Kinetic feedback design for polynomial systems

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Abstract

New computational methods are proposed in this paper to construct polynomial feedback controllers for the stabilization of polynomial systems with linear input structure around a positive equilibrium point. Using the theory of chemical reaction networks (CRNs) and previous results on dynamical equivalence, a complex balanced or weakly reversible zero deficiency closed loop realization is achieved by computing the gain matrix of a polynomial feedback using optimization. It is shown that the feedback resulting in a complex balanced closed loop system having a prescribed equilibrium point can be computed using linear programming (LP). The robust version of the problem, when a convex set of polynomial systems is given over which a stabilizing controller is searched for, is also solvable with an LP solver. The feedback computation for rendering a polynomial system to deficiency zero weakly reversible form can be solved in the mixed integer linear programming (MILP) framework. It is also shown that involving new monomials (complexes) into the feedback does not improve the solvability of the problems. The proposed methods and tools are illustrated on simple examples, including stabilizing an open chemical reaction network .

Key words: nonnegative systems, kinetic systems, optimization, chemical reaction networks, feedback equivalence, feedback design

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1 Introduction

Polynomial systems form a well-investigated class of smooth nonlinear systems that enable us to apply computationally efficient methods for their dynamic analysis and control [4], and at the same time, have practically important applications in the field of process, mechanical, (bio)chemical etc. control. Within this class, positive polynomial systems play an important role in the applications, where the value of the variables is positive by nature, such as pressure, temperature, composition etc.

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) form a wide class of nonnegative polynomial systems. CRNs are able to produce all the important qualitative phenomena present in nonlinear systems, so they form a relatively rich sub-class there. At the same time, CRNs are closed lumped process systems under isothermal and isobaric conditions [21], that exhibit polynomial nonlinearities. A recent survey shows [2] that CRNs are also widely used in other areas than chemical reaction kinetics or process systems that include biological applications, such as to model the dynamics of intracellular processes and metabolic or cell signalling pathways [19].

The theory of chemical reaction networks has significant results relating network structure and the qualitative properties of the corresponding dynamics [26,15]. However, the network structure corresponding to a given dynamics is generally not unique [8]. Recently, optimization-based computational methods were proposed for dynamically equivalent network structures with given preferred properties (see, e.g. [41,43,42,32]).

The field of feedback controller design for nonlinear systems in general, and process systems in particular has been continuously developing in recent decades, because of its practical importance and challenging theoretical nature. It is well-known that the utilization of the physical and/or structural specialities of different nonlinear system classes greatly helps in obtaining theoretically well-grounded, powerful and practically still feasible control methods. In general control theory we have sound methods of nonlinear feedback design for smooth input-affine systems [29], flat systems [33], Hamiltonian or port-Hamiltonian systems [5,46], or that for Euler-Lagrange systems [38]. Utilizing the engineering insight into the physics and chemistry of the system, the thermodynamic passivity approach [47] as a special control approach has been proposed for nonlinear process systems that is based on controlling its inventories [30]. Further improvements of the physically motivated nonlinear controller design have been achieved by using passivity [24], control Lyapunov [12] and Hamiltonian approaches [9,23,39,40] to nonlinear process systems.

The control design of positive polynomial systems - to which CRNs belong - has become quite popular recently (see e.g. [45]), that is explained by the great practical importance and wide expressive power of such systems. An introduction and overview on the analysis and design of polynomial control systems using dissipation inequalities is given in [10]. The computational tools used for both the stability analysis and feedback design for such systems is the semidefinite programming and the sum of squares decomposition [4], that is computationally hard, therefore, generally not feasible for large-scale problems. It is shown in [37] that the stabilizing control of quasi-polynomial (QP) process models can be solved through bilinear matrix inequalities. A recent paper proposes approximate but computationally feasible methods for optimally controlling polynomial systems [28]. An LMI (linear matrix inequalities) technique for the global stabilization of nonlinear polynomial systems using a quadratic control Lyapunov function candidate is reported in [3].

Motivated by the above results, the general purpose of our work is to construct polynomial feedback controllers to polynomial systems to achieve a closed loop system in a CRN form with given advantageous structural properties. In [44], the problem of obtaining a closed loop system in CRN form was addressed in the framework of mixed integer linear programming. The idea has been further extended to cover feedback design to achieve weak reversibility and minimal deficiency in the closed loop CRN form in [34]. The aim of the present paper is to propose a a systematic approach for the optimization-based state feedback computation for polynomial systems to achieve structural stability utilizing the prescribed properties of the closed loop CRN form of the system.

2 Reminder on polynomial systems assosciated with chemical reaction networks

This section is devoted to the notions and tools applied in the theory of *positive (or nonnegative) polynomial systems*, that are widely applied in process control. The main emphasis is put on the most important subclass of positive polynomial systems, that are chemical reaction networks with mass action law (abbreviated as MAL-CRN). The notations used in this section are mainly based on Lecture 4 in [14] and on [18].

2.1 Kinetic systems, their dynamics and structure

Let us consider a polynomial nonlinear system that can be described in the form of an ODE

$$\dot{x} = f(x) = M \cdot \varphi(x), \tag{1}$$

where $x \in \mathbb{R}^n$ is the state variable, $M \in \mathbb{R}^{n \times l}$, and $\varphi : \mathbb{R}^n \mapsto \mathbb{R}^l$ is a polynomial mapping.

A polynomial system has a kinetic realization, if a suitable MAL-CRN model can be constructed for it. The problem of kinetic realizability of polynomial ODE models was first examined and solved in [27] where it was shown, that the necessary and sufficient condition for kinetic realizability of a polynomial vector field is that all coordinates functions of f in (1) must have the form

$$f_i(x) = -x_i g_i(x) + h_i(x), \ i = 1, \ldots, n \tag{2}$$

where g_i and h_i are polynomials with nonnegative coefficients. It's easy to prove that kinetic systems are nonnegative [20].

2.1.1 CRN systems

If the condition (2) is fulfilled for a polynomial dynamical system, then it can always be written into the form

$$\dot{x} = Y \cdot A_k \cdot \psi(x), \tag{3}$$

where $x \in \mathbb{R}^n$ is the vector of state variables, $Y \in \mathbb{Z}_{\geq 0}^{n \times m}$ with distinct columns is the so-called *complex composition matrix*, $A_k \in \mathbb{R}^{m \times m}$ contains the information corresponding to the weighted directed graph, the reaction graph, of the reaction network (see below). As it will be visible later, the generally non-unique factorization (3) is particularly useful for prescribing structural constraints using optimization. According to the original chemical meaning of this system class, the state variables x_i represent the concentrations of the chemical *species* denoted by X_i, for $i = 1, \ldots, n$. Moreover, $\psi : \mathbb{R}^n \mapsto \mathbb{R}^m$ is a mapping given by

$$\psi_j(x) = \prod_{i=1}^{n} x_i^{Y_{ij}}, \quad j = 1, \ldots, m. \tag{4}$$

A_k is a column conservation matrix (i.e. the sum of the elements in each column is zero) defined as

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1, l \neq i}^{m} k_{il}, & \text{if } i = j \\ k_{ji}, & \text{if } i \neq j \end{cases} \tag{5}$$

where $k_{ij} \geq 0, \ i \neq j$. Note that A_k is also called as the *Kirchhoff matrix* of the network.

The *complexes* are formally defined as nonnegative integer linear combinations

of the species in the following way:

$$C_i = \sum_{j=1}^{n} Y_{ji} X_j, \;\; i = 1, \ldots, m \tag{6}$$

Note, that a column (let's say column i) of the matrix Y may be equal to the zero vector. In such a case, complex C_i is called the *zero complex*.

2.1.2 The reaction graph and its incidence matrix

The structure of MAL-CRNs is well characterized by a weighted directed graph, called the *reaction graph*, and by its *complex composition matrix*.

The weighted directed graph (or reaction graph) of kinetic systems is $G = (V, E)$, where $V = \{C_1, C_2, \ldots, C_m\}$ and E denotes the set of vertices and directed edges, respectively. The directed edge (C_i, C_j) (also denoted by $C_i \mapsto C_j$) belongs to the reaction graph if and only if $[A_k]_{ji} > 0$. In this case, the weight assigned to the directed edge $C_i \mapsto C_j$ is $[A_k]_{ji}$. Naturally, $[A_k]_{ji} = 0$ means that $(C_i, C_j) \notin E$.

In addition to the Kirchhoff matrix of the system, one can characterize the reaction graph using its incidence matrix $B_G \in \{-1, 0, 1\}^{m \times r}$ where r is the number of reactions. Each reaction in the CRN is represented by the appropriate column of B_G as follows. Let the ℓ-th reaction in the CRN be $C_j \mapsto C_i$ for $1 \leq \ell \leq r$. Then the ℓ-th column vector of B_G is characterized as: $[B_G]_{i\ell} = 1$, $[B_G]_{j\ell} = -1$, and $[B_G]_{k\ell} = 0$ for $k = 1, \ldots, r$, $k \neq i, j$. It is clear from the above description that the *unweighted directed graph structure* of a kinetic system can be characterized by the matrix pair (Y, B_G).

2.2 Stoichiometric subspace and compatibility classes

The stoichiometric subspace is defined as

$$S = span\left\{[Y]_{\cdot,j} - [Y]_{\cdot,i} \mid \exists C_i \mapsto C_j\right\} \tag{7}$$

where $[Y]_{\cdot,i}$ denotes the ith column of Y. The *rank* (or *dimension*) of a reaction network denoted by s is the dimension of the stoichiometric subspace.

The stoichiometric compatibility classes of a chemical reaction network are the following affine spaces

$$S_p = (p + S) \cap \mathbb{R}^n_{\geq 0}, \tag{8}$$

where the elements of p are nonnegative. These classes are forward invariant to the system (3).

2.3 Dynamical equivalence and different realizations of MAL-CRNs

It is a known result of chemical reaction network theory that a reaction graph corresponding to a given set of kinetic ODEs is generally not unique [8,41]. Moreover, the kinetic realizability of a polynomial dynamical system is not coordinate-independent and it is preserved only up to the reordering and positive rescaling of the state variables [11].

Based on the above, a CRN realization (Y, A'_k) is called *dynamically equivalent* to a kinetic system of the form (1) if A'_k is an $m \times m$ Kirchhoff matrix, and $Y \in \mathbb{Z}_{\geq 0}^{n \times m}$ such that

$$M \cdot \varphi(x) = Y \cdot A'_k \cdot \psi(x), \quad \forall x \in \mathbb{R}_{\geq 0}^n \tag{9}$$

where ψ is defined as in Eq. (4). We note that the vector functions φ in Eq. (1) and ψ in (9) are not necessary identical, since the monomials corresponding to product complexes without any outgoing reaction do not appear in the kinetic differential equations.

2.4 Weak reversibility, complex balance and deficiency

Important dynamic properties of a MAL-CRN depend on some of the structural properties of the reaction graph, most notably on its connectivity and on its strong components.

A CRN is called *weakly reversible* if whenever there exists a directed path from C_i to C_j in its reaction graph, then there exists a directed path from C_j to C_i, too. In graph theoretic terms, this means that all components of the reaction graph are strongly connected components. A MAL-CRN is called *reversible*, if for each reaction $C_i \mapsto C_j$ there exists another (reverse) reaction $C_j \mapsto C_i$. It is well-known from the literature (see Theorem 3.1 of [16] and Proposition 4.1 of [14]) that a CRN is weakly reversible if and only if there is a strictly (elementwise) positive vector q^* in the kernel of A_k.

The equilibrium points of the system (3) can be obtained by solving the nonlinear set of algebraic equations

$$Y \cdot A_k \cdot \psi(x^*) = 0, \tag{10}$$

with (4) for an element-wise non-negative x^*. Note that several equilibrium points may exist due to the possible rank deficiency of the matrices Y and A_k, and the nonlinearity of ψ.

The notion of complex balance originally comes from the study of the thermo-

dynamic compatibility of reaction networks. An equilibrium point $x^* \in \mathbb{R}^n_{>0}$ of the system (3) is called *complex balanced* if $A_k \cdot \psi(x^*) = 0$. It is known that if any equilibrium point of a CRN given by the pair (Y, A_k) is complex balanced, then all other equilibrium points are complex balanced, too. It is an important result from the literature that complex balance implies weak reversibility, since the kernel condition of weak reversibility is fulfilled [25].

Deficiency δ is a fundamental property of a reaction network and it is defined as [15]:

$$\delta = m - l - s, \tag{11}$$

where m is the number of complexes (vertices) in the reaction graph, l is the number of linkage classes (graph components) and s is the rank of the reaction network. Another equivalent definition of deficiency [2] is

$$\delta = \dim(\mathrm{Ker}(Y) \cap \mathrm{Im}(B_G)) \tag{12}$$

where Y is the complex composition matrix and B_G is the incidence matrix of the reaction network. It is easy to see from (11) and (12) that deficiency depends only on the complex composition (Y) and the network structure (i.e. on the unweighted reaction graph), but not on the values of the reaction rate coefficients. The deficiency is a very useful measure for studying the dynamical properties of reaction networks and for establishing parameter-independent (at least) local stability conditions.

It is important to remark that weak reversibility, complex balance and deficiency are all realization-dependent properties and not the inherent properties of the kinetic differential equations [32,35]. This structural non-uniqueness will be utilized for feedback design in Section 3.1.

2.5 Qualitative dynamical properties of MAL-CRNs

A central problem in CRN theory is the relation between the network structure/ parametrization and the qualitative properties of the dynamics. From the numerous results and conjectures in the field, we only mention those that are directly related to the forthcoming feedback design methods.

According to the *Global Attractor Conjecture*, for any complex balanced CRN and any positive initial condition $x(0)$, the equilibrium point x^* is a global attractor in the corresponding positive stoichiometric compatibility class [7]. Important special cases were proven in [1] and [17]. Moreover, the possible general proof of the conjecture has recently appeared in [6].

A fundamental result of Chemical Reaction Network Theory is the *Deficiency*

Zero Theorem (Theorem 6.1.1 in [15]), that proves a robust stability property of a certain class of kinetic systems. Here we recall that the reaction rate coefficient k_{ij} (that is the weight of the directed edge $C_i \longrightarrow C_j$ in the reaction graph) is equal to $[A_k]_{ji}$. Part (iii) of the Deficiency Zero Theorem says that deficiency zero weakly reversible networks possess precisely exactly one equilibrium point in each stoichiometric compatibility class, and these equilibria are at least locally stable with a known logarithmic Lyapunov function that is also independent of the rate coefficients. To connect complex balance and the deficiency zero weak reversibility condition, we also recall from [25] and [13] that a mass action reaction network is complex balanced for any positive choice of rate constants if and only if it is weakly reversible and has a deficiency of zero.

The above results motivate us to design such feedbacks that are able to ensure the complex balanced or deficiency zero weakly reversible properties.

3 Kinetic feedback forms

In order to be able to design any feedback controllers, one should extend the closed autonomous form (1) of the system with a suitable input structure. This is followed by the description of the proposed static and dynamic kinetic state feedback structures in this section.

3.1 Open MAL-CRNs as process systems

The aim is to construct a nonlinear state equation in the case when the system is open under the following conditions:

(1) isothermal and isobaric conditions,
(2) constant physico-chemical properties (density, reaction rate coefficients),
(3) only inlet and outlet convection and chemical reactions are taking place.

The model is constructed from the overall mass balance and from the component mass balances for all n components as follows.

Assuming liquid in- and outflows with the same density, the overall mass balance is in the following form

$$\frac{dV}{dt} = \sum_{j=1}^{n} F_{j,IN} - F_{OUT} \tag{13}$$

where $F_{j,IN}$ is the inlet volumetric flow rate containing the jth component and possibly a liquid inert solvent in units $[\frac{m^3}{s}]$, F_{OUT} is the outlet volumetric flow rate, that contains all components in the reactor, and V is the volume of the liquid in the reactor.

The component molar balances are of an open MAL-CRN, are constructed from the CRN model (1) augmented with in- and outflows [21]:

$$\frac{dm_i}{dt} = F_{i,IN}x_{i,IN} - F_{OUT}x_i + V[M]_{i,\cdot}\varphi(x) \quad , \quad i = 1, ..., n \tag{14}$$

where m_i is the mole number of the ith component in the reactor, $x_{i,IN}$ is its inlet concentration, x_i is its concentration, and $[M]_{i,\cdot}$ is the ith row of matrix M. One can use the fact, that $m_i = Vx_i$ to derive a simpler form of (14), by substituting Eq. (13) for $\frac{dV}{dt}$ into it to obtain:

$$\frac{dx_i}{dt} = \frac{F_{i,IN}}{V}x_{i,IN} - \left(\sum_{j=1}^{n}\frac{F_{j,IN}}{V}\right)x_i + [M]_{i,\cdot}\varphi(x) \quad , \quad i = 1, ..., n \tag{15}$$

3.1.1 Transformation into polynomial form

Let us introduce a new dynamic variable $z = \frac{1}{V}$, and transform both (13) and (15) to obtain

$$\frac{dz}{dt} = z^2\left(F_{OUT} - \sum_{j=1}^{n}F_{j,IN}\right) \tag{16}$$

$$\frac{dx_i}{dt} = F_{i,IN}x_{i,IN}z - \left(\sum_{j=1}^{n}F_{j,IN}\right)x_i z + [M]_{i,\cdot}\varphi(x) \quad , \quad i = 1, ..., n \tag{17}$$

3.1.2 The nonlinear state equations

The form of the nonlinear state equation depends on our choice of the manipulable input variables. Two cases are considered here:

(1) inlet volumetric flow rates as manipulable inputs,
(2) inlet concentrations as manipulable inputs (but keeping V constant).

Inlet volumetric flow rates as manipulable inputs Assume that the inlet concentrations are constant, i.e. $x_{i,IN} = K_i,\ i = 1, ..., n$ and let the inputs be

$$u_i = F_{i,IN}z \ , \ i = 1, ..., n \quad , \quad u_z = F_{OUT}z \tag{18}$$

Then we can use u_z to stabilize z at an arbitrary steady state point using the equation

$$\frac{dz}{dt} = z\left(u_z - \sum_{j=1}^{n} u_j\right) \tag{19}$$

Then the component molar balances take the form

$$\frac{dx_i}{dt} = K_i u_i - \left(\sum_{j=1}^{n} u_j\right) x_i + [M]_{i,\cdot}\varphi(x) \quad , \quad i = 1, ..., n \tag{20}$$

Inlet concentrations as manipulable inputs In order to obtain a time-invariant (i.e. constant parameter) model, let us assume that the inlet and outlet volumetric flow rates are kept constant such that $k_i = F_{i,IN},\ i = 1, ..., n$ with $K_z = \sum_{j=1}^{n} F_{j,IN}$, and let the inputs be

$$u_i = x_{i,IN} z \ , \ i = 1, ..., n \quad , \quad u_z = F_{OUT} \tag{21}$$

Then we can use u_z to stabilize z at an arbitrary steady state point using the equation

$$\frac{dz}{dt} = u_z z^2 - K_z z^2 \tag{22}$$

Furthermore, the component molar balances take the form

$$\frac{dx_i}{dt} = k_i u_i - K_z x_i z + [M]_{i,\cdot}\varphi(x) \quad , \quad i = 1, ..., n \tag{23}$$

It is important to remark, that both model structures are*hierarchically decomposed* the same way as in [22]. This enables to control the mass/volume separately and treat the component mass balances on the top of them. Therefore, from now on we assume that z is perfectly controlled and constant in our models. To relax this assumption, one has to prove that the subsystem (23) stabilized with inputs u_i is input to state stable for the additional input z. Another possibility is to include (22) into the entire feedback computation model considering z formally a 'pseudo concentration', since z is a positive variable, and the right hand side of (22) is kinetic.

3.2 Open loop model form

The analysis of the possible input structures of open MAL-CRNs presented in subsection 3.1 showed that *a simple linear input term with constant coefficients is chemically plausible when the inlet concentrations are chosen as manipulable*

inputs. Therefore, we assume for the feedback design that the equations of the open loop polynomial system with linear input structure are given as

$$\dot{x}_p = M_p \cdot \psi_p(x_p) + B_p u_p, \tag{24}$$

where $x_p \in \mathbb{R}^{n_p}$ is the plant state vector, $u_p \in \mathbb{R}^{r_p}$ is the input, $\psi_p \in \mathbb{R}^{n_p} \to \mathbb{R}^{m_p}$ contains the monomials of the open-loop system, $M_p \in \mathbb{R}^{n_p \times m_p}$ and $B_p \in \mathbb{R}^{n_p \times r_p}$.

It is important to note that the state equation (24) of open MAL-CRNs originating from component molar balances (23) when the inlet concentrations are used as manipulable inputs can be simply derived from these molar balances in the following steps assuming that the volume has been stabilized to a steady-state value V^* giving rise to a given value of $z^* = \frac{1}{V^*}$.

- The vector of state variables x_p is formed from the concentrations, so $x_p = x$ and $\dim(x_p) = n$.
- If all inlet concentrations are manipulable, then $\dim(u_p) = n$, and the constant input matrix B_p is a diagonal matrix with the positive constant $k_i = F_{i,IN}$ in its diagonal elements, i.e. $[B_p]_{ii} = k_i$.
- The monomial vector $\psi_p(x_p)$ is extended by the one specie monomials $C_{i'} = X_i$ if they were not present already. The corresponding coefficient in the coefficient matrix M_p is obtained by subtracting the positive term $K_z z^*$ from the MAL-CRN coefficient matrix M in Eq. (23), i.e. $[M_p]_{ii'} = [M]_{ii'} - K_z z^*$.

Parametric uncertainty in the open loop model In this case, we assume that the coefficient matrix M_p is not known exactly, but it is an element of the polytopic set

$$\mathcal{M} = \Big\{ \sum_{i=1}^{L} \alpha_i M_p^{(i)} \;\; | \;\; (\forall i : \alpha_i \geq 0) \;\wedge\; \sum_{i=1}^{L} \alpha_i = 1 \Big\} \tag{25}$$

where $M_p^{(i)} \in \mathbb{R}^{n_p \times m_p}$ for $i = 1 \ldots, L$ are the vertex points.

A simple example of the uncertainty described by Eq. (25) is the class of models, where the elements of M are assumed to belong to predefined intervals [36]. These intervals may easily come from parameter estimation as a result of uncertainty (covariance) analysis of the estimate, since model (24) is linear in the parameter matrix M_p. On the other hand, if the open-loop model (24) is a reaction network, and some uncertain reaction rate coefficients (i.e. the elements of matrix A_k) are modeled as intervals, we also obtain a polytopic model of the form (25) for matrix M_p.

3.3 The state feedback law

We assume a polynomial dynamic feedback of the form

$$u_p = K \cdot \psi(x) \tag{26}$$

where $x = [x_p \ x_c]^T$ is the overall state vector with the *state of the controller* $x_c \in \mathbb{R}^{n_c}$, $\psi(x) = [\psi_p(x_p) \ \psi_c(x_p, x_c)]^T$ is the overall monomial vector with $\psi_c : \mathbb{R}^{n_p+n_c} \to \mathbb{R}^{m_c}$ containing *possible additional monomials* for the feedback, and $K \in \mathbb{R}^{r_p \times (m_p+m_c)}$ is a *constant feedback gain*. The state equations of the controller are

$$\dot{x}_c = M_c \cdot \psi(x) \tag{27}$$

where $M_c \in \mathbb{R}^{n_c \times (m_p+m_c)}$ and $\psi(x)$ is the overall monomial vector containing ψ_p and ψ_c. We can partition K and M_c into two blocks as $K = [K_p \ K_c]^T$ and $M_c = [M_{cp} \ M_{cc}]^T$ where $K_p \in \mathbb{R}^{r_p \times m_p}$, $K_c \in \mathbb{R}^{r_p \times m_c}$, $M_{cp} \in \mathbb{R}^{n_c \times m_p}$ and $M_{cc} \in \mathbb{R}^{n_c \times m_c}$. In that case the equations of the closed loop system are given by

$$\dot{x} = \begin{bmatrix} M_p + B_p K_p & B_p K_c \\ M_{cp} & M_{cc} \end{bmatrix} \cdot \begin{bmatrix} \psi_p(x_p) \\ \psi_c(x_p, x_c) \end{bmatrix} = M \cdot \psi(x). \tag{28}$$

The aim is to *set the closed loop coefficient matrix M by choosing a suitable feedback gain K such that it defines a kinetic system with prescribed properties (e.g. complex balance)* such that the overall complex composition matrix Y is compatible with ψ. It is clear from subsection 2.1 that this is possible if and only if M can be factorized as $M = Y \cdot A_k$ where $Y \in \mathbb{Z}_{\geq 0}^{(n_p+n_c)\times(m_p+m_c)}$ is the given complex composition matrix (which generates $\psi(x)$ in (28)) , and $A_k \in \mathbb{R}^{(m_p+m_c)\times(m_p+m_c)}$ is a valid Kirchhoff matrix. In the following, let $n_p + n_c = n$ and $m_p + m_c = m$.

3.4 The effect of feedback structure on the closed loop dynamics

The results in this subsection show that involving new monomials (complexes) into the feedback law in (26) does not improve the solvability of the feedback problem from the point of view of weak reversibility, deficiency or complex balance. In the following, by *additional complexes*, we mean complexes corresponding to the monomials of ψ_c in (28). Therefore, a *closed loop system without additional complexes* means a controlled system of the form (28), where $K_c = \mathbf{0}$ and $M_c = \mathbf{0}$. Note that this is a technical solution in order to keep the dimension of the state vector and the Kirchhoff matrix of the closed loop

system constant in the calculations. In this case, the complexes corresponding to ψ_c are naturally isolated in the reaction graph.

Lemma 1 *Consider the open loop system* (24) *and the feedback law* (26). *Assume that there exist a closed loop system with feedback parameters* K, M_c, *and it has a realization* (Y, A_k) *where the* j*th complex* C_j *is an additional source complex (i.e.* $[A_k]_{jj} \neq 0$*). Then, there exist other feedback parameters* K' *and* M_c' *such that the corresponding closed loop system has a realization* (Y, A_k'), *where* A_k' *is given by*

$$[A_k']_{\cdot,i} = [A_k]_{\cdot,i} + \frac{[A_k]_{ji}}{-[A_k]_{jj}}[A_k]_{\cdot,j}, \quad \forall i. \tag{29}$$

Remark It is visible from (29) that the jth complex is isolated in the realization (Y, A_k'), since $[A_k']_{ji} = 0$ and $[A_k']_{ij} = 0$ for all i.

Proof of Lemma 1 It can be seen from (29) that the matrix A_k' is Kirchhoff, because the sum of its columns is zero and the off-diagonal elements are positive due to $[A_k']_{ji} = 0$ for all i.
First, we can write (29) in the following compact form

$$A_k' = A_k + \frac{1}{-[A_k]_{jj}}[A_k]_{\cdot,j} \cdot [A_k]_{j,\cdot}. \tag{30}$$

Then, we can construct the feedback gain K' as

$$K' = K + \frac{1}{-[A_k]_{jj}}K_{\cdot,j} \cdot [A_k]_{j,\cdot} \tag{31}$$

and the matrix M_c' as

$$M_c' = M_c + \frac{1}{-[A_k]_{jj}}[M_c]_{\cdot,j} \cdot [A_k]_{j,\cdot}. \tag{32}$$

Then, the matrix M' is given by

$$M' = M + \frac{1}{-[A_k]_{jj}} \begin{bmatrix} B_p K \\ M_c \end{bmatrix}_{\cdot,j} [A_k]_{j,\cdot} \tag{33}$$

which can be written as

$$M' = Y \cdot A_k + \frac{1}{-[A_k]_{jj}} Y \cdot [A_k]_{\cdot,j} \cdot [A_k]_{j,\cdot} = Y \cdot A_k'. \tag{34}$$

Therefore, M' has the realization A'_k. $\square$

Lemma 2 *Let A_k and A'_k be Kirchhoff matrices where the matrix A'_k is constructed by* (29)*. Then $Ker(A_k) \subseteq Ker(A'_k)$.*

Proof Let us take an element p of $\mathrm{Ker}(A_k)$, then

$$p_j = \sum_{i \neq j} p_i \frac{[A_k]_{ji}}{-[A_k]_{jj}}. \tag{35}$$

Let us consider the product $A'_k \cdot p$:

$$\sum_{i=1}^{m} p_i [A'_k]_{\cdot,i} = \sum_{i \neq j} p_i [A_k]_{\cdot,i} + \sum_{i \neq j} p_i \frac{[A_k]_{ji}}{-[A_k]_{jj}} [A_k]_{\cdot,j}. \tag{36}$$

We can now substitute (35) into (36) to obtain

$$\sum_{i=1}^{m} p_i [A'_k]_{\cdot,i} = \sum_{i \neq j} p_i [A_k]_{\cdot,i} + p_j [A_k]_{\cdot,j} = 0 \tag{37}$$

that means $p \in \mathrm{Ker}(A'_k)$. $\square$

Theorem 3 *Consider the open loop system* (24) *and the feedback law* (26)*. Then the following statements apply.*

(a) If there exists a weakly reversible closed loop system (28) *with additional complexes, then there exists another weakly reversible closed loop system without additional complexes.*
(b) Suppose there exists a weakly reversible closed loop system (28) *with additional complexes and deficiency δ. Then there exists another weakly reversible closed loop system without additional complexes, and it has deficiency δ' such that $\delta' \leq \delta$.*
(c) Suppose there exists a complex balanced closed loop system (28) *with additional complexes and equilibrium points in the set E. Then there exists another complex balanced closed loop system without additional complexes and it has equilibrium points E' such that $E \subseteq E'$.*

Proof

(a) If there exists a closed loop system with a weakly reversible realization (Y, A_k), then there exists another one with realization (Y, A'_k) where the additional complexes are isolated (Lemma 1) and $\mathrm{Ker}(A_k) \subseteq \mathrm{Ker}(A'_k)$ (Lemma

2.). A Kirchhoff matrix is weakly reversible if and only if there exists a positive vector in its kernel. Therefore, matrix A'_k is weakly reversible, too.

(b) If there exists a closed loop system with a weakly reversible realization (Y, A_k), then there exists another one with realization (Y, A'_k) where the additional complexes are isolated (Lemma 1). Let us denote the corresponding incidence matrices by B_G and B'_G. The columns of matrix B'_G are linear combinations of the columns of matrix B_G by construction. Therefore, $\mathrm{Im}(B'_G) \subseteq \mathrm{Im}(B_G)$. By the definition of deficiency $\delta = \dim(\mathrm{Ker}(Y) \cap \mathrm{Im}(B_G))$ and $\delta' = \dim(\mathrm{Ker}(Y) \cap \mathrm{Im}(B'_G))$. So $\delta' \leq \delta$.

(c) If there exists a closed loop system with a weakly reversible realization (Y, A_k), then there exists another one with realization (Y, A'_k) where the additional complexes are isolated (Lemma 1) and $\mathrm{Ker}(A_k) \subseteq \mathrm{Ker}(A'_k)$ (Lemma 2.). According to the assumption, (Y, A_k) is complex balanced, therefore the set of equilibrium points of (28) can be described as $E = \{x \mid A_k \cdot \psi(x) = \mathbf{0}\}$. Since, $\mathrm{Ker}(A_k) \subseteq \mathrm{Ker}(A'_k)$, then A'_k is complex balanced and $E \subseteq E'$. □

The kinetic feedback structure The theoretical results described in this section can be summarized in the following simple statements to determine the structure of the kinetic feedback, if one wants to achieve complex balanced closed loop MAL-CRN structure, or a weakly reversible zero deficiency closed loop MAL-CRN structure.

(1) There is not necessary to apply dynamic feedback to achieve complex balance or weak reversibility with zero deficiency for the closed loop system.
(2) *It is sufficient to use only the monomials of the open loop system* (24) *in the monomial function* $\psi(x)$ *of the static feedback* (26).

However, increasing the degrees of freedom of the control design with additional state variables, monomials and the corresponding extra parameters using the general form (28) might be advantageous to achieve additional goals, such as improving the time-domain performance of the closed loop system.

4 Feedback computation

In this section, the optimization problems for the design of kinetic feedback are described. First the control problem statement is described and analysed, that is followed by the optimization problems.

Based on the structure of the open loop system and that of the polynomial feedback described before in Section 3, let us consider

- a polynomial system with linear constant parameter input-affine structure as the open loop system (24) with its parameter matrices (M_p, B_p, Y),
- and a static positive polynomial feedback law (26) with the monomials of the open loop system. In that case the only design parameter is the feedback gain matrix $K = K_p$.

The aim of the feedback is to set a region in the state space, where $x^* \in \mathbb{R}^n_{>0}$ is an (at least) locally asymptotically stable equilibrium point of the closed loop system. This will be achieved in two different ways:

(i) to find a feedback gain K such that the closed loop system has a MAL-CRN complex balanced realization with a given equilibrium point x^*,
(ii) to compute the feedback gain K such that the closed loop system is weakly reversible with deficiency zero.

In the following, two realization computation problems are proposed for dynamically equivalent network structures that solve the feedback gain computation problem for the above two cases. It will be shown in the following sub-sections that one can apply linear programming (LP or MILP) optimization approaches to compute the feedback gain K.

It is important to note that no control performance requirement is set besides stabilizing the system, but one can additionally specify one on the price of making the related feedback gain computation problem possibly more complex.

Besides of the above general feedback design problem statement, the proposed linear programming based approach is capable of handling additional *constraints on the feedback gain*. These can serve to achieve a physically realizable feedback (in case of non-negativity) or to find a feedback with low gain (when minimizing the l_1 norm).

- **Non-negativity of the feedback**
  In many cases non-negativity of the input is a necessary condition of physical realizability. When the closed loop system is kinetic then its states are non-negative. Therefore the feedback $u_p = K\psi(x)$ is non-negative if the elements of the matrix K are non-negative

$$K_{ij} \geq 0, \quad \forall i = 1, \ldots, n, \ j = 1, \ldots, m. \tag{38}$$

- **Minimization of the l_1-norm of the feedback gain**

A suitable objective function of the optimization is the l_1-norm of the matrix K

$$f_{obj} = \sum_{i=1}^{n} \sum_{j=1}^{m} |K_{ij}|. \tag{39}$$

The minimization of this objective function can be easily implemented in the LP framework.

4.2 Complex balanced closed loop

In this case, the equilibrium point x^* of the closed loop system is a design parameter, so it is assumed to be known before the optimization. A complex balanced equilibrium point is (at least) locally asymptotically stable in its stoichiometric compatibility class. Therefore, the aim of the feedback is to set the vector x^* to be a complex balanced equilibrium point of the controlled system.

The linear optimization problem to be solved is described in terms of the linear constraints that express the requirements in the feedback design. The *first set of constraints is responsible for the dynamical equivalence*

$$\begin{cases} M_p + B_p K = Y \cdot A_k \\ \mathbf{1}^T \cdot A_k = \mathbf{0}^T \\ [A_k]_{ij} \geq 0 \quad i,j = 1,\ldots,m,\ i \neq j \end{cases} \tag{40}$$

where the elements of K and A_k are the continuous decision variables of the optimization problem, and $\mathbf{0}$ and $\mathbf{1}$ are column vectors with all of their elements being 0 and 1, respectively.

The vector x^* is a *complex balanced equilibrium point* of the closed loop system if and only if $A_k \cdot \psi(x^*) = \mathbf{0}$. This is also a *linear constraint*

$$A_k \cdot q^* = \mathbf{0} \tag{41}$$

where $q^* = \psi(x^*)$ is a priori known.

Finally, *by minimizing the objective function* (39)*, the feedback gain K can be computed (if it exists) in a LP framework* using the linear constraints (40) and (41).

With the resulting feedback gain K, the point x^* will be an equilibrium point of the closed loop system, and x^* will be locally asymptotically stable in the region $\mathcal{S} = (x^* + S) \cap \mathbb{R}^n_{\geq 0}$, where S is the stoichiometric subspace of the closed

loop system. We remark that the stability is proven to be global if the closed loop system consists of one linkage class [1].

4.3 Handling the parametric uncertainty in the complex balanced closed loop case

In this subsection, the above feedback computation method will be extended by handling parametric uncertainty. The uncertainty is modelled by the polytopic set given in Eq. (25).

Lemma 4 *Let x^* be a joint complex balanced equilibrium point of the realizations $(Y, A_k^{(1)})$ and $(Y, A_k^{(2)})$. Then x^* is a complex balanced equilibrium point of the realization $(Y, A_k^{(3)})$ where $A_k^{(3)}$ is the convex combination of the matrices $A_k^{(1)}$ and $A_k^{(2)}$.*

Proof It is clear that $A_k^{(3)}$ is a Kirchhoff matrix. Then we have to show that $A_k^{(3)} \cdot \psi(x^*) = \mathbf{0}$ is fulfilled:

$$A_k^{(3)} \cdot \psi(x^*) = (\lambda A_k^{(1)} + (1-\lambda) A_k^{(2)}) \cdot \psi(x^*) = \mathbf{0}. \tag{42}$$

for any $\lambda \in [0, 1]$. $\square$

The above convexity result shows that it is enough to compute a complex balanced realization $(Y, A_k^{(h)})$ with the joint equilibrium point x^* in each vertex $M_p^{(h)}$ ($h = 1, ..., L$ where L is the number of vertices of the convex set) with the same feedback gain matrix K. This gives the following *constraints*

$$\begin{cases} M_p^{(h)} + B_p K = Y \cdot A_k^{(h)} \\ \mathbf{1}^T \cdot A_k^{(h)} = \mathbf{0}^T \\ [A_k^{(h)}]_{ij} \geq 0 \quad i, j = 1, \ldots, m, \ i \neq j \\ A_k^{(h)} \cdot q^* = \mathbf{0} \end{cases} \tag{43}$$

where $q^* = \psi(x^*)$ is known and $h = 1, \ldots, L$.

Finally, *by minimizing the objective function* (39)*, the feedback gain K can be computed (if it exists) in a LP framework using the linear constraints* (43).

With the resulting feedback gain K, the point x^* will be an equilibrium point of all possible closed loop systems, and x^* will be locally asymptotically stable in the region $\mathcal{S} = (x^* + S) \cap \mathbb{R}^n_{\geq 0}$, where S is the stoichiometric subspace of the closed loop system.

In this case, the only computational goal is weak reversibility and zero deficiency, but the equilibrium points are *arbitrary*, i.e. they are not specified in advance. We recall that if a kinetic system is weakly reversible and has zero deficiency, then its equilibrium points are complex balanced and they are asymptotically stable within the appropriate stoichiometric compatibility classes. Therefore, the aim of the feedback is to transform the open loop system into a weakly reversible kinetic system with zero deficiency.

A Kirchhoff matrix A_k is weakly reversible if and only if there exist a positive vector $p \in \mathbb{R}^n_{>0}$ in its kernel. This condition is nonlinear because the vector p is unknown, too. Therefore, we use the solution proposed in [31] as follows. In order to construct linear constraints, we are going to transform the decision variables, the elements of the matrices K and A_k by $\mathrm{diag}(p)$ (a diagonal matrix with the vector elements $p_i > 0$ in its diagonal) where $p \in \mathbb{R}^n_{>0}$ to form $A'_k = A_k \cdot \mathrm{diag}(p)$ and $K' = K \cdot \mathrm{diag}(p)$. Then A'_k has same structure as A_k and $A_k \cdot p = \mathbf{0}$ if and only if $A'_k \cdot \mathbf{1} = \mathbf{0}$. Then the resulting *linear constraints of dynamical equivalence* are

$$\begin{cases} M_p \cdot \mathrm{diag}(p) + B_p \cdot K' = Y \cdot A'_k \\ \mathbf{1}^T \cdot A'_k = \mathbf{0}^T \\ [A'_k]_{ij} \geq 0 \quad i,j = 1,\ldots,m,\ i \neq j \\ p > \mathbf{0} \end{cases} \tag{44}$$

where the elements of K' and A'_k are the continuous decision variables.

The *linear constraint of weak reversibility* is

$$A'_k \cdot \mathbf{1} = \mathbf{0}. \tag{45}$$

thanks to the suitable transformation of A_k to A'_k.

The MILP constraints of zero deficiency are taken from [35] in the form of

$$\begin{cases} \tilde{y}^{(\ell)} = \eta^{(\ell)} + Y^T \cdot \alpha^{(\ell)}, \quad \ell = 1,\ldots,m - \mathrm{rank}(Y) \\ [A'_k]_{ij} \leq U_1 \cdot \Theta_{ij} \quad i,j = 1,\ldots,m \\ \mid \eta_i^{(\ell)} - \eta_j^{(\ell)} \mid \leq 2 \cdot U_2(1 - \Theta_{ij}) \quad i,j = 1,\ldots,m, \quad \ell = 1,\ldots,m - \mathrm{rank}(Y). \end{cases} \tag{46}$$

The constant vectors $\tilde{y}^{(\ell)} \in \mathbb{R}^m$ for $\ell = 1,\ldots,m - \mathrm{rank}(Y)$ span the kernel of the matrix Y. The bounds U_1 and U_2 are positive real constants, and by increasing these bounds the optimization problem will be less conservative. The continuous decision variables are $\alpha^{(\ell)} \in \mathbb{R}^n$ and $\eta_i^{(\ell)} \in \mathbb{R}^m$ for

$\ell = 1, \ldots, m - \text{rank}(Y)$ and $i = 1, \ldots, m$. Additionally, $\Theta_{i,j}$ for $i, j = 1, \ldots, m$ are the binary decision variables.

By minimizing *the objective function* (39)*, the feedback gain K can be computed (if it exists) in a MILP framework using the linear constraints* (44)-(46). Note, that the resulting equilibrium point can also be computed from the optimization results.

It is important to observe, that the design based on achieving a weakly reversible closed loop with zero deficiency has generally less strict constraints - even the equilibrium point cannot be specified - than that of the complex balanced closed loop case, therefore it may be feasible when the latter is not. At the same time, the underlying optimization problem is a MILP problem, that is computationally much harder than the LP problem required to solve the feedback design in the complex balanced closed loop case. However, we can still check the existence of a weakly reversible closed loop system in polynomial time by checking the feasibility of the linear constraints (44) and (45), since they do not contain integer variables. If no weakly reversible solution exists, then it is unnecessary to run the MILP optimization.

Finally, we recall that none of the feedback computation methods described in this Section require that the open loop system is kinetic, therefore, generally, no initial graph structure is assumed for it. The computation of the feedback and the desired graph structure/parametrization of the closed loop system is performed in one optimization step in all cases.

5 Case studies

The proposed methods are illustrated by two computational examples, and a simple process control example in this section.

5.1 Computational examples

In this section, two simple examples are presented to highlight the feedback computation in both the complex balanced and the weakly reversible zero deficiency closed loop case. The purpose of these simple examples is to illustrate the developed computational methods in the case of stabilizing general polynomial systems.

5.1.1 Robust, complex balanced closed loop

In this example the robust design case is considered, when the uncertain coefficient matrix of a polynomial system is characterized as the convex combination constant matrices of appropriate dimensions. Let the open-loop system be given as

$$\dot{x}_p = M_p \underbrace{\begin{bmatrix} x_{p_1}x_{p_2} \\ x_{p_2}x_{p_3} \\ x_{p_1} \end{bmatrix}}_{\psi_p(x_p)} + \underbrace{\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}}_{B_p} u_p \tag{47}$$

where M_p is the arbitrary convex combination of the following three matrices

$$M_p^{(1)} = \begin{bmatrix} -1 & 1 & 0 \\ 2 & 1 & 2 \\ 1 & -1 & 0 \end{bmatrix}, \quad M_p^{(2)} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}, \quad M_p^{(3)} = \begin{bmatrix} 0 & 1 & -1 \\ 2 & 0 & 3 \\ 0 & -1 & 1 \end{bmatrix}.$$

Let the desired equilibrium point be chosen as $x^* = [1\ 1\ 1]^T$.

We are looking for a feedback law with the gain K that transforms the systems characterized by the matrices $M_p^{(i)}$ into a complex balanced kinetic system with the given equilibrium point.

By solving the feedback design LP optimization problem using the linear constraints (43), we obtain the following feedback

$$u_p = \begin{bmatrix} -2 & -1 & -2 \end{bmatrix} \psi_p(x_p). \tag{48}$$

Fig. 1. depicts a complex balanced realization of the closed loop system in the case $M_p = 0.6M_p^{(1)} + 0.2M_p^{(2)} + 0.2M_p^{(3)}$. The obtained closed loop system in an inner point of the convex set $\mathcal{M}$ has the following stoichiometric subspace:

$$S = \text{span}(\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ -1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}). \tag{49}$$

Therefore, the equilibrium point x^* will be asymptotically stable in the region $\mathcal{S} = (x^* + S) \cap \mathbb{R}^n_{\geq 0}$. Therefore, if the initial value is chosen from the set $\mathcal{S}$, then the corresponding solution will converge to the desired equilibrium point x^* . Fig. 2 shows the time domain behaviour of the perturbed system.

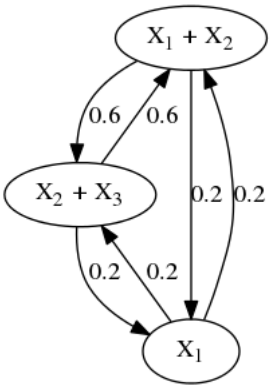

Figure 1. Complex balanced realization of the closed loop system (of subsection 5.1.1) in the case $M_p = 0.6M_p^{(1)} + 0.2M_p^{(2)} + 0.2M_p^{(3)}$

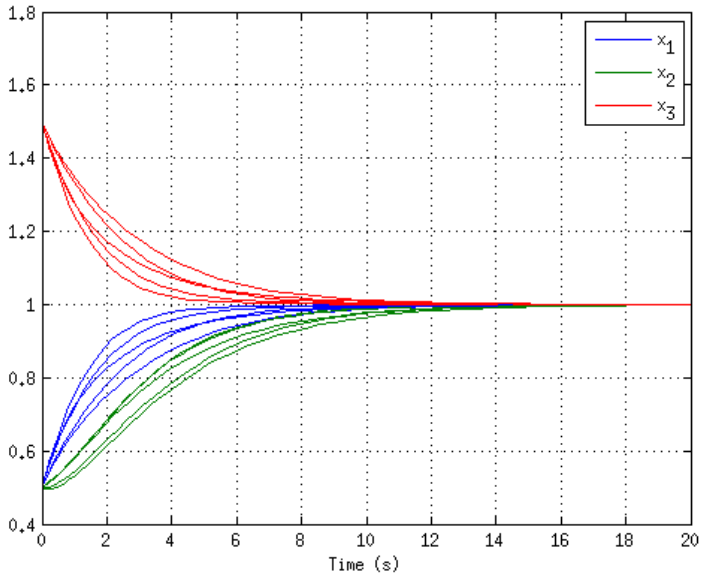

Figure 2. Time domain simulation of the perturbed closed loop system (of subsection 5.1.1) with the initial value $x_0 = [0.5\ 0.5\ 1.5]$.

5.1.2 Weakly reversible closed loop with zero deficiency

Let us consider the following polynomial system

$$\dot{x}_{p_1} = -x_{p_1}x_{p_2} + 2x_{p_2}^2 x_{p_3} \tag{50}$$
$$\dot{x}_{p_2} = -4x_{p_2}^2 x_{p_3} - 6x_{p_2}^2 x_{p_3} + u_{p_1} \tag{51}$$
$$\dot{x}_{p_3} = -1 + x_{p_1}x_{p_2} - 4x_{p_2}^2 x_{p_3} - 3x_{p_2}x_{p_3}^2 + u_{p_2} \tag{52}$$

It is easy to see from (52) that for $u_{p_1} = 0$, $u_{p_2} = 0$, the system has no equilibrium points in the nonnegative orthant. Using the notations of Section

3.2, we have:

$$\psi_p(x_p) = [1 \; x_{p_1}x_{p_2} \; x_{p_2}^2 x_{p_3} \; x_{p_2}x_{p_3}^2]^T,$$
$$M_p = \begin{bmatrix} 0 & -1 & 2 & 0 \\ 2 & 0 & -6 & 0 \\ -1 & 1 & -4 & -3 \end{bmatrix}, \quad B_p = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Then, after performing the procedure presented in Section 4, we find that the MILP optimization problem is feasible, and the resulted feedback is

$$u_p = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 \end{bmatrix} \psi_p(x_p). \tag{53}$$

Fig. 3. depicts the resulted weakly reversible realization with zero deficiency of the closed loop system.

The obtained closed loop system has the following stoichiometric subspace:

$$S = \text{span}(\begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 0 \\ -2 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ -1 \end{bmatrix}, \begin{bmatrix} 0 \\ -1 \\ -2 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}). \tag{54}$$

It is easy to see that the dimension of S is 3. Therefore, the system has only one equilibrium point in the positive orthant which is complex balanced and asymptotically stable: $x^* = \left[2(1/3)^{2/3} \; (1/3)^{1/3} \; (1/3)^{1/3}\right]^T$.

Fig. 4 shows the time domain behaviour of the closed loop system.

5.2 A process control example

Let us consider an open chemical reaction network in which the chemical reactions

$$2X_1 + X_3 \mapsto X_1 + X_2 \quad , \quad X_1 + X_2 \mapsto X_1 + 2X_3 \quad , \quad X_1 + 2X_3 \mapsto X_1 + X_2$$
$$X_1 + 2X_2 \mapsto X_1 + X_2 \quad , \quad X_1 + 2X_2 \mapsto X_1 + 2X_3$$

take place under isothermal conditions, where all the reaction rate constants are equal to 1. Fig. 5 shows the reaction graph of the above CRN without any in- and outflow. Let us choose the inlet concentrations of the species X_1

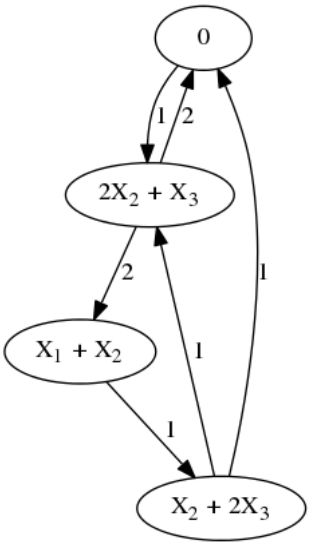

Figure 3. Weakly reversible realization with zero deficiency of the closed loop system (of subsection 5.1.2)

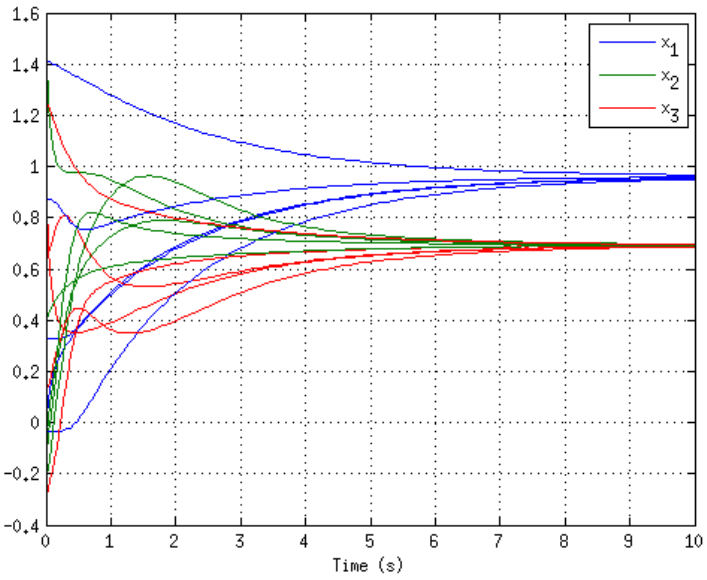

Figure 4. Time domain simulation of closed loop system (of subsection 5.1.2) with five different initial values.

and X_2 as input variables and assume constant volume in the open chemical reaction network.

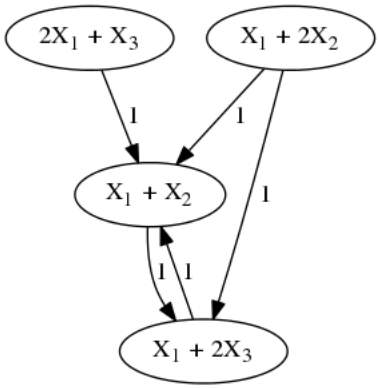

Figure 5. The reaction graph of the CRN in the process system example (of subsection 5.2)

Then the open-loop system model is in the following form

$$\dot{x}_p = \underbrace{\begin{bmatrix} -1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & -1 & -3 & 1 & 0 & -1 & 0 \\ -1 & 2 & 2 & -2 & 0 & 0 & -1 \end{bmatrix}}_{M_p} \cdot \underbrace{\begin{bmatrix} x_{p_1}^2 x_{p_3} \\ x_{p_1} x_{p_2} \\ x_{p_1} x_{p_2}^2 \\ x_{p_1} x_{p_3}^2 \\ x_{p_1} \\ x_{p_2} \\ x_{p_3} \end{bmatrix}}_{\psi_p(x_p)} + \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}}_{B_p} u_p. \tag{55}$$

We are looking for the non-negative feedback gain K which transforms the system into a complex balanced one with the desired equilibrium point $x_p^* = [1\ 1\ 1]$.

The computed feedback gain is

$$K = \begin{bmatrix} 0\ 0\ 0\ 0\ 1\ 0\ 1 \\ 1\ 0\ 0\ 0\ 0\ 1\ 1 \end{bmatrix} \tag{56}$$

and the corresponding feedback is

$$u_{p_1} = x_{p_1} + x_{p_3} \tag{57}$$
$$u_{p_2} = x_{p_1}^2 x_{p_3} + x_{p_2} + x_{p_3}. \tag{58}$$

The above equation (58) ensures the nonnegativity of the input variables, that are the inlet concentrations of X_1 and X_2.

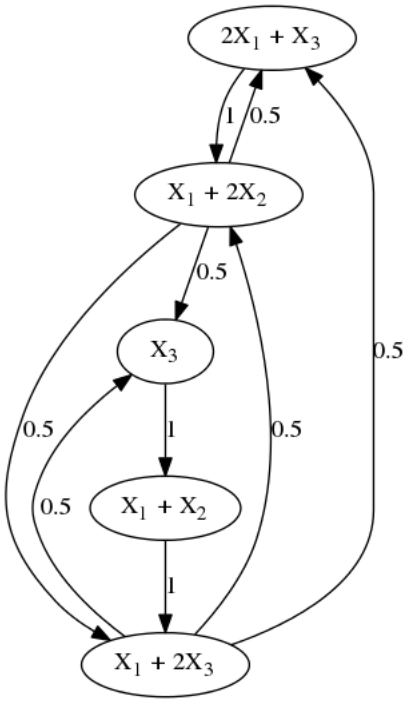

Figure 6. Complex balanced realization of the closed loop process system (of subsection 5.2)

The closed loop system has a complex balanced realization which is depicted in Fig. 6.

The dimension of the stoichiometric subspace of the closed loop system is 3, so it has only one positive equilibrium point $x_p^* = [1\ 1\ 1]^T$ which is asymptotically stable. Fig. 7. shows the time domain simulation under different initial conditions.

Finally, it is important to remark here that all three closed loop systems in the examples of this section are globally stable, since their reaction graphs contain only one linkage class.

6 Conclusions

A novel approach is proposed in this paper to asymptotically stabilize polynomial systems with linear constant parameter input terms around a positive equilibrium point. The stabilization is achieved by constructing a polynomial state feedback that results in a closed loop system that has a MAL-CRN realization with prescribed advantageous properties.

Based on the theory of MAL-CRN systems and the phenomenon of dynamical equivalence, a complex balanced or weakly reversible zero deficiency realization

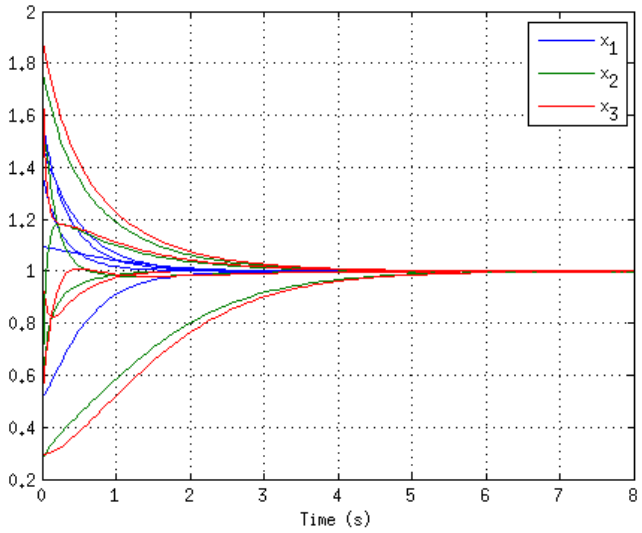

Figure 7. Time domain simulation of closed loop system (of subsection 5.2) with five different initial values.

is aimed at by computing the feedback gain of a polynomial feedback using optimization. First the sufficient feedback structure is determined by proving that it is enough to apply a static feedback with constant gains containing only the monomials that are present in the open loop polynomial system.

The case of requiring a closed loop system with complex balanced MAL-CRN realization having a prescribed equilibrium point results in a linear optimization problem that is solvable in the LP framework. The robust version of the problem, when a convex set of polynomial systems is given over which an asymptotically stabilizing controller is searched for, is also solvable with a LP solver.

If the complex balanced case has no solution, one can attempt to solve another case with weaker but still linear constraint set to obtain a closed loop system that has a weakly reversible realization with zero deficiency. Although this also guarantees asymptotic stability around a positive steady state point, but this point is not arbitrarily chosen, and the resulting optimization problem is only solvable in a MILP framework. The proposed methods and tools are illustrated on two simple examples, and on a process system case study.

The input structure and the proposed optimization framework technically allows us to exclude certain (e.g. non-measured) state variables from the feedback law, since the feedback expression (26) may contain the linear combination of arbitrary monomials. Clearly, the assumptions of Theorem 3 would be no longer valid in such a case. This situation would raise the problem of new monomial selection, therefore, it will be a target of future research.

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