

Stability results on a chemical system

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In this paper, we first use the small gain theorem to present some sufficient conditions for global asymptotic stability of an equilibrium point of the bromate-malonic acid-ferroin system. Then we give an estimate of ultimate bounded set of this system.

KEY WORDS: bromate-malonic acid-ferroin system, global asymptotic stability, small gain theorem; ultimate bound set

1. Introduction

The Belousov–Zhabotinsky (B–Z) reaction (oxidation of organic reagents by bromate, catalyzed by metal ions) is the best-known chemical system in which various concentration oscillations can be observed [1]. For the typical B–Z reaction, i.e. bromate-malonic acid-ferroin system, some regular transient oscillations were reported by experimental results in [1] (Strzhak and Kawczynski). To explain the phenomena, the authors of Ref. 1 proposed a model described by the following equations:

$$\begin{aligned}\dot{x} &= f_1(x, y, z) = a(y - x^3 + \mu_1 x), \\ \dot{y} &= f_2(x, y, z) = \mu_2 x - y + z + \delta, \\ \dot{z} &= f_3(x, y, z) = \gamma(x - z).\end{aligned}\tag{1.1}$$

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where $a > 0$, $\gamma > 0$, μ_2 , μ_1 , and δ are guiding parameters. Moreover in [1], the authors showed that system (1.1) is the simplest system, in which mixed-mode oscillations (MMO) and deterministic chaos are observed. In [2], the authors found that system (1.1) can describe different modes observed in nonlinear chemical reactions because their kinetic schemes may be reduced to this system. Therefore it is significant to study system (1.1).

In this paper, we focus on the global asymptotic stability of an equilibrium point of system (1.1) and estimates of an ultimate bounded set of system (1.1). First we study the global asymptotic stability of the equilibrium point of system (1.1) by the small gain theorem, because the stability of the equilibrium point, i.e. the steady state plays a key role in the qualitative analysis of chemical systems. Then we investigate estimates of an ultimate bounded set of system (1.1), which is important in chaos control, chaos synchronization and their applications.

This paper is organized as follows. In section 2, we recall the small gain theorem given in [3]. In section 3, we present some sufficient conditions for the global asymptotic stability of the equilibrium point of system (1.1) by the small gain theorem. In section 4 we give an estimate of an ultimate bounded set of system (1.1).

2. Preliminaries

In this section, we review the small gain theorem given in [3], which is useful in the following arguments.

Consider the following interconnected system:

$$\begin{aligned}\dot{x}_1 &= g_1(x_1, x_2), \\ \dot{x}_2 &= g_2(x_1, x_2, u)\end{aligned}\tag{2.1}$$

with state $x = (x_1, x_2)^T$ and input $u \in \mathbb{R}^m$, where $x_1 \in \mathbb{R}^{n_1}$, $x_2 \in \mathbb{R}^{n_2}$, $u \in \mathbb{R}^m$ and $g_1(0, 0) = 0$, $g_2(0, 0, 0) = 0$.

Before stating the small gain theorem, we introduce the following definition and theorem obtained in [3].

Definition 2.1. (Alberto, Isidori [3]). A C^1 function $V : \mathbb{R}^{n_1+n_2} \rightarrow \mathbb{R}$ is called an ISS-Lyapunov function for system (2) if there exist class κ_∞ functions $\underline{\alpha}(\cdot)$, $\bar{\alpha}(\cdot)$, $k(\cdot)$, and a class κ function $\chi(\cdot)$ such that

$$\underline{\alpha}(\|x\|) \leq V(x) \leq \bar{\alpha}(\|x\|) \quad \text{for all } x = (x_1, x_2)^T \in \mathbb{R}^{n_1+n_2},$$

and

$$\|x\| \geq \chi(\|u\|) \Rightarrow \frac{\partial V}{\partial x} g(x, u) \leq -k(\|x\|) \text{ for all } x = (x_1, x_2)^T \in \mathbb{R}^{n_1+n_2},$$

where $g(x) = (g_1(x_1, x_2), g_2(x_1, x_2, u))^T$.

Theorem 2.1. (Alberto,Isidori [3]). A system is input-to-state stability if and only if there exists an ISS-Lyapunov function for the system.

Now for system (2.1) we make the following assumptions.

Assumption H₁. The x_1 -subsystem of system (2.1), viewed as a system with internal state x_1 and input x_2 , is input-to-state stable.

Assumption H₂. The x_2 -subsystem of system (2.1), viewed as a system with internal state x_2 and inputs x_1 and u , is input-to-state stable.

In view of Assumption H₁, definition 2.1 and Theorem 2.1, we have that for the x_1 -subsystem of system (2.1) there exist class κ_∞ functions $\underline{\alpha}(\cdot), \bar{\alpha}(\cdot), \alpha_1(\cdot)$, and a class κ function $\chi_1(\cdot)$ and an ISS-Lyapunov function $V_1 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} \underline{\alpha}_1(\|x_1\|) &\leq V_1(x_1) \leq \bar{\alpha}_1(\|x_1\|), \\ \|x_1\| \geq \chi_1(\|x_2\|) &\Rightarrow \frac{\partial V_1}{\partial x_1} g_1(x_1, x_2) \leq -k_1(\|x_1\|). \end{aligned}$$

Likewise, for the x_2 -subsystem of system (2.1) there exist class κ_∞ functions $\underline{\alpha}(\cdot), \bar{\alpha}(\cdot), \alpha_2(\cdot)$, and class κ function $\chi_2(\cdot)\chi_u(\cdot)$ and an ISS-Lyapunov function $V_2 : \mathbb{R}^{n_2} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} \underline{\alpha}_2(\|x_2\|) &\leq V_2(x_2) \leq \bar{\alpha}_2(\|x_2\|), \\ \|x_2\| \geq \max\{\chi_2(\|x_1\|), \chi_u(\|u\|)\} &\Rightarrow \frac{\partial V_2}{\partial x_2} g_2(x_1, x_2, u) \leq -k_2(\|x_2\|). \end{aligned}$$

Now we state the small gain theorem.

Theorem 2.2. (Small gain theorem) (Alberto,Isidori [3]). Suppose H₁ and H₂ hold, let

$$\gamma_1(r) = \underline{\alpha}_1^{-1} \circ \bar{\alpha}_1 \circ \chi_1(r), \tag{2.2}$$

$$\gamma_2(r) = \underline{\alpha}_2^{-1} \circ \bar{\alpha}_2 \circ \chi_2(r). \tag{2.3}$$

If the condition

$$\gamma_2(\gamma_1(r)) < r, \tag{2.4}$$

holds for all $r > 0$, then system (2.1), viewed as a system with state (x_1, x_2) and input u , is input-to-state stable.

Remark 2.1. When $u = 0$, the input-to-state stability implies the global asymptotic stability. (For more details see [3]).

3. The global asymptotic stability based on the small gain theorem

In this section we use the small gain theorem to discuss the global asymptotic stability of the equilibrium point of system (1.1). First we find the equilibrium point of system (1.1). To this end, we let

$$f_1(x, y, z) = a(y - x^3 + \mu_1 x) = 0, \quad (3.1)$$

$$f_2(x, y, z) = \mu_2 x - y + z + \delta = 0, \quad (3.2)$$

$$f_3(x, y, z) = \gamma(x - z) = 0. \quad (3.3)$$

According to (3.1)–(3.3), we have

$$x^3 - \mu x - \delta = 0, \quad (3.4)$$

where $\mu = (1 + \mu_1 + \mu_2)$. From (3.4), we have that the coordinate x of the equilibrium point depends only on μ and δ . The two other coordinate is determined by the following equations:

$$y = (\mu_2 + 1)x + \delta,$$

$$z = x.$$

Since we concern with the global asymptotic stability of the equilibrium point of the chemical system (1.1) in this section, we only consider this case that equation (3.4) has a unique positive real root.

Lemma 3.1. Consider equation (3.4), if $\mu < 0$ and $\delta > 0$ or $\mu > 0$ and $\delta > \frac{2}{3}\mu\sqrt{\frac{\mu}{3}}$ hold, then equation (3.4) has a unique positive real root x_0 , where

$$x_0 = \sqrt[3]{\frac{\delta}{2} + \sqrt{\frac{1}{4}\delta^2 - \frac{1}{27}\mu^3}} + \sqrt[3]{\frac{\delta}{2} - \sqrt{\frac{1}{4}\delta^2 - \frac{1}{27}\mu^3}}.$$

The above lemma 3.1 is easy to be proven, thus its proof is omitted.

The associated equilibrium point of system (1.1) with x_0 is denoted by (x_0, y_0, z_0) , where $y_0 = (\mu_2 + 1)x_0 + \delta$, $z_0 = x_0$. To analyze the global asymptotic stability of this equilibrium point (x_0, y_0, z_0) , we make the following translation:

$$x \rightarrow x - x_0, \quad y \rightarrow y - y_0, \quad z \rightarrow z - z_0.$$

Thus under this translation system (1.1) can be written as

$$\begin{aligned} \dot{x} &= a(y - x^3 + \mu_1 x - 3x^2 x_0 - 3xx_0^2), \\ \dot{y} &= \mu_2 x - y + z, \\ \dot{z} &= \gamma(x - z). \end{aligned} \tag{3.5}$$

Therefore we easily see that the global asymptotical stability of the equilibrium point $(0, 0, 0)$ of system (3.5) is equivalent to the global asymptotical stability of the equilibrium point (x_0, y_0, z_0) of system (1.1). Below we use the small gain theorem to discuss the global asymptotic stability of the equilibrium point $(0, 0, 0)$ of system (3.5). The following theorem 3.1 is obtained.

Theorem 3.1. Suppose that the conditions stated in lemma (3.1) hold, if $\mu_1 < \frac{3}{4}x_0^2$ and $d(\mu_2^2 + 1) < \frac{1}{16}c^4$ hold, where $x_0 = \sqrt[3]{\frac{\delta}{2} + \sqrt{\frac{1}{4}\delta^2 - \frac{1}{27}\mu^3}} + \sqrt[3]{\frac{\delta}{2} - \sqrt{\frac{1}{4}\delta^2 - \frac{1}{27}\mu^3}}$, $c^2 = 2(\frac{3}{4}x_0^2 - \mu_1)$ and $d = \max\{\gamma, \frac{1}{\gamma}\}$, then the equilibrium point $(0, 0, 0)$ of system (3.5) is globally asymptotically stable.

Proof. We consider the following two cases.

Case (1). $\gamma \geq 1$. For the y -subsystem and z -subsystem, we give the following ISS–Lyapunov function

$$V_1(y, z) = \frac{1}{2} \left(y^2 + \frac{z^2}{\gamma} \right) \tag{3.6}$$

and obtain

$$\begin{aligned} \dot{V}_1 &= \mu_2 xy - y^2 + yz + xz - z^2 \\ &\leq (\mu_2 x)^2 + x^2 - \frac{1}{4}y^2 - \frac{1}{4}z^2. \end{aligned}$$

We Choose $0 < \varepsilon < \frac{1}{4}$ and observe that if

$$(\mu_2 x)^2 + x^2 < \left(\frac{1}{4} - \varepsilon \right) (y^2 + z^2), \tag{3.7}$$

then

$$\dot{V}_1 \leq -\varepsilon(y^2 + z^2).$$

By $\gamma \geq 1$ and (3.6), we have

$$\frac{1}{2\gamma} (y^2 + z^2) \leq V_1(y, z) \leq \frac{1}{2} (y^2 + z^2). \tag{3.8}$$

From (3.7) and (3.8), we have

$$\underline{\alpha}_1(r) = \frac{1}{2\gamma}(r), \quad \bar{\alpha}_1(r) = \frac{1}{2}r^2, \quad \chi_1(r) = \sqrt{\frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}}r.$$

By (2.2), we have

$$\gamma_1(r) = \sqrt{\gamma \frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}}r.$$

For the x -subsystem, we present the following ISS-Lyapunov function

$$V_2(x) = \frac{1}{2}\alpha x^2 \tag{3.9}$$

and obtain

$$\begin{aligned} \dot{V}_2 &= xy + \mu_1 x^2 - x^2 \left(x^2 + 3xx_0 + \frac{9}{4}x_0^2 - \frac{9}{4}x_0^2 \right) - 3x^2x_0^2 \\ &\leq xy + \mu_1 x^2 - \frac{3}{4}x^2x_0^2 \\ &\leq \left(\mu_1 - \frac{3}{4}x_0^2 + \frac{1}{4}c^2 \right) x^2 + \frac{y^2 + z^2}{c^2}, \end{aligned}$$

where the constant c satisfies the following inequality

$$\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 > 0.$$

It is obvious that if $\mu_1 < \frac{3}{4}x_0^2$, then the above constant c is existent. We Choose $0 < \varepsilon < \frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2$ and observe that if

$$\frac{y^2 + z^2}{c^2} \leq \left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon \right) x^2, \tag{3.10}$$

then

$$\dot{V}_2 \leq \left(\mu_1 - \frac{3}{4}x_0^2 + \frac{1}{4}c^2 \right) x^2 + \frac{y^2 + z^2}{c^2} \leq -\varepsilon x^2.$$

By (3.9) and (3.10), we have

$$\underline{\alpha}_2(r) = \frac{1}{2a}r^2, \quad \bar{\alpha}_2(r) = \frac{1}{2a}r^2, \quad \chi_2(r) = \sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon \right) c^2}}r.$$

By (2.3), we have

$$\gamma_2(r) = \sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon\right) c^2}} r.$$

By the small gain condition, i.e. (2.4), we have

$$\gamma_2(\gamma_1(r)) = \sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon\right) c^2}} \sqrt{\gamma \frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}} r < r.$$

Further we have

$$\sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon\right) c^2}} \sqrt{\gamma \frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}} < 1.$$

Setting $\frac{1}{4}c^2 = \frac{1}{2} \left(\frac{3}{4}x_0^2 - \mu_1\right)$, we have

$$\gamma \left(\mu_2^2 + 1\right) < c^2 \left(\frac{1}{4}c^2 - \varepsilon\right) \left(\frac{1}{4} - \varepsilon\right). \tag{3.11}$$

Since $\varepsilon > 0$ is arbitrary small, by (3.11) we have

$$\gamma \left(\mu_2^2 + 1\right) < \frac{1}{16}c^4. \tag{3.12}$$

Therefore in this case by the small gain theorem, we have that if (3.12) holds, then the equilibrium point $(0, 0, 0)$ of system (3.5) is globally asymptotically stable.

Case (2). $\gamma \leq 1$. In this case, we choose the same ISS-Lyapunov functions $V_1(y, z)$ and $V_2(x)$. By $\gamma \leq 1$, we rewrite (3.8) in the following form

$$\frac{1}{2} \left(y^2 + z^2\right) \leq V_1(y, z) \leq \frac{1}{2\gamma} \left(y^2 + z^2\right). \tag{3.13}$$

Then

$$\underline{\alpha}_1(r) = \frac{1}{2}(r), \quad \bar{\alpha}_1(r) = \frac{1}{2\gamma}r^2.$$

Hence by the previous similar arguments, we have

$$\begin{aligned} \chi_1(r) &= \sqrt{\frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}} r, & \gamma_1(r) &= \sqrt{\frac{1}{\gamma} \frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}} r, \\ \chi_2(r) = \gamma_2(r) &= \sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon\right) c^2}} r. \end{aligned}$$

By the small gain condition, i.e. (2.4), we have

$$\gamma_2(\gamma_1(r)) = \sqrt{\frac{1}{\left(\frac{3}{4}x_0^2 - \mu_1 - \frac{1}{4}c^2 - \varepsilon\right) c^2}} \sqrt{\frac{1}{\gamma} \frac{\mu_2^2 + 1}{\frac{1}{4} - \varepsilon}} r < r.$$

By the above similar analysis, we have

$$\frac{1}{\gamma} (\mu_2^2 + 1) < \frac{1}{16} c^4. \tag{3.14}$$

Therefore in this case by the small gain theorem, we have that if (3.14) holds, then the equilibrium point $(0, 0, 0)$ of system (3.5) is globally asymptotically stable. The proof is complete. \square

Remark 3.1. When the conditions of Theorem 3.1 hold, we easily see that the equilibrium point (x_0, y_0, z_0) of system (1) is globally asymptotically stable. Thus system (1.1) does not exhibit chaotic behaviors under these conditions.

Remark 3.2. When $a = 18.7, \gamma = 4.35, \mu_1 = 0.44, \mu_2 = -1.43$ and $\delta = 0.0186$, we find that $x_0 < 0.4$ and $\frac{3}{4}x_0^2 - \mu_1 < 0$. This shows that the above parameters do not satisfy conditions of Theorem 3.1. In fact, it was shown in [2, 4] that under the above parameters system (1.1) exhibits chaotic behaviors.

4. Estimates of the ultimate bound of system (1.1)

In this section, we present an estimate of an ultimate bounded set of the chemical system (1.1). First we give the definition of ultimate bounded set.

Definition 4.1. A bounded closed set Ω is an ultimate bounded set for system $\dot{x} = f(x)$, where

$f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a continuous function, if for every initial value $x_0 \in \mathbb{R}^n$,

$$\lim_{t \rightarrow +\infty} \rho(x(t, x_0), \Omega) = 0$$

where $\rho(., .)$ is the Euclidian distance, $x(x_0, t)$ denotes the trajectory of system $\dot{x} = f(x)$ with initial value x_0 .

Now we state our result.

Theorem 4.1. Let $\Omega = \{(x, y, z) | V \leq M\}$, where $M = \max_{(x,y,z) \in \Omega} V(x, y, z)$,

$$V(x, y, z) = \frac{1}{2} \left(\frac{x^2}{a} + y^2 + \frac{z^2}{\gamma} \right),$$

$$\Omega = \left\{ (x, y, z) \mid (x^2 - \beta)^2 + \left((\mu_2 + 1)x - \frac{1}{2}y \right)^2 + \left(\frac{1}{2}y - \delta \right)^2 + \frac{1}{2}(x - z)^2 + \frac{1}{2}(y - z)^2 \leq \delta^2 + \beta^2 \right\},$$

$\beta = \frac{1}{2} \left(\mu_1 + \frac{1}{2} + (\mu_2 + 1)^2 \right)$. Then the set Ω is an ultimate bounded set of system (1.1).

Proof. We construct the following Lyapunov function

$$V(x, y, z) = \frac{1}{2} \left(\frac{x^2}{a} + y^2 + \frac{z^2}{\gamma} \right). \tag{4.1}$$

Then its time derivative along the trajectories of system (1) is

$$\begin{aligned} \dot{V} &= \frac{\partial V}{\partial x} f_1 + \frac{\partial V}{\partial y} f_2 + \frac{\partial V}{\partial z} f_3 \\ &= xy - x^4 + \mu_1 x^2 + \mu_2 xy - y^2 + yz + \delta y + xz - z^2 \\ &= (\mu_2 + 1)xy - x^4 + \mu_1 x^2 - \frac{1}{2}y^2 + \delta y + xz - \frac{1}{2}z^2 - \frac{1}{2}(z - y)^2 \\ &= (\mu_2 + 1)xy - x^4 + (\mu_1 + 1)x^2 - \frac{1}{2}y^2 + \delta y - \frac{1}{2}(x - z)^2 - \frac{1}{2}(z - y)^2 \\ &= -(x^2 - \beta)^2 - \left((\mu_2 + 1)x - \frac{1}{2}y \right)^2 - \left(\frac{1}{2}y - \delta \right)^2 \\ &\quad - \frac{1}{2}(x - z)^2 - \frac{1}{2}(z - y)^2 + \delta^2 + \beta^2, \end{aligned} \tag{4.2}$$

where $\beta = \frac{1}{2} \left(\mu_1 + \frac{1}{2} + (\mu_2 + 1)^2 \right)$.

We let

$$\Lambda = \{(x, y, z) \mid (x^2 - \beta)^2 + \left((\mu_2 + 1)x - \frac{1}{2}y \right)^2 + \left(\frac{1}{2}y - \delta \right)^2 + \frac{1}{2}(x - z)^2 + \frac{1}{2}(y - z)^2 \leq \delta^2 + \beta^2\}.$$

It is easy to see that Λ is a bounded closed set. Thus by the continuity of the function $V(x, y, z)$, there exists $(x_0, y_0, z_0) \in \Lambda$ such that

$$V(x_0, y_0, z_0) = \max_{(x, y, z) \in \Lambda} V(x, y, z) = M.$$

By (4.2), we have that if $(x, y, z) \in \Lambda^c$, then $\dot{V}(x, y, z) < 0$, where Λ^c is the complement of the set Λ .

Hence we have

$$\limsup_{t \rightarrow \infty} V \leq M.$$

Therefore the trajectories of system (1.1) is ultimately contained in the set

$$\Omega = \{(x, y, z) \mid V \leq M\},$$

that is, the set $\Omega = \{(x, y, z) \mid V \leq M\}$ is an ultimate bounded set of system (1.1). The proof is complete. \square

Remark 4.1. When $a = 18.7, \mu_1 = 0.44, \mu_2 = -1.43, \gamma = 4.35, \delta = 0.0186$, it was shown in [2, 4] that system (1.1) exhibits chaotic behaviors. By theorem 4.1 the trajectories of the chaotic system (1.1) is ultimately contained in the set $\Omega = \{(x, y, z) \mid V \leq 0.6759\}$, that is, the set $\Omega = \{(x, y, z) \mid V \leq 0.6759\}$ is an ultimate bounded set of system (1.1) under the above parameters. Therefore under the above parameters chaos takes place only in the set $\Omega = \{(x, y, z) \mid V \leq 0.6759\}$.

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