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A Balanced Shaping Method for Stabilizing Chemical Reaction Networks

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Abstract

A balanced shaping method for stabilizing open mass action systems is proposed in this paper. Since complex balanced systems are locally asymptotically stable, the closed loop system, which is dynamically equivalent to a complex balanced system under state feedback, is also stable. Essentially, the stabilization process is to find a target system such that the matching equation is satisfied. We show that balanced shaping control is an equivalent method of kinetic feedback design for stabilizing open mass action systems. In addition, controller design based on solving convex quadratic programming is also presented. Lastly, we illustrate the effectiveness of balanced shaping control with two examples.

1 Introduction

Chemical reaction networks (CRNs) arise abundantly in process systems and biological applications, the theory related to it has attracted a growing interest from engineering [17, 26], and even mathematics [1, 7, 24] in recent decades.

Research on CRNs was initiated and developed by Horn, Jackson [19], and Feinberg [14–16]. Structurally, each CRN corresponds to a directed graph, namely reaction graph. Reactions are associated with directed edges, while reactants and products (namely

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complexes) are associated with vertexes. This graph representation provides a clear insight on the mathematical structure of CRNs, since weakly reversible CRNs contribute to digraphs with each connected component to be a strongly connected one. Besides reaction graph, there exist other graph representations for CRNs, such as species-reaction graph [6] and species-reaction Petri net [2,3]. These two kinds of graphs were used to analyze the existence of multiple equilibria and develop checkable conditions for persistence of CRNs in [3] and [6] respectively. A CRN together with mass action law give rise to a mass action system. The dynamics of some mass action systems have been known to us. In [19], it was shown that mass action systems contain certain stability property, i.e., self-sustaining oscillation and bistability are precluded from complex balanced systems, and mass action systems admitting quasi-thermodynamic condition are locally asymptotically stable. Feinberg [13] reported the famous Deficiency Zero Theorem, saying that for each mass action system for which the underlying CRN is weakly reversible and has deficiency zero, then there exists a unique locally asymptotically stable equilibrium in each positive stoichiometric compatibility class. He extended it to the Deficiency One Theorem in [16], which gives weaker conditions for the existence and uniqueness of equilibrium in each positive stoichiometric compatibility class, i.e., weakly reversible but not necessary zero-deficient. The same results were established for complex balanced systems [19, 25, 33]. Furthermore, if complex balanced systems are assumed to be persistent, then the stability is global [1, 24]. The Lyapunov function used in all the above works is a logarithmic function, referred to as the Gibbs' free energy hereinafter. Recently, the famous global attractor conjecture has been proven by Craciun with toric differential inclusions [8], which implies complex balanced systems are globally asymptotically stable in each positive stoichiometric compatibility class.

A mass action system is a nonnegative polynomial system [5]. Mass action systems can be regarded as a possible prototype of nonlinear systems [11], since they have the ability to produce qualitative phenomena such as stable and unstable equilibria, multiple equilibria, bifurcation, oscillatory and even chaotic behavior [10, 11], which are important for us to study and understand nonlinear processes. In addition, a lot of nonnegative polynomial systems can be realized by mass action systems, i.e., for a nonnegative polynomial system, there exists a mass action system can realize its dynamics if some conditions are satisfied [18, 28]. Hence, we can investigate nonnegative polynomial systems from the perspective

of mass action systems [12].

Owing to such practical conclusions on mass action systems and strong relationship between mass action systems and nonnegative polynomial systems stated above, we can design controllers for open loop polynomial systems. In [31], the authors have considered an open loop system with linear input structure, both static and dynamic state feedback controllers were designed such that the closed loop system is dynamically equivalent to a weakly reversible mass action system. In another literature [22], the same strategies were applied to achieve weakly reversible mass action systems with minimal deficiency.

In this paper, we deal with the problem of stabilizing open mass action systems. If the closed loop system under control is dynamically equivalent to a system, which is stable at the desired state, then the former is also stable. Inspired by this fact, we stabilize open mass action systems by state feedback. Since complex balanced systems are stable at each equilibrium, we can choose them as target systems. More precisely, we look for a proper state feedback such that the closed loop system is dynamically equivalent to a mass action system with complex balanced structure. Therefore, control action is taken to shape the closed loop system, and hence we call this control method balanced shaping control. Mathematically, balanced shaping is equivalent to the solution of a set of nonlinear algebraic equations. By fixing the complex stoichiometric matrix of the target system, these nonlinear constraints change to be linear ones, then we can compute a target system which is as similar to the mass action system related to the open loop system as possible through solving convex quadratic programming problem, thus the controller is designed based on optimization.

The rest of this paper is organized as follows. Section 2 gives a brief introduction on CRNs. In section 3, we propose the theoretical framework for shaping closed loop systems such that they have complex balanced target systems under state feedback. Next, optimization based controller design is presented in section 4. Finally, balanced shaping control is applied to two examples in section 5. Section 6 concludes the paper.

Notation: Throughout the paper, $\mathbb{R}^n$, $\mathbb{R}^n_{>0}$, $\mathbb{R}^n_{\geq 0}$, $\mathbb{Z}^n$, and $\mathbb{Z}^n_{\geq 0}$ denote the space of n-dimensional real, positive real, non-negative real, integer and nonnegative integer vectors respectively; $A_{\cdot i}$ means the ith column of matrix A; $\mathbb{1}_n$ and $\mathbb{0}_n$ denote n-dimensional vector with all elements being 1 and 0, respectively; matrix $D = \mathrm{diag}(d_i) \in \mathbb{R}^{n\times n}$ is a diagonal matrix with the i_{th} diagonal element to be d_i.

2 Preliminaries on chemical reaction networks

In this section, we will sketch the mathematical structure of CRNs and the related results on stability analysis. All CRNs investigated are governed by mass action kinetics in this paper.

For a CRN involving n species $X_i (i = 1, \cdots, n)$, c complexes $\mathcal{C}_l (l = 1, \cdots, c)$ and r reactions $\mathcal{R}_j (j = 1, \cdots, r)$, we suppose the jth reaction is associated with complexes $\mathcal{C}_j$ and $\mathcal{C}_{j'}$, then it can be represented by

$$\mathcal{R}_j : \quad \sum_{i=1}^{n} Z_{ij} X_i \longrightarrow \sum_{i=1}^{n} Z_{ij'} X_i \,, \tag{1}$$

where $Z_{ij}, Z_{ij'} \in \mathbb{Z}_{\geq 0}$ are called stoichiometric coefficients. The stoichiometric coefficients not only define the complex stoichiometric matrix $Z \in \mathbb{Z}_{\geq 0}^{n \times c}$ with $Z_{\cdot l}$ expressing the lth complex $\mathcal{C}_l$ in the n species, but also define the stoichiometric matrix $S \in \mathbb{Z}^{n \times r}$ with $S_{\cdot j} = Z_{\cdot j'} - Z_{\cdot j}$. Using a slight abuse of notation, we will also refer to the vector $Z_{\cdot l}$ as the complex $\mathcal{C}_l$ in the context.

Definition 1. *A CRN $\mathcal{N} = \{\mathcal{X}, \mathcal{C}, \mathcal{R}\}$ is composed of three finite sets:*

(1) *A set $\mathcal{X} = \bigcup_{i=1}^{n} X_i$ of species;*

(2) *A set $\mathcal{C} = \bigcup_{j=1}^{r} \{Z_{\cdot j}, Z_{\cdot j'}\}$ of complexes with $\bigcup_{j=1}^{r} \{j, j'\} = \{1, \cdots, c\}$ and $Z_{\cdot j}$, $Z_{\cdot j'} \in \mathbb{Z}_{\geq 0}^{n}$;*

(3) *A set $\mathcal{R} = \bigcup_{j=1}^{r} \{Z_{\cdot j} \to Z_{\cdot j'}\}$ of reactions, such that for any $Z_{\cdot j} \in \mathcal{C}$, $Z_{\cdot j} \to Z_{\cdot j} \notin \mathcal{R}$, and there must exist a $Z_{\cdot j'} \in \mathcal{C}$ satisfying either $Z_{\cdot j} \to Z_{\cdot j'} \in \mathcal{R}$ or $Z_{\cdot j'} \to Z_{\cdot j} \in \mathcal{R}$.*

Matrices S and Z can be connected by

$$S = ZB, \tag{2}$$

where $B \in \mathbb{R}^{c \times r}$ is the incidence matrix [4] of reaction graph $G(V, E)$ of $\mathcal{N}$. Structurally, $G(V, E)$ is a digraph, where V is the set of vertexes with each vertex corresponding to a complex and E is the set of edges with each edge corresponding to a reaction. For reaction graph G, its incidence matrix B is defined as $B_{lj} = 1$ (and -1) if complex $\mathcal{C}_l$ acts as product (and reactant) complex for reaction $\mathcal{R}_j$, and $B_{lj} = 0$ otherwise [25].

Definition 2. *A CRN $\mathcal{N}$ is weakly reversible if for each reaction $Z_{\cdot j} \to Z_{\cdot j'} \in \mathcal{R}$, there exists a sequence of reactions in $\mathcal{R}$, which starts with $Z_{\cdot j'}$ and ends with $Z_{\cdot j}$, i.e., $Z_{\cdot j'} \to$*

$Z_{\cdot j_1} \in \mathcal{R}$, $Z_{\cdot j_1} \to Z_{\cdot j_2} \in \mathcal{R}$, $\cdots$, $Z_{\cdot j_{(k-1)}} \to Z_{\cdot j_k} \in \mathcal{R}$, $Z_{\cdot j_k} \to Z_{\cdot j} \in \mathcal{R}$. $\mathcal{N}$ *is reversible if* $Z_{\cdot j} \to Z_{\cdot j'} \in \mathcal{R}$ *indicates* $Z_{\cdot j'} \to Z_{\cdot j} \in \mathcal{R}$.

In a view of graph theory, $\mathcal{N}$ is weakly reversible if and only if each component of reaction graph G is a strongly connected one. Obviously, reversible CRNs are also weakly reversible in the view of graph theory.

With mass balance, the dynamics of a CRN can be modeled by

$$\dot{x} = Sv(x), \tag{3}$$

where $x \in \mathbb{R}^n_{\geq 0}$ is the concentration vector with x_i representing the concentration of species X_i, $v(x)$ is the reaction rate vector with $v_j(x)$ representing the rate function of $\mathcal{R}_j$.

Definition 3. *The linear subspace* Im S *is called the stoichiometric subspace of* $\mathcal{N}$. *For any* $x_0 \in \mathbb{R}^n_{>0}$, $\mathscr{S}(x_0) = \{x_0 + \xi | \xi \in \text{Im } S\}$ *is named the stoichiometric compatibility class of* x_0, *and* $\mathscr{S}(x_0) \cap \mathbb{R}^n_{>0}$ *is called the positive stoichiometric compatibility class of* x_0.

Integrating (3) with respect to time yields

$$x - x_0 = \sum_{j=1}^{r} S_{\cdot j} \int_0^t v_j(\tau) d\tau,$$

where $x_0 = x(0)$ is the initial condition. Therefore, the state remains within $\mathscr{S}(x_0)$ for all time if the system starts with x_0.

Rate function $v_j(x)$ is related to the kinetics. Under mass action kinetics, the reaction rate obeys power law in the concentrations of species. For $\mathcal{R}_j$, the reaction rate is

$$v_j(x) = k_{jj'} \prod_{i=1}^{n} x_i^{Z_{ij}}, \tag{4}$$

where $k_{jj'}$ is the reaction rate coefficient. Therefore, dynamics of CRNs governed by mass action kinetics can be captured by the following complex centered formulation [28]

$$\dot{x} = Z\mathcal{L}\Psi(x), \tag{5}$$

where $\mathcal{L} \in \mathbb{R}^{c \times c}$ is a Kirchhoff matrix with

$$\mathcal{L}_{ij} = \begin{cases} k_{ji} & i \neq j, \\ -\sum_{k \neq j}^{c} \mathcal{L}_{kj} & i = j. \end{cases} \tag{6}$$

and $\Psi(x) \in \mathbb{R}^c$ is the kinetic vector given by

$$\Psi(x) = \begin{bmatrix} \prod_{i=1}^{n} x_i^{Z_{i1}} \\ \vdots \\ \prod_{i=1}^{n} x_i^{Z_{ic}} \end{bmatrix}. \tag{7}$$

Here, k_{ji} is the reaction rate coefficient of $Z_{\cdot j} \to Z_{\cdot i}$. Obviously, $\mathcal{L}$ reports the structure of $\mathcal{N}$, i.e., $\mathcal{L}_{ij} \neq 0$ if and only if there exists a reaction from complex $Z_{\cdot j}$ to complex $Z_{\cdot i}$, and $\Psi(x)$ is solely determined by Z. Denote the set of k_{ji} as $\mathcal{K}$, i.e., $\mathcal{K} = \bigcup_{i,j=1,i\neq j}^{c} k_{ji}$, then we can define mass action system as following.

Definition 4. *A CRN $\mathcal{N} = \{\mathcal{X}, \mathcal{C}, \mathcal{R}\}$ together with mass action kinetics give rise to a mass action system $\mathcal{M} = \{\mathcal{X}, \mathcal{C}, \mathcal{R}, \mathcal{K}\}$ admitting*

$$\dot{x} = Z\mathcal{L}\Psi(x). \tag{8}$$

$\mathcal{M}$ is called weakly reversible if $\mathcal{N}$ is weakly reversible.

Both complex balanced systems and detailed balanced systems are weakly reversible, the definitions of them are given below.

Definition 5. *For a mass action system $\mathcal{M}$ captured by (8), $x^* \in \mathbb{R}^n_{>0}$ is a complex balanced equilibrium of $\mathcal{M}$ if $\mathcal{L}\Psi(x^*) = \mathbb{0}_c$. Mass action systems admitting a complex balanced equilibrium are named complex balanced systems.*

Definition 6. *For a mass action system $\mathcal{M}$ captured by (8), $x^* \in \mathbb{R}^n_{>0}$ is a detailed balanced equilibrium of $\mathcal{M}$ if $\Lambda\mathcal{L}^\top = \mathcal{L}\Lambda$, where $\Lambda = \mathrm{diag}(\Psi_i(x^*)) \in \mathbb{R}^{c\times c}$. Mass action systems admitting a detailed balanced equilibrium are named detailed balanced systems.*

Detailed balanced systems are definitely complex balanced systems, while some other conditions should be satisfied for a complex balanced system to be detailed balanced [9]. For these two classes of balanced systems, the stability has been known.

Lemma 1. [8, 19, 25] For a complex balanced system $\mathcal{M}$ governed by (8), suppose $x^* \in \mathbb{R}^n_{>0}$ is an equilibrium, then x^* is the unique equilibrium in $\mathscr{S}(x^*) \cap \mathbb{R}^n_{>0}$, and moreover, it is locally asymptotically stable with respect to all initial conditions in $\mathscr{S}(x^*) \cap \mathbb{R}^n_{>0}$ near x^*. Further, under persistence x^* is globally asymptotically stable with respect to all initial conditions in $\mathscr{S}(x^*) \cap \mathbb{R}^n_{>0}$.

The proof of the **Lemma 1** is carried through with Lyapunov function

$$G(x) = x^\top[\mathrm{Ln}(x) - \mathrm{Ln}(x^*)] - (x - x^*)^\top \mathbb{1}_n, \tag{9}$$

which is referred to as the Gibbs' free energy in the context.

Corollary 1. [8,9,32] For any detailed balanced system, there exists a unique equilibrium in each positive stoichiometric compatibility class. Moreover, every equilibrium is locally asymptotically stable. The result is further enhanced to globally asymptotic stability with persistence support.

3 Balanced shaping control

Though complex balanced systems are locally asymptotically stable, the stability of mass action systems that are not complex balanced is not known to us yet. This together with the demand that a system should work at a certain positive equilibrium motivate us to consider the following control problem: For a positive state $x^\dagger \in \mathbb{R}^n_{>0}$, how to stabilize the closed loop system at $x^\dagger$ with a controller? This problem formulation captures well the actual requirement of system biology and chemical engineering. In this section, we stabilize mass action systems through balanced shaping. Firstly, we give a formulation of open mass action system following the literature [23]. Then balanced shaping control strategy is proposed.

3.1 Open mass action systems

Open mass action systems (reactions contained in $\mathcal{M}$ are taking place in a reactor) are process systems under the following assumptions:

(1) the system is isothermal and isobaric,

(2) constant physico-chemical properties, such as density and reaction rate coefficients,

(3) only inlet and outlet convection and reactions are taking place.

With overall mass balance and component mass balances, the open system can be model by [23]

$$\begin{cases} \dot{x} = Z\mathcal{L}\Psi(x) - y(\sum_{i=1}^n F_i)x + y\bar{F}x_{in}, \\ \dot{y} = y^2(F_{out} - \sum_{i=1}^n F_i), \end{cases} \tag{10}$$

where $x \in \mathbb{R}^n_{\geq 0}$ is the state vector, Z, $\mathcal{L}$ and $\Psi(x)$ are matrices related to mass action system $\mathcal{M}$, $y = \frac{1}{V}$ where V is the volume of the liquid in the reactor, $\bar{F} = \mathrm{diag}(F_i) \in \mathbb{R}^{n\times n}_{\geq 0}$ where F_i is the inlet volumetric flow rate containing species X_i, F_{out} is the outlet volumetric flow rate containing all components in the reactor, and $x_{in} = [x_{1,in}, \cdots, x_{n,in}]^\top \in \mathbb{R}^n_{\geq 0}$ where $x_{i,in}$ is the inlet concentration of species X_i.

Assume F_i is kept constant for all $i = 1, \cdots, n$, then we can use F_{out} to stabilize y at any $y^* \in \mathbb{R}_{>0}$ using the equation $\dot{y} = y^2(F_{out} - \sum_{i=1}^{n} F_i)$. Therefore, we assume y is perfectly controlled and constant in our model, without loss of generality, we assume $y = y^* = 1$. Hence we can model open mass action systems by the following linear input affine system

$$\dot{x} = Z\mathcal{L}\Psi(x) - fx + gu, \tag{11}$$

where $f = (\sum_{i=1}^{n} F_i)$ is constant, $g = \bar{F}$ is the linear input structure, and $u = x_{in}$ is the input. It is important to remark that we choose inlet concentrations as manipulable input but keep V constant to model open mass action systems here.

Eq. (11) is a fully actuated system, there is a designed input for each of the n states. However, this is not practical since not all inlet concentrations are manipulable. Therefore, a general model for the open mass action system is needed. Denote $\mathcal{E}$ ($|\mathcal{E}| = p$) as the index set of manipulable variables, i.e.,

$$\mathcal{E} = \{i | i \in \mathcal{E} \text{ if and only if } x_{i,in} \text{ is munipulable}\}. \tag{12}$$

Then a general model for the open mass action system is

$$\dot{x} = Z\mathcal{L}\Psi(x) - \hat{f}x + \hat{g}\hat{u}, \tag{13}$$

where $\hat{f} = \sum_{i\in\mathcal{E}} F_i$, $\hat{g} = \{\bar{F}_{\cdot i} | \hat{g}_{\cdot j} = \bar{F}_{\cdot i} \text{ if and only if } i \in \mathcal{E},\ j = 1, \cdots, p\}$ is the linear input structure, $\hat{u} = \{x_{i,in} | \hat{u}_j = x_{i,in} \text{ if and only if } i \in \mathcal{E},\ j = 1, \cdots, p\}$ is the input. Moreover, $\hat{g}$ is of full column rank, i.e., $\text{rank}(\hat{g}) = p$. For example, if $x_{1,in}$ is the manipulable inlet concentration for reaction

$$X_1 \xrightarrow{k_{12}} X_2 \xrightarrow{k_{23}} X_3 \tag{14}$$

taking placing in the reactor, then the corresponding $\hat{f}$, $\hat{g}$ and $\hat{u}$ are

$$\hat{f} = F_1, \quad \hat{g} = \begin{bmatrix} F_1 \\ 0 \\ 0 \end{bmatrix}, \quad \hat{u} = x_{1,in}. \tag{15}$$

Denote $\mathcal{N}_1 = \{ X_i \xrightarrow{\hat{f}} \mathcal{C}_0 , i = 1, \cdots, n\}$, and $\mathcal{M}_1$ as the mass action system for which the underlying CRN is $\mathcal{N}_1$, then $\dot{x} = -\hat{f}x$ is dynamically equivalent to $\mathcal{M}_1$. Let $\hat{\mathcal{M}}$ be the mass action system consists of $\mathcal{M}$ and $\mathcal{M}_1$, then $\dot{x} = Z\mathcal{L}\Psi(x) - \hat{f}x$ is dynamically equivalent to mass action system $\hat{\mathcal{M}}$. Hence, (13) can be rewritten as

$$\dot{x} = \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\hat{u}, \tag{16}$$

where $\hat{Z}$, $\hat{\mathcal{L}}$ and $\hat{\Psi}(x)$ are matrices related to mass action system $\hat{\mathcal{M}}$. Take the mass action system represented by (14) for example, by choosing $x_{1,in}$ as manipulable inlet concentration, then the corresponding mass action system $\mathcal{M}_1$ is

$$\begin{array}{ccccc} X_1 & \xrightarrow{k_{12}} & X_2 & \xrightarrow{k_{23}} & X_3, \\ & \searrow^{F_1} & \downarrow{\scriptstyle F_1} & \swarrow_{F_1} & \\ & & \mathcal{C}_0 & & \end{array} \tag{17}$$

and the open mass action system can be modeled by (16), where $\hat{Z}$ and $\hat{\mathcal{L}}$ are

$$\hat{Z} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \hat{\mathcal{L}} = \begin{bmatrix} -(F_1 + k_{12}) & 0 & 0 & 0 \\ k_{12} & -(F_1 + k_{23}) & 0 & 0 \\ 0 & k_{23} & -F_1 & 0 \\ F_1 & F_1 & F_1 & 0 \end{bmatrix}.$$

3.2 Balanced shaping control strategy

For open loop system (16), if we stabilize it with state feedback $\hat{u} = \alpha(x)$, then the closed loop system is

$$\dot{x} = \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\alpha(x). \tag{18}$$

Furthermore, if system (18) is dynamically equivalent to a system

$$\dot{x} = f(x), \tag{19}$$

which is stable at $x^\dagger$, then closed loop system (18) will also be stable at $x^\dagger$.

Since complex balanced systems are locally asymptotically stable at each equilibrium, they are naturally candidate systems for (19). Specifically, if system (18) is dynamically equivalent to a complex balanced system $\tilde{\mathcal{M}} = \{\mathcal{X}, \tilde{\mathcal{C}}, \tilde{\mathcal{R}}, \tilde{\mathcal{K}}\}$ modeled by

$$\dot{x} = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x), \tag{20}$$

where $x \in \mathbb{R}^n_{\geq 0}$ is the state, $\tilde{Z}$, $\tilde{\mathcal{L}}$ and $\tilde{\Psi}(x)$ are defined as in section 2. Then we get

$$\hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\alpha(x) = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x). \tag{21}$$

As $\hat{g}$ is of full column rank, $\hat{g}^\top\hat{g}$ is nonsingular, we can rewrite (21) as

$$\begin{aligned} \alpha(x) &= (\hat{g}^\top\hat{g})^{-1}\hat{g}^\top\left(\tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x) - \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x)\right) \\ &= (\hat{g}^\top\hat{g})^{-1}Q\Phi(x), \end{aligned} \tag{22}$$

where $Q \in \mathbb{R}^{p\times q}$ is a matrix with constant elements, $\Phi(x) \in \mathbb{R}^q_{\geq 0}$ is a nonnegative vector with distinct elements (nonnegative monomials).

For open mass action system, we choose inlet concentrations as manipulable inputs in section 2, hence $\hat{u} = \alpha(x)$ should be nonnegative in a necessary condition of physical realizability. Since $\hat{g}^\top \hat{g}$ is a positive diagonal matrix, a sufficient condition for $\alpha(x)$ given by (22) to be nonnegative is that Q is a nonnegative matrix, i.e., $Q \in \mathbb{R}^{p\times q}_{\geq 0}$.

Based on the above analysis, we have the following control strategy.

Theorem 1. *For open mass action system modeled by (16), $x^\dagger \in \mathbb{R}^n_{>0}$ is a desired equilibrium point, if there exist $\tilde{Z} \in \mathbb{Z}^{n\times \tilde{c}}_{\geq 0}$ and $\tilde{\mathcal{L}} \in \mathbb{R}^{\tilde{c}\times\tilde{c}}$ such that*

(i) $\tilde{\mathcal{L}}\tilde{\Psi}(x^\dagger) = \mathbb{0}_{\tilde{c}}$,

(ii) $\mathbb{1}_{\tilde{c}}^\top \tilde{\mathcal{L}} = \mathbb{0}_{\tilde{c}}^\top$ *and* $\tilde{\mathcal{L}}_{ij} \geq 0,\ \forall\ i \neq j$,

(iii) $\hat{g}^\perp \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) = \hat{g}^\perp \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x)$ *(we call it matching equation),*

(iv) Q *is a nonnegative matrix, i.e.,* $Q \in \mathbb{R}^{p\times q}_{\geq 0}$,

where $\hat{g}^\perp \in \mathbb{R}^{(n-p)\times n}$ is a left annihilator of $\hat{g}$ with $\mathrm{rank}(\hat{g}^\perp) = n - p$. *Then the closed loop system is stable at $x^\dagger$ under state feedback*

$$\hat{u} = (\hat{g}^\top \hat{g})^{-1} Q\Phi(x), \tag{23}$$

where Q and $\Phi(x)$ are given by (22).

Proof. Conditions (i) and (ii) ensure that mass action system $\tilde{\mathcal{M}} = \{\mathcal{X}, \tilde{\mathcal{C}}, \tilde{\mathcal{R}}, \tilde{\mathcal{K}}\}$ modeled by $\dot{x} = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x)$ is complex balanced at $x^\dagger$.

Since $\hat{g}^\perp$ is a left annihilator of $\hat{g}$, i.e., $\hat{g}^\perp \hat{g} = \mathbb{0}_{(n-p)\times p}$, this together with condition (iii) indicate that there exists $\alpha(x)$ such that

$$\tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x) - \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) = \hat{g}\alpha(x), \tag{24}$$

or equivalently $\hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\alpha(x) = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x)$, which means complex balanced system $\tilde{\mathcal{M}}$ is dynamically equivalent to the closed loop system $\dot{x} = \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\alpha(x)$. According to **Lemma 1**, $\tilde{\mathcal{M}}$ is locally asymptotically stable at each equilibrium, therefore, the closed loop system will also be stable at $x^\dagger$ with state feedback $\hat{u} = \alpha(x)$. While $\mathrm{rank}(\hat{g}) = p$, $\hat{g}^\top \hat{g}$ is nonsingular, we get

$$\begin{aligned} \alpha(x) &= (\hat{g}^\top \hat{g})^{-1} \hat{g}^\top \left(\tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x) - \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) \right) \\ &= (\hat{g}^\top \hat{g})^{-1} Q\Phi(x) \end{aligned} \tag{25}$$

from (24), and the nonnegativity of $\alpha(x)$ follows from condition (iv). This completes the proof. □

Remark 1. It is important to observe that we can compute $\hat{g}^{\perp}$ with identity matrix E and $\mathcal{E}$ defined by (12), i.e.,

$$\hat{g}^{\perp} = \{E_{i\cdot} | [\hat{g}^{\perp}]_{\cdot j} = E_{i\cdot} \text{ if and only if } i \in \{1, \cdots, n\} \backslash \mathcal{E},\ j = 1, \cdots, n-p\}. \tag{26}$$

Take the input structure $\hat{g}$ in (15) as an example, a left annihilator is

$$\hat{g}^{\perp} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Since detailed balanced systems are also complex balanced systems, we have the following conclusion for a detailed balanced system to be the target system.

Corollary 2. For open mass action system modeled by (16), $x^{\dagger} \in \mathbb{R}^n_{>0}$ is a desired equilibrium point, if there exist $\tilde{Z} \in \mathbb{Z}^{n\times\tilde{c}}_{\geq 0}$ and $\tilde{\mathcal{L}} \in \mathbb{R}^{\tilde{c}\times\tilde{c}}$ such that

(i) $\tilde{\Lambda}\tilde{\mathcal{L}}^{\top} = \tilde{\mathcal{L}}\tilde{\Lambda}$,

(ii) $\mathbb{1}_{\tilde{c}}^{\top}\tilde{\mathcal{L}} = \mathbb{0}_{\tilde{c}}^{\top}$ and $\tilde{\mathcal{L}}_{ij} \geq 0,\ \forall\ i \neq j$,

(iii) $\hat{g}^{\perp}\hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) = \hat{g}^{\perp}\tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x)$,

(iv) Q is a nonnegative matrix, i.e., $Q \in \mathbb{R}^{p\times q}_{\geq 0}$,

where $\tilde{\Lambda} = \mathrm{diag}(\tilde{\Psi}_i(x^{\dagger})) \in \mathbb{R}^{\tilde{c}\times\tilde{c}}$, then the closed loop system is stable at $x^{\dagger}$ under state feedback (23).

Theorem 1 provides a controller design method for stabilizing open loop system (16) at $x^{\dagger}$. Since the closed loop system is dynamically equivalent to a locally asymptotically stable target system, which in fact is a complex balanced system, we would like to call this control method balanced shaping. Under control action $\hat{u} = \alpha(x)$, the closed loop system works like a complex balanced system, therefore, the complex balanced structure is shaped through $\alpha(x)$.

Generally, conditions given by **Theorem 1** is less strict than that reported in **Corollary 2**, since detailed balanced systems are definitely complex balanced.

Remark 2. A strongly related notion of balanced shaping control is kinetic feedback design [23]. For an open loop polynomial system with nonnegative integer exponents

$$\dot{x} = \tilde{M}\tilde{\Psi}(x) + \hat{g}\hat{u}, \tag{27}$$

where $\tilde{M} \in \mathbb{R}^{n\times\tilde{c}}$ is a constant matrix, $\tilde{\Psi}(x) \in \mathbb{R}^{\tilde{c}}$ contains monomials of the open loop system, $\hat{g} \in \mathbb{R}^{n\times p}$ is the linear input structure, $\hat{u} \in \mathbb{R}^{p}$ is the input, Lipták et al [23] proposed a kinetic design method for stabilizing the system at a desired positive equilibrium point $x^{\dagger}$. With static polynomial feedback law

$$\hat{u} = K\tilde{\Psi}(x), \tag{28}$$

where K is a constant feedback gain to be determined, the closed loop system is

$$\dot{x} = (\tilde{M} + \hat{g}K)\tilde{\Psi}(x). \tag{29}$$

As $\tilde{\Psi}(x)$ is determined by a matrix $\tilde{Z} \in \mathbb{Z}_{\geq 0}^{n\times\tilde{c}}$, if there exist K and Kirchhoff matrix $\tilde{\mathcal{L}}$ such that the closed loop system is dynamically equivalent to a complex balanced system $\tilde{\mathcal{M}}$ characterized by the pair $(\tilde{Z}, \tilde{\mathcal{L}})$, i.e.,

$$(\tilde{M} + \hat{g}K)\tilde{\Psi}(x) = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x), \tag{30}$$

then the closed loop system will be stable at $x^{\dagger}$, since $\tilde{\mathcal{M}}$ is stable at $x^{\dagger}$. Compared with kinetic feedback design, balanced shaping control is an equivalent method for stabilizing open mass action systems by supposing $\tilde{Z} = \hat{Z}$. According to **Theorem 1**, the following conditions should be fulfilled with $\tilde{Z} = \hat{Z}$

$$\begin{cases} \tilde{\mathcal{L}}\hat{\Psi}(x^{\dagger}) = \mathbb{0}_{\hat{c}}, & \text{(31a)} \\ \mathbb{1}_{\hat{c}}^{\top}\tilde{\mathcal{L}} = \mathbb{0}_{\hat{c}}^{\top}, & \text{(31b)} \\ \tilde{\mathcal{L}}_{ij} \geq 0,\ \forall\ i \neq j, & \text{(31c)} \\ \hat{g}^{\perp}\hat{Z}(\hat{\mathcal{L}} - \tilde{\mathcal{L}}) = \mathbb{0}_{(n-p)\times\hat{c}}, & \text{(31d)} \\ [\hat{g}^{\top}\hat{Z}(\tilde{\mathcal{L}} - \hat{\mathcal{L}})]_{ij} \geq 0,\ \forall\ i = 1, \cdots, p,\ j = 1, \cdots, \hat{c}. & \text{(31e)} \end{cases}$$

While the conditions (i.e. Eqs. (38), (40) and (41) in [23]) should be fulfilled for kinetic feedback design are

$$\begin{cases} \tilde{\mathcal{L}}\hat{\Psi}(x^{\dagger}) = \mathbb{0}_{\hat{c}}, & \text{(32a)} \\ \mathbb{1}_{\hat{c}}^{\top}\tilde{\mathcal{L}} = \mathbb{0}_{\hat{c}}^{\top}, & \text{(32b)} \\ \tilde{\mathcal{L}}_{ij} \geq 0,\ \forall\ i \neq j, & \text{(32c)} \\ (\tilde{M} + \hat{g}K) = \hat{Z}\tilde{\mathcal{L}}, & \text{(32d)} \\ K_{ij} \geq 0,\ \forall\ i = 1, \cdots, p,\ j = 1, \cdots, \hat{c}. & \text{(32e)} \end{cases}$$

Next, we prove that conditions (31d) and (31e) are equivalent to (32d) and (32e). If there exists a Kirchhoff matrix $\tilde{\mathcal{L}}$ such that Eqs. (31d) and (31e) are satisfied, then there exists

a $\hat{K}$ such that $\hat{Z}(\hat{\mathcal{L}}-\tilde{\mathcal{L}})=\hat{g}\hat{K}$, since $\hat{g}^{\perp}$ is the left annihilator of $\hat{g}$. Let $K=-\hat{K}$, then (32d) is fulfilled (here $\tilde{M}=\hat{Z}\hat{\mathcal{L}}$). Moreover, we have $\hat{K}=-(\hat{g}^{\top}\hat{g})^{-1}\hat{g}^{\top}\hat{Z}(\tilde{\mathcal{L}}-\hat{\mathcal{L}})$, it follows that (32e) is satisfied since $\hat{g}^{\top}\hat{g}$ is a positive diagonal matrix. On the other hand, if there exist $\tilde{\mathcal{L}}$ and K such that conditions (32d) and (32e) are satisfied, then (31d) is straightforward since $\tilde{M}=\hat{Z}\hat{\mathcal{L}}$, and we can get $K=(\hat{g}^{\top}\hat{g})^{-1}\hat{g}^{\top}\hat{Z}(\tilde{\mathcal{L}}-\hat{\mathcal{L}})$. While $K_{ij}\geq 0$ and $\hat{g}^{\top}\hat{g}$ is a positive diagonal matrix, (31e) is fulfilled. Therefore, balanced shaping control and kinetic feedback design are equivalent methods for stabilizing open mass action systems. Though these two methods have the same design goal, i.e., the closed loop system is dynamically equivalent to a complex balanced system $\tilde{\mathcal{M}}$. However, $\tilde{\mathcal{L}}$ is the only variable to be determined in balanced shaping control, we characterize the existence and positivity of $\hat{u}$ i.e., (31d) and (31e), with the help of $\hat{g}^{\perp}$, hence balanced shaping control may has advantage in computation in this sense.

Remark 3. Balanced shaping control can also be applied to stabilize affine system like

$$\dot{x}=\hat{f}(x)+\hat{g}\hat{u}, \tag{33}$$

where $\hat{g}\in\mathbb{R}^{n\times p}$ is the linear input structure with full column rank, $\hat{u}\in\mathbb{R}^{p}$ is the input, and $\hat{f}(x)\in\mathbb{R}^{n}$ is a kinetically realizable polynomial vector field [18], i.e., $\hat{f}(x)$ has the form

$$\hat{f}_i(x)=-x_i\mu_i(x)+\nu_i(x),\quad i=1,\cdots,n \tag{34}$$

where $\mu_i(x)$ and $\nu_i(x)$ are polynomials with nonnegative coefficients. In this case, system $\dot{x}=\hat{f}(x)$ can be kinetically realized by a mass action system $\hat{\mathcal{M}}$, hence (33) can be rewritten as

$$\dot{x}=\hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x)+\hat{g}\hat{u},$$

where $\hat{Z}$, $\hat{\mathcal{L}}$ and $\hat{\Psi}(x)$ are matrices related to $\hat{\mathcal{M}}$. Thus, balanced shaping control is applicable to this case.

4 Optimization based controller design

Since the target system fulfilled for conditions in **Theorem 1** and **Corollary 2** may not be unique, it follows that there may exist several controllers. In order to get an appropriate controller, we propose a systematic method for computing complex balanced (or detailed balanced) target system based on optimization in this section.

As $\tilde{\Psi}(x)$ is determined by $\tilde{Z}$, conditions (i) and (iii) in **Theorem 1** are nonlinear constraints involving $\tilde{Z}$ and $\tilde{\mathcal{L}}$. For simplicity, we can fix $\tilde{Z} = \hat{Z}$, and then look for a solution of the following linear constraints:

$$\begin{cases} \tilde{\mathcal{L}}\hat{\Psi}(x^\dagger) = \mathbb{0}_{\hat{c}}, \\ \mathbb{1}_{\hat{c}}^\top \tilde{\mathcal{L}} = \mathbb{0}_{\hat{c}}^\top, \\ \tilde{\mathcal{L}}_{ij} \geq 0, \ \forall\ i \neq j, \\ \hat{g}^\perp \hat{Z}(\hat{\mathcal{L}} - \tilde{\mathcal{L}}) = \mathbb{0}_{(n-p)\times\hat{c}}, \\ [\hat{g}^\top \hat{Z}(\hat{\mathcal{L}} - \tilde{\mathcal{L}})]_{ij} \geq 0, \ \forall\ i = 1, \cdots, p, \ j = 1, \cdots, \hat{c}. \end{cases} \tag{35}$$

In this case, the stabilizer (23) changes to be

$$\hat{u} = (\hat{g}^\top \hat{g})^{-1} \hat{g}^\top \hat{Z}(\tilde{\mathcal{L}} - \hat{\mathcal{L}})\hat{\Psi}(x), \tag{36}$$

since $Q = \hat{g}^\top \hat{Z}(\tilde{\mathcal{L}} - \hat{\mathcal{L}})$ and $\Phi(x) = \hat{\Psi}(x)$.

We hope to find a proper target system which is as similar to $\hat{\mathcal{M}}$ as possible, and hence the control cost may be cut down. The reasons are: (a) Balanced shaping control strategy can be considered as control action is taken such that $\hat{\mathcal{M}}$ is shaped into $\tilde{\mathcal{M}}$ since $\hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\alpha(x) = \tilde{Z}\tilde{\mathcal{L}}\tilde{\Psi}(x)$. (b) The controller given by (36) containing $\tilde{\mathcal{L}} - \hat{\mathcal{L}}$, which is the only difference between $\hat{\mathcal{M}}$ and $\tilde{\mathcal{M}}$ since $\tilde{Z} = \hat{Z}$. An available performance index function is

$$J(\tilde{\mathcal{L}}) = \frac{1}{2} \sum_{i,j=1}^{\hat{c}} (\tilde{\mathcal{L}}_{ij} - \hat{\mathcal{L}}_{ij})^2. \tag{37}$$

Based on the objective function (37) and constraints given by (35), an optimization based systematic method for computing complex balanced target system is

$$\min_{\tilde{\mathcal{L}}} \quad J(\tilde{\mathcal{L}}) \tag{**CB**}$$

$$\text{s.t.} \begin{cases} \tilde{\mathcal{L}}\hat{\Psi}(x^\dagger) = \mathbb{0}_{\hat{c}}, \\ \mathbb{1}_{\hat{c}}^\top \tilde{\mathcal{L}} = \mathbb{0}_{\hat{c}}^\top, \\ \tilde{\mathcal{L}}_{ij} \geq 0, \ \forall\ i \neq j, \\ \hat{g}^\perp \hat{Z}(\hat{\mathcal{L}} - \tilde{\mathcal{L}}) = \mathbb{0}_{(n-p)\times\hat{c}}, \\ [\hat{g}^\top \hat{Z}(\tilde{\mathcal{L}} - \hat{\mathcal{L}})]_{ij} \geq 0, \ \forall\ i = 1, \cdots, p, \ j = 1, \cdots, \hat{c}, \end{cases} \tag{38}$$

where $\hat{Z}$, $\hat{\mathcal{L}}$, $\hat{\Psi}(x^\dagger)$ and $\hat{g}^\perp$ are known, $x^\dagger$ is the desired equilibrium point.

By solving the optimization problem **CB**, we get $\tilde{L}$ firstly, then we can compute $\hat{u}$ according to (36).

Remark 4. Target system $\tilde{\mathcal{M}}$ is a complex balanced realization of the closed loop system in balanced shaping control. The problem of finding realizations of kinetic systems was

first addressed by Szederkényi et al. In [27], Szederkényi developed mixed integer linear programming (MILP) algorithm capable of determine sparse and dense realizations. In another paper [29], MILP was applied to find maximal and minimal realizations. Based on MILP, various realization properties can be reached, such as complex balanced systems [28], weakly reversible mass action systems [30], linearly conjugate mass action systems [20], weakly reversible linearly conjugate mass action systems [21].

Analogously, an optimization based systematic method for computing detailed balanced target system is

$$\min_{\tilde{\mathcal{L}}} \quad J(\tilde{\mathcal{L}}) \tag{\textbf{DB}}$$

$$\text{s.t.} \begin{cases} \hat{\Lambda}\tilde{\mathcal{L}}^\top = \tilde{\mathcal{L}}\hat{\Lambda}, \\ \mathbb{1}_{\hat{c}}^\top \tilde{\mathcal{L}} = \mathbb{0}_{\hat{c}}^\top, \\ \tilde{\mathcal{L}}_{ij} \geq 0, \ \forall\, i \neq j, \\ \hat{g}^\perp \hat{Z}(\hat{\mathcal{L}} - \tilde{\mathcal{L}}) = \mathbb{0}_{(n-p)\times\hat{c}}, \\ [\hat{g}^\top \hat{Z}(\tilde{\mathcal{L}} - \hat{\mathcal{L}})]_{ij} \geq 0, \ \forall\, i = 1, \cdots, p, \ j = 1, \cdots, \hat{c}, \end{cases} \tag{39}$$

where $\hat{Z}$, $\hat{\mathcal{L}}$, $\hat{\Lambda} = \mathrm{diag}(\hat{\Psi}_i(x^\dagger))$ and $\hat{g}^\perp$ are known.

5 Illustrative examples

In this section, balanced shaping control is applied to two examples, the first one is a process system, while the second one is a polynomial system.

5.1 Balanced shaping control for stabilizing a process system

Consider the open mass action system given by Lipták et al. (in section 5.2 in [23]), the following chemical reactions are taking placing in the reactor

$$2X_1 + X_3 \xrightarrow{1} X_1 + X_2 \underset{1}{\overset{1}{\rightleftharpoons}} X_1 + 2X_3. \qquad X_1 + 2X_2 \xrightarrow{1} X_1 + X_2 \tag{40}$$

Suppose the inlet volumetric flow rates $F_1 = F_2 = 0.5\mathrm{m}^3/\mathrm{s}$, and the desired positive equilibrium point $x^\dagger = [1, 1, 1]^\top$. By choosing inlet concentrations $x_{1,in}$ and $x_{2,in}$ as manipulable variables, the open mass action system can be modeled by

$$\dot{x} = \hat{Z}\hat{\mathcal{L}}\hat{\Psi}(x) + \hat{g}\hat{u}, \tag{41}$$

where

$$\hat{Z} = \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2 & 0 & 1 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad \hat{\mathcal{L}} = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}, \tag{42}$$

$$\hat{g} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \\ 0 & 0 \end{bmatrix}, \quad \hat{u} = \begin{bmatrix} x_{i,in} \\ x_{2,in} \end{bmatrix},$$

in which $\hat{Z}$ and $\hat{\mathcal{L}}$ correspond to mass action system $\hat{\mathcal{M}}$

$$2X_1 + X_3 \xrightarrow{1} X_1 + X_2 \underset{1}{\overset{1}{\rightleftharpoons}} X_1 + 2X_3, \qquad X_1 \xrightarrow{1} \mathcal{C}_0 \xleftarrow{1} X_2, \tag{43}$$

$$X_1 + 2X_2 \xrightarrow{1} X_1 + X_2, \qquad X_3 \xrightarrow{1} \mathcal{C}_0$$

where $\mathcal{C}_0$ is the zero complex. According to **Remark 1**, a left annihilator of $\hat{g}$ is

$$\hat{g}^{\perp} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}. \tag{44}$$

Now we design controller for the open loop system by utilizing the systematic method proposed in section 4, which is based on optimization. By solving the corresponding optimization problem **CB**, we get

$$\tilde{\mathcal{L}} = \begin{bmatrix} -1 & 0 & 0.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0.4294 & -1 & 0 & 0 & 0.096 & 0.0678 & 0.339 & 0.0678 \\ 0 & 1 & -1.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0.4294 & 0 & 0.5 & -1.5 & 0.096 & 0.0678 & 0.339 & 0.0678 \\ 0.1412 & 0 & 0 & 0 & -0.1921 & 0 & 0.0508 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1356 & 0.1356 & 0 \\ 0 & 0 & 0.5 & 0.5 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.1356 & -0.1356 \end{bmatrix}. \tag{45}$$

Hence, the optimization based controller is

$$\hat{u} = \begin{bmatrix} 1.9998x_1 + 0.2712x_2 + 1.4576x_3 + 0.2712 \\ 0.5764x_1^2x_3 + 0.576x_1 + 2.1356x_2 + 2.3052x_3 + 0.4068 \end{bmatrix}. \tag{46}$$

With initial state $x_0 = [0.5, 1.2, 1.5]^{\top}$, Fig. 1 shows the states simulation of the closed loop system. As one expects, the trajectories convergent to the desired point $x^{\dagger}$.

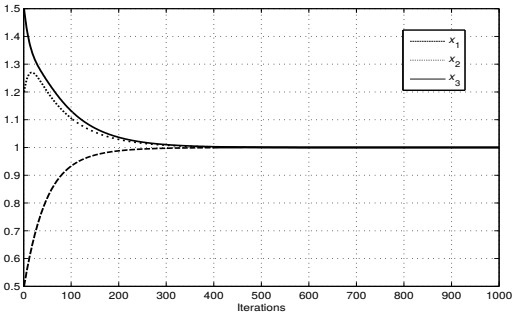

Figure 1. States simulation of the closed loop system in section 5.1 with initial value $x_0 = [0.5, 1.2, 1.5]^\top$.

5.2 Application to a polynomial system

Another example is the following open loop polynomial system

$$\dot{x} = \hat{f}(x) + \hat{g}\hat{u}, \tag{47}$$

where

$$\hat{f}(x) = \begin{bmatrix} -0.6x_1x_2 + 0.8x_2x_3 - 0.2x_1 \\ -0.5x_1x_2 - 0.5x_2x_3 + 0.2x_1 \\ 0.6x_1x_2 - 0.8x_2x_3 + 0.2x_1 \end{bmatrix}, \quad \hat{g} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \hat{u} \in \mathbb{R}. \tag{48}$$

According to **Remark 3**, $\dot{x} = \hat{f}(x)$ is kinetically realizable, and the realization is

$$\begin{array}{ccccc} \mathcal{C}_0 & \xleftarrow{0.2} & X_1 & \xrightarrow{0.2} & X_1 + X_3 \\ & & \underset{0.2}{\overset{0.5}{\rightleftharpoons}} & & \\ X_2 & \xleftarrow{0.6} & X_1 + X_2 & \xrightarrow{0.6} & X_1 + X_2 + X_3 \\ & \nwarrow^{0.8} & & \nearrow_{0.8} & \\ & & X_2 + X_3 & \xrightarrow{0.5} & X_3, \end{array} \tag{49}$$

which is characterized by

$$\hat{Z} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}, \quad \hat{\mathcal{L}} = \begin{bmatrix} -1.7 & 0 & 0 & 0 & 0.2 & 0 & 0 & 0 \\ 0.6 & 0 & 0.8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2.1 & 0 & 0 & 0 & 0 & 0 \\ 0.6 & 0 & 0.8 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 & -0.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2 & 0 & 0 & 0 \end{bmatrix}. \tag{50}$$

Suppose $x^\dagger = [1,1,1]^\top$ is the desired equilibrium point, we use the systematic method proposed in section 4 to design controller for the open loop system. By solving the optimization problem **CB**, we get

$$\tilde{\mathcal{L}} = \begin{bmatrix} -0.6 & 0 & 0.6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.45 & 0 & -0.8 & 0 & 0.2 & 0 & 0.15 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.2 & 0 & -0.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.15 & 0 & 0 & 0 & 0 & 0 & -0.15 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{51}$$

Therefore, the complex balanced target system $\tilde{\mathcal{M}}$ is

$$X_1 \underset{0.2}{\overset{0.2}{\rightleftharpoons}} X_2 + X_3 \underset{0.45}{\overset{0.6}{\rightleftharpoons}} X_1 + X_2. \qquad 0.15 \uparrow \quad \swarrow 0.15 \qquad X_3 \tag{52}$$

Hence the optimization based controller is

$$\hat{u} = \left[0.35x_1x_2 + 0.3x_2x_3 + 0.15x_3\right]. \tag{53}$$

Finally, we simulate the states with initial value $x_0 = [1.5, 1.2, 0.5]^\top$. Fig. **2** shows that all trajectories convergent to $x^\dagger$.

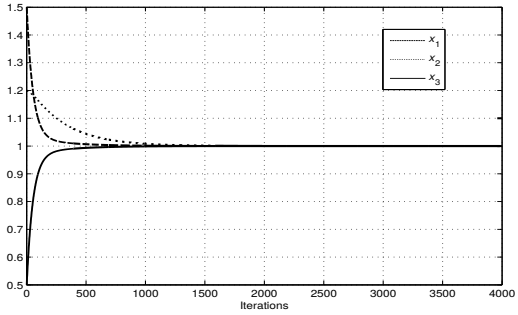

Figure 2. States simulation of the closed loop system in section 5.2 with initial value $x_0 = [1.5, 1.2, 0.5]^\top$.

6 Conclusion

In the present work, we have developed a theoretical framework for stabilizing open mass action systems at the desired state. Since complex balanced systems are locally asymptot-

ically stable, we try to shape the closed loop systems such that the target systems have a complex balanced structure, and hence the closed loop systems are also stable. More precisely, control action is taken such that the closed loop system is dynamically equivalent to a complex balanced system. Therefore, the effectiveness of balanced shaping control is equivalent to the existence of proper state feedback and target system. By fixing the complex stoichiometric matrix of the target system, balanced shaping control results in a set of linear constraints, and we have proposed a systematic method for computing the Kirchhoff matrix of the target system through solving optimization problem, i.e., convex quadratic programming. In this case, we have shown that balanced shaping control is an equivalent method of kinetic feedback design for stabilizing open mass action systems. Finally, two examples have been given to illustrate the effectiveness of balanced shaping control.

In this paper, we keep the inlet volumetric flow rates constant, and choose the inlet concentrations as manipulable inputs, thus the open loop model for open mass action system is a linear input affine system. If the inlet concentrations are kept constant and the inlet volumetric flow rates are chosen as manipulable inputs, then the model for open mass action system is an affine system with nonlinear input structure. In the near future, we will consider this nonlinear case, and try to stabilize it by balanced shaping with the help of mass conservation law.

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