organized as follows. Section 2 presents some notations and the problem for-

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mulation. Section 3 presents the adaptive extremum seeking controller and the stability and convergence of the closed-loop extremum seeking system. A numerical simulation is shown in Section 4 followed by brief conclusions in Section 5.

2. PROBLEM

We focus on a class of nonisothermal continuous stirred-tank reactor models described by

$$\dot{x} = -Dx + KC(x, T) + U_{in} \quad (1)$$

$$\dot{T} = -DT + \lambda^T C(x, T) + u \quad (2)$$

where $x \in S_x \subset \mathbb{R}^n$ denote the concentration of chemical components in the reaction mixture taking value in compact subset S_x of \mathbb{R}^n . The temperature is denoted by T , it takes values on a compact subset S_T of \mathbb{R}^+ , the positive reals. $K \in \mathbb{R}^{n \times r}$ is the $n \times r$ matrix of stoichiometric coefficients for each n components on r chemical reactions. The vector $C(x, T) \in \mathbb{R}^r$ summarizes the temperature dependent chemical kinetics for r chemical reactions of the reaction network under study. D is the CSTR dilution rate. $U_{in} \in \mathbb{R}^n$ gives the rate of addition of each n components. The vector $\lambda \in \mathbb{R}^r$ provide the heats of reaction for each reaction. The control input u is assumed to be the rate of heating and cooling. The control objective is to design a controller, u , such that the function $y = Hx$, where $H \in \mathbb{R}^{1 \times n}$, achieves its maximum at steady-state. We consider the extremum-seeking problem for the nonisothermal CSTR with unknown chemical reaction kinetics, $C(x, T)$. It is assumed that the stoichiometry of the reaction network (summarized by the matrix K) and the heats of reaction, λ , are known. The nonisothermal CSTR is initially assumed to operate at constant flowrate.

The problem is solved by first expressing the equilibrium concentrations in the reaction mixture as function of temperature, T . We assume that there exists a vector-valued function, $\pi(T)$, that solves the following equation

$$-D\pi(T) + KC(\pi(T), T) + U_{in} = 0. \quad (3)$$

The solution $\pi(T)$ is assumed to be continuous on S_T . More specifically, we require the following.

Assumption 2.1. The function $H\pi(T)$ is continuously differentiable and it admits a maximum on $\Psi_T = \{x \in S_x | x = \pi(T)\}$.

By Assumption 2.1, we consider only cases where $H\pi(T)$ is a continuously differentiable convex function of T .

We consider systems where the isothermal reaction kinetics are stable. We state this requirement as follows.

Assumption 2.2. Consider the reaction kinetics dynamics eq.(1). There exists a positive definite function $V(x) \in C^1$ such that

$$c_1 \|x\|^2 \leq V(x) \leq c_2 \|x\|^2$$

and

$$\dot{V} \leq -c_3 \|x - \pi(T)\| + c_4 \|x\| \|\pi(T)\|$$

for positive nonzero constants c_1, c_2, c_3 and c_4 .

Assumption 2.2 provides a minimum-phase property of the reaction kinetics that guarantees converge of the compositions, x , to a neighbourhood of the equilibrium $x = \pi(T)$.

The temperature dynamics eq.(2) subject to the equilibrium condition eq.(3) are written as

$$\begin{aligned} \dot{T} = & -DT + \lambda^T K^+ D\pi(T) - \lambda^T K^+ U_{in} \\ & + u + \lambda^T (C(x, T) - C(\pi(T), T)) \end{aligned} \quad (4)$$

We assume that the following holds.

Assumption 2.3. $\forall x \in S_x$ and $\forall T \in S_T$, \exists a positive nonzero constant L_1 such that

$$\|C(x, T) - C(\pi(T), T)\| \leq L_1 \|x - \pi(T)\|. \quad (5)$$

The strategy developed in this paper consists in approximating the steady-state, or equilibrium, composition $\pi(T)$ using a linear approximation technique such as neural networks. Radial basis function (RBF) neural networks presented in (Sanner and Slotine 1992) and (Seshagiri and Khalil 2000) shall be used to approximate a continuous function $\phi : \mathbb{R}^p \rightarrow \mathbb{R}$ as

$$\phi(z) = W^{*T} S(z) + \mu_l(t) \quad (6)$$

with NN approximation error $\mu_l(t)$, and basis function vector

$$\begin{aligned} S(z) = & [s_1(z), s_2(z), \dots, s_l(z)]^T \\ s_i(z) = & \exp \left[\frac{-(z - \varphi_i)^T (z - \varphi_i)}{\sigma_i^2} \right], \quad i = 1, 2, \dots, l \end{aligned} \quad (7)$$

where φ_i is the center of the receptive field, and σ_i is the width of the Gaussian function. The ideal weight W^* in (6) is defined as

$$W^* := \arg \min_{W \in \Omega_w} \left\{ \sup_{z \in \Omega} \left| W^T S(z) - \phi(z) \right| \right\} \quad (8)$$

where Ω is a compact subset of R^p and

$$\Omega_w = \left\{ W \mid \|W\| \leq w_m \right\}$$

with positive constant w_m to be chosen at the design stage. Universal approximation results stated in (Funahashi 1989) (Kosmatopoulos *et al.* 1995) indicate that, if l is chosen sufficiently large, then $W^T S(z)$ can approximate any continuous function to any desired accuracy on a compact set.

We apply eq.(6) to develop an approximation of the objective function $y = H\pi(T)$ given by

$$H\pi(T) = W_p^{*T} S(T) + \mu_p(t) \quad (9)$$

where W_p^* and S are as defined in eqs.(7)-(8). Since it is assumed that the reaction kinetics are unknown, we need to approximate the term $D\lambda^T K^+ \pi(T)$. To allow for the simultaneous approximation of the objective function and the regulation of the system temperature, we breakdown the heat of reaction term as follows,

$$\lambda^T K^+ \pi(T) = \lambda^T K^+ H^T W_p^{*T} S(T) + W_o^{*T} S(T) + \mu_l(t).$$

We make the following assumption about the approximation error terms $\mu_p(t)$ and $\mu_l(t)$.

Assumption 2.4. The NN approximation errors satisfies $|\mu_p(t)| \leq \bar{\mu}_p$ and $|\mu_l(t)| \leq \bar{\mu}_l$ with constants $\bar{\mu}_p > 0$ and $\bar{\mu}_l > 0$ over the compact set $\Omega_w \times S_T$.

3. CONTROLLER DESIGN

In this section, we design a control strategy that tracts the unknown optimum of y . We first develop the parameter estimation algorithm for the unknown parameter vector W^* . Let \hat{W} denote the estimate of the true parameter W^* and let \hat{T} the predictions of T . Using eqs.(9)-(10) and eq.(4), the temperature dynamics are written as,

$$\begin{aligned} \dot{T} = & -DT + F(T)W^* + D\mu_l(t) - \lambda^T K^+ U_{in} + u \\ & + \lambda(C(x, T) - C(\pi(T), T)) \end{aligned} \quad (10)$$

where $F(T) = [DS(T)^T, D\lambda^T K^+ H^T S(T)^T]$ and $W^{*T} = [W_p^{*T}, W_o^{*T}]$.

The predicted state \hat{T} is generated by

$$\begin{aligned} \dot{\hat{T}} = & -D\hat{T} + F(\hat{T})\hat{W} - \lambda^T K^+ U_{in} + u \\ & + k_T(T - \hat{T}) + c_1(t)\dot{\hat{W}} \end{aligned} \quad (11)$$

with gain function $k_T > 0$ and prediction error $e_T = T - \hat{T}$. The vector-valued time-varying function $c_1(t)$ is to be assigned. It follows from (2)-(11) that

$$\begin{aligned} \dot{e}_T = & F(T)\tilde{W} + D\mu_l(t) - k_T e_T \\ & + \lambda^T (C(x, T) - C(\pi(T), T)) - c_1(t)\dot{\hat{W}} \end{aligned} \quad (12)$$

where $\tilde{W} = W^* - \hat{W}$.

The objective of the extremum-seeking control is stabilize the closed-loop system around a point where the gradient of $y = H\pi(T)$ with respect to T vanishes while attenuating the effect of the modelling uncertainty $\mu_l(t)$.

Using the approximation eq.(9), the objective function given by

$$y = H\pi(T) = W_p^{*T} S(T) + \mu_p(t)$$

is approximated by

$$y_e = \hat{W}_p^T S(T)$$

where \hat{W}_p is an estimate of the optimal weight W_p^* . The estimated gradient of y_e with respect to T is given by

$$z = \frac{\partial y_e}{\partial T} = \hat{W}_p^T dS(T) \quad (13)$$

where $dS(T) = \frac{\partial S(T)}{\partial T}$. The Hessian of y_e with respect to T is given by

$$\frac{\partial^2 y_e}{\partial T^2} = \hat{W}_p^T d^2 S(T) = \Gamma_2 \quad (14)$$

where $d^2 S(T) = \frac{\partial^2 S(T)}{\partial T^2}$

Define

$$z_s = \hat{W}_p^T dS(T) - d(t) \quad (15)$$

where $d(t) \in C^1$ is an excitation signal to be assigned. In the remainder, the dependence of the radial basis functions S on the temperature is implied and we write S , dS and $d^2 S$.

To address the controller design, we define the following auxiliary signals

$$\eta_1 = e_T - c_1(t)^T \tilde{W} \quad (16)$$

$$\eta_2 = z_s - c_2(t)^T \tilde{W} \quad (17)$$

where $c_2(t)$ is a time-varying vector valued function to be assigned in the design.

We propose the Lyapunov function candidate

$$V = \frac{1}{2}\eta_1^2 + \frac{1}{2}\eta_2^2. \quad (18)$$

The following dynamic controller is considered

$$\dot{d}(t) = c_2(t)^T \dot{\hat{W}} - k_z z_s - k_d |\Gamma_2| d(t) - \Gamma_2 a(t) \quad (19)$$

$$u = DT - F(T)\hat{W} + \lambda^T K^+ U_{in} - k_d \text{sgn}(\Gamma_2) d(t) - a(t) \quad (20)$$

where $k_z > 0$ and $k_d > 0$ are gain function to be assigned in the sequel, sgn is the sign function. The signal $a(t)$ acts as a secondary dither signal that is used to generate information about the unknown nonlinearities associated with the reaction kinetics. The dynamics of the time-varying functions $c_1(t)$ and $c_2(t)$ are assigned as follows

$$\dot{c}_1(t)^T = -k_T c_1(t)^T + F(T) \quad (21)$$

$$\dot{c}_2(t)^T = -k_z c_2(t)^T + \Gamma_2 F(T) \quad (22)$$

Taking the time derivative of V and substitution of eqs.(19)-(22) gives

$$\begin{aligned} \dot{V} = & -k_T \eta_1^2 - k_z \eta_2^2 + (\eta_1 + \Gamma_2 \eta_2) \\ & \times [D\mu_l(t) + \lambda^T (C(x, T) - C(\pi(T), T))] \end{aligned} \quad (23)$$

From Assumption 2.2 it follows that

$$\sup_{x \in S_x, T \in S_T} \|x - \pi(T)\| = C_1$$

exists and is finite. By Assumption 2.3, we get

$$\begin{aligned} \dot{V} \leq & -k_T \eta_1^2 - k_z \eta_2^2 + (\eta_1 + \Gamma_2 \eta_2) D\mu_l(t) \\ & + (|\eta_1| + |\Gamma_2| \|\eta_2\|) \|\lambda\| L_1 C_1 \end{aligned} \quad (24)$$

Completing the squares and applying the gain functions

$$k_T = k_{T0} + \frac{k_4}{2} D^2 + \frac{k_5}{2} \|\lambda\|^2, \quad (25)$$

$$k_z = k_{z0} + \frac{k_7}{2} \|\lambda\|^2 \Gamma_2^2, \quad (26)$$

we obtain the following inequality

$$\begin{aligned} \dot{V} \leq & -k_{T0} \eta_1^2 - k_{z0} \eta_2^2 + \left(\frac{1}{2k_4} + \frac{1}{2k_5} \right) \mu_l(t)^2 \\ & + \left(\frac{1}{2k_6} + \frac{1}{2k_7} \right) L_1^2 C_1^2 \end{aligned} \quad (27)$$

where $k_{T0} > 0$, $k_{z0} > 0$, $k_4 > 0$, $k_5 > 0$, $k_6 > 0$ and $k_7 > 0$ are constants. Eq.(27) establishes that the state, η , converges to a small neighborhood of the origin. It remains to show that the original state variables, e_T and z_s and the parameter estimation errors \tilde{W} converge to a small neighborhood of the origin. To this end, we derive a persistency of excitation condition that guarantees

the convergence of the parameter estimates to the ideal weights, W^* .

Consider the following matrix,

$$\Upsilon(t) = \begin{bmatrix} c_1(t)^T \\ c_2(t)^T \end{bmatrix}$$

By construction, this matrix solves the matrix differential equation

$$\dot{\Upsilon}(t) = -K(t)\Upsilon(t) + B(t) \quad (28)$$

where

$$K(t) = \begin{bmatrix} k_T & 0 \\ 0 & k_z \end{bmatrix}, \quad B(t) = \begin{bmatrix} F(T) \\ \Gamma_2 F(T) \end{bmatrix}.$$

A bound on the parameter estimates \hat{W} can be ensured by choosing the following parameter update law.

$$\dot{\hat{W}} = \begin{cases} \gamma_w \Gamma & \text{if } \|\hat{W}\| \leq w_m \text{ or} \\ & \text{if } \|\hat{W}\| = w_m \text{ and } \hat{W}^T \Gamma \leq 0 \\ \gamma_w \left(I - \frac{\hat{W} \hat{W}^T}{\hat{W}^T \hat{W}} \right) \Gamma & \text{otherwise} \end{cases} \quad (29)$$

where $\Gamma = \Upsilon(t)^T e$ Eq.(29) is a projection algorithm which ensures that $\|\hat{W}\| \leq w_m$. The convergence of the parameter estimation scheme is considered in the sequel.

By the property of the projection algorithm and for the specific choice of basis function it is possible to show that the norm of $B(t)$ is bounded. Using the bound on $B(t)$, an explicit bound for the solution of eq.(28) can be obtained as follows,

$$\|\Upsilon(t)\| \leq C_2 e^{-\lambda_2(t-t_0)} + C_2 \frac{B_M}{\lambda_2}. \quad (30)$$

where $C_2 = \|\Upsilon(t_0)\| > 0$ and $\lambda_2 > 0$ is a positive constant. Next, we want to show that the parameter estimation error \tilde{W} converges to a neighborhood of the origin.

Substituting for $e = \eta + \Upsilon(t)\tilde{W}$ we obtain the perturbed dynamics

$$\begin{aligned} \dot{\tilde{W}} = & -\gamma_w \Upsilon(t)^T \Upsilon(t) \tilde{W} - \gamma_w \Upsilon(t)^T \eta \\ & + \begin{cases} 0 & \text{if } \|\hat{W}\| \leq w_m \text{ or} \\ & \text{if } \|\hat{W}\| = w_m \text{ and } \hat{W}^T \Upsilon(t)^T e \leq 0 \\ \gamma_w \frac{\hat{W} \hat{W}^T}{\hat{W}^T \hat{W}} \left(\Upsilon(t)^T \Upsilon(t) \tilde{W} + \Upsilon(t)^T \eta \right) & \text{otherwise} \end{cases} \end{aligned} \quad (31)$$

To establish the convergence of the parameter estimation, we make the following persistency of excitation assumption.

Assumption 3.1. The solution of eq.(28) is such that there exists positive constants $T > 0$ and $k_N > 0$ such that

$$\int_t^{t+T} \Upsilon(\tau)^T \Upsilon(\tau) d\tau \geq k_N I_N \quad (32)$$

where I_N is the N-dimensional identity matrix.

By a standard adaptive control argument, the persistency of excitation condition guarantees that the origin of the differential equation

$$\dot{\tilde{W}} = -\gamma_w \Upsilon(t)^T \Upsilon(t) \tilde{W} \quad (33)$$

is an exponentially stable equilibrium. Since $B(t)$ is a bounded function, it is shown that the parameter estimation error is guaranteed to decay exponentially as

$$\|\tilde{W}\| \leq \alpha_4 e^{-\lambda_4(t-t_0)} + \frac{|\bar{\mu}_l| + L_1 C_1}{\sqrt{2kmc_3}} \quad (34)$$

Hence the parameter estimation error and the redefined state variables, η , converge exponentially fast to an adjustable neighbourhood of the origin. By definition, convergence of η and \tilde{W} to a neighbourhood of the origin implies that $\|e\| \leq \|\eta\| + \|\Upsilon(t)\| \|\tilde{W}\|$. Substituting for $\|\eta\|$, $\|\Upsilon(t)\|$ and \tilde{W} , we obtain

$$\|e\| \leq \alpha_5 e^{-\lambda_5(t-t_0)} + \beta_5 \quad (35)$$

where $\alpha_5 > 0$ and $\beta_5 > 0$ are computable positive constants. The convergence of the error vector, e , implies that the convergence of the prediction error, e_T and the exponential convergence of the closed-loop system to an adjustable neighbourhood of the unknown steady-state optimum. We summarize the result of the above analysis as follows.

Theorem 3.1. Consider the nonisothermal continuous stirred tank reactor model eqs.(1)-(2) in closed-loop with the state prediction eq.(11), the controller eq.(20), the dither signal eq.(19) and the adaptive learning law eq.(29). Assume that the signal $a(t)$ is such that

$$\int_t^{t+T} \Upsilon(\tau)^T \Upsilon(\tau) d\tau \geq k_N I_N \quad (36)$$

for positive constants $T > 0$ and $k_N > 0$ where $\Upsilon(t)$ is the solution of eq.(28). Then

- the error dynamics eq.(12) converge exponentially to a small neighbourhood of the origin
- the parameter estimation errors \tilde{W} converge exponentially to a small neighbourhood of the origin

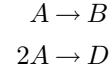
Parameter	Value
k_{10}, E_1	$1.287 \times 10^{12}, 9758.3$
k_{20}, E_2	$1.287 \times 10^{12}, 9578.3$
k_{30}, E_3	$9.043 \times 10^9, 8560.0$

Table 4.1. Kinetic Parameters of the van de Vusse reactor

- the tracking error from the unknown steady-state, z_s , converges exponentially to a small neighbourhood of the origin.

4. SIMULATION RESULTS

In this section, we demonstrate the effectiveness in simulation of the proposed adaptive extremum-seeking control. We consider the standard van de Vusse chemical reaction. The reaction scheme for this reactor is given by



The reaction kinetics are summarized by

$$K = \begin{bmatrix} -1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix}, \quad C(x, T) = \begin{bmatrix} k_{10} e^{-\left(\frac{E_1}{T}\right)} x_1 \\ k_{20} e^{-\left(\frac{E_2}{T}\right)} x_2 \\ k_{30} e^{-\left(\frac{E_3}{T}\right)} x_1^2 \end{bmatrix}$$

where x_1 and x_2 are the concentrations of components A and B, respectively, T is the reactor temperature, k_{10} , k_{20} and k_{30} are the pre-exponential factors, E_1 , E_2 and E_3 are the activation energies. The numerical values used for simulation are listed in Table 4.1.

The dilution rate, D , is 14.19 hr^{-1} . The latent heat of reaction is given by $\lambda^T = [-4.2, 11.0, -41.85]/\rho/C_p$ where $\rho = 0.9342$ and $C_p = 3.01$. The pseudo-inverse of K is given by

$$K^+ = \begin{bmatrix} -0.333 & 0.333 \\ -0.333 & -0.667 \\ -0.667 & -0.333 \end{bmatrix}$$

The objective is to steer the system to the maximum steady-state concentration of B, that is $H = [0, 1]$.

We consider the initial conditions, $x_1(0) = 1$, $x_2(0) = 0$, $T(0) = 25$. The centers of the linear approximation are evenly spaced points on the interval $[75, 125]$, $\sigma_i^2 = 10$ for $1 \leq i \leq l$. The six(6) centers, ω_i , are picked evenly at spaced points on that interval. The dither signal was set to

$$a(t) = \exp(-0.1t) \sum_{i=1}^6 (\sin((0.5i)t) + \cos((0.5i)t))$$

The simulation results are shown in Figures 1 to 3. The concentration of component B is shown in Figure 1. Figure 2 shows the reactor temperature profile. The required control action is given in Figure 3. The true optimum concentration of B is 1.09. As shown in Figure 1, the adaptive controller recovers the unknown optimum in a relatively short time. The control profile and the temperature profile demonstrate that the control is physically realizable.

5. CONCLUSION

We have solved a class of extremum seeking control problems for continuous stirred tank reactors represented by an unknown growth kinetic model. It has been shown that when the external dither signal is designed such that a persistent of excitation condition is satisfied, the proposed adaptive extremum seeking controller guarantees the exponential convergence to an adjustable neighborhood of its optimum.

6. REFERENCES

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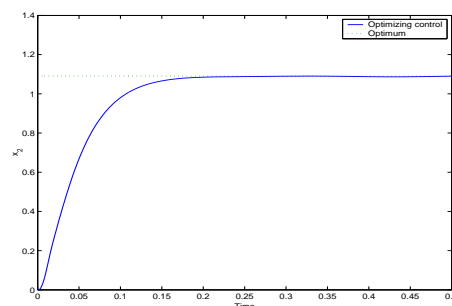


Fig. 1. Concentration of B

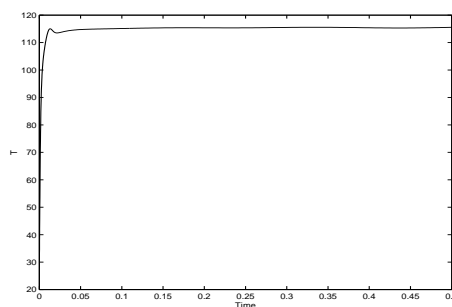


Fig. 2. Temperature Response

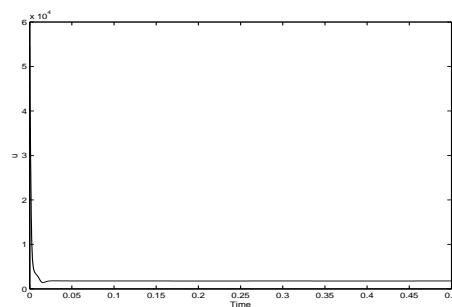


Fig. 3. Control, u