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# 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.


## 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-, or (bio)chemical-control, etc. 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 non-negative 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. [41–43,32]).

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 specialties 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

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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 [2].

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 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 associated with chemical reaction networks

This section is devoted to the notions and tools applied in the theory of *positive (or non-negative) 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

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

where $g_i$ and $h_i$ are polynomials with non-negative coefficients. It is easy to prove that kinetic systems are non-negative [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 non-negative 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 $\ell$-th reaction in the CRN be $C_j \mapsto C_i$ for $1 \leq \ell \leq r$. Then the $\ell$-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

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

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