Hamiltonian Feedback Design for Mass Action Law Chemical Reaction Networks

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Abstract: A special polynomial state feedback structure is proposed for open chemical reaction networks obeying the mass action law (MAL-CRNs) that stabilizes them for any of their admissible positive set of parameters. The proposed feedback makes the closed-loop system a reversible CRN that enables a generalized Hamiltonian description assuming that their number of reversible reactions is less or equal that the number of species. The design is based on solving a mixed integer linear optimization problem (MILP).
A simple example is used to illustrate the basic concepts and the design method.

Keywords: Process control; Hamiltonian control; Modelling; Chemical Reaction Networks

1. INTRODUCTION

Process systems are often highly nonlinear with a wide range of nonlinear phenomena that make their dynamic analysis and control a challenging task. At the same time, they have a characteristic nonlinear structure that is determined by the laws of thermodynamics, that opens the possibility to apply physically inspired special approaches (e.g. Lagrangian or Hamiltonian methods [19], [11]) for their dynamic analysis and controller design.

The major sources of the nonlinearity in process systems are the chemical reactions. A separate special positive nonlinear system class, the chemical reaction networks (CRN) with mass action law (MAL) kinetics is suitable to characterize their nonlinear dynamic behavior. It has been shown that the MAL CRN system class is a wide class, that is often used to model complex biological mechanisms [18], or even models of application fields far from chemistry such as mechanical or electrical systems [22]. The increasing interest for this field is shown by numerous surveys and tutorials in different journals [25], [5], [2].

Motivated by the fact that MAL CRNs exhibit all the qualitative dynamic behavior patterns (e.g. oscillations, chaotic behavior, stable and unstable equilibrium points) that a lumped process system with smooth nonlinearities may show, the possibility of deriving a MAL CRN representation i.e. a model in MAL CRN form for them has been proposed recently [15].

The idea of constructing a Hamiltonian description of process systems is not new [13], but it has become popular in recent years (see e.g. [21], [16]). However, no feasible way of constructing a Hamiltonian description of a general lumped process system has been found so far, but only for some special cases (e.g. isothermal, one balance volume, constant mass holdup etc). For the special case of reversible chemical reaction networks it was shown [20] that they admit a generalized Hamiltonian description if the number of reversible reactions is less or equal than the number of species in the system. Very recently, a port-Hamiltonian description of close complex balanced chemical reaction networks have also been proposed [24].

The aim of this paper is to propose a method for kinetic nonlinear feedback design to the simplest case of a lumped process system that enables to have a generalized Hamiltonian structure for the closed-loop system. The basic idea is similar to the one applied earlier to general polynomial systems (see e.g. [17]), namely to use a specially designed polynomial feedback to the open loop system that makes the closed loop system to have a desired property, a generalized Hamiltonian structure in our case.

2. BASIC NOTIONS

Consider a specially opened chemical reaction network, where the reactions are taking place in a perfectly stirred (lumped) reactor with the possibility of feeding in some of the pure components (species). This corresponds to the fed-batch operation case in the terminology of process systems engineering.

Then the dynamic model is in the form of a set of ordinary differential equations (possibly equipped with algebraic equations, but we assume that these can be substituted into the balance equations). In order to have the simplest

⋆ This work was supported in part by the Hungarian Research Fund through grant 83440.

possible case, the following ***general assumptions*** are made:

(1) constant temperature, i.e. no energy balance equations are considered,
(2) constant pressure (in-compressible fluid phases),
(3) the presence of an inert solvent with great excess such that the reactor has constant overall volume despite of the feed,
(4) chemical reactions obey the mass action law (MAL),
(5) constant physico-chemical properties.

This way we assume that the system is open with an inflow of pure species, where the number of species is n. Then we can describe the open-loop system by the following variables and parameters:

- the specie mass flow rates of component (or specie) A_s denoted by $v_{I,s},\ s = 1, ..., n$ (measured in kg/s), that are the manipulable inlet variables,
- the concentration (measured in $\frac{mol}{m^3}$) of component (or specie) A_s that is denoted by $x_s,\ s = 1, ..., n$.
- the reaction rate constants denoted by $k_{\ell,l}$, where the pair ℓ, l is the identifier of the reaction.

2.1 Dynamic model equations

Under the general assumptions above, the model equations originate from the component mass balances for the considered balance volume. These dynamic balances are of the following general form for lumped balance volumes [14]:

$$\left\{ \begin{matrix} \textit{rate of} \\ \textit{change} \end{matrix} \right\} = \left\{ \begin{matrix} \textit{in-} \\ \textit{flow} \end{matrix} \right\} \pm \left\{ \begin{matrix} \textit{source} \\ \textit{sink} \end{matrix} \right\} \qquad (1)$$

The first term on the right-hand side of the above equation corresponds to the inbound convection term, while in the source or sink terms may correspond to various other mechanisms. For the sake of simplicity we only assume to have chemical reactions obeying the mass action law.

It is important to note that the convective component mass inflow rate $v_{I,s}$ corresponds to the concentration inflow $x_{I,s} = \frac{v_{I,s}}{V}$ for the chemical specie A_s, where the volume of the reactor is V.

2.2 Chemical reaction networks and the reaction graph

A CRN obeying the mass action law is a closed system where chemical species $\mathrm{A}_s,\ s = 1, ..., n$ take part in r chemical reactions. The concentrations of the species denoted by $x_s,\ (s = 1, ..., n)$ form the state vector x. The *elementary reaction steps* have the following form:

$$\sum_{s=1}^{n} \alpha_{sj} \mathrm{A}_s \to \sum_{s=1}^{n} \beta_{sl} \mathrm{A}_s, \qquad (2)$$

where α_{sj} is the so-called *stoichiometric coefficient* of component A_s in reaction $C_j \to C_l$, and β_{sl} is the stoichiometric coefficient of the product A_s. The linear combinations of the species in Eq. (2), namely $C_j = \sum_{s=1}^{n} \alpha_{sj} \mathrm{A}_s$ and $C_l = \sum_{s=1}^{n} \beta_{sl} \mathrm{A}_s$ are called the *complexes* and are denoted by $C_1, C_2, \ldots, C_m$. Reactions may share complexes in complex reaction schemes, therefore m is generally not equal to the number of reactions. Moreover, reactions are assumed to be irreversible in classical reaction kinetic systems, therefore *the stoichiometric coefficients are always nonnegative integers.*

The *reaction rates* of the individual reactions $C_j \longrightarrow C_l$ can be described as

$$\rho_{jl}(x) = k_{j,l} \prod_{s=1}^{n} x_s^{\alpha_{sj}} \qquad (3)$$

where $k_{j,l} > 0$ is the *reaction rate coefficient* of the reaction, and x_s is the concentration of specie A_s.

In our computations, the following form will be used for the description of the dynamics of CRNs obeying the mass action law [8]:

$$\dot{x} = M \cdot \varphi(x) = Y \cdot A_k \cdot \varphi(x) \qquad (4)$$

where $\alpha_{sj} = Y_{sj},\ Y \in \mathbb{R}^{n \times m}$ stores the stoichiometric composition of the complexes, $A_k \in \mathbb{R}^{m \times m}$ contains information about the structure of the reaction network, and $\varphi : \mathbb{R}^n \mapsto \mathbb{R}^m$ is a monomial-type vector mapping given by

$$\varphi_j(x) = \prod_{s=1}^{n} x_s^{\alpha_{sj}}, \quad j = 1, \ldots, m \qquad (5)$$

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

$$[A_k]_{lj} = \begin{cases} -\sum\limits_{\substack{\ell = 1 \\ \ell \neq j}}^{m} k_{l,\ell}, & \text{if } l = j \\ k_{j,l}, & \text{if } l \neq j \end{cases} \qquad (6)$$

where $[A_k]_{lj}$ denotes the ljth element of the matrix A_k. It is important to note that the pair (Y, A_k) uniquely characterizes a particular CRN with its structure and parameters.

To handle the exchange of materials between the environment and the reaction network, the so-called "zero-complex" can be introduced and used which is a special complex where all stoichiometric coefficients are zero i.e., it is represented by a zero column vector in the Y matrix [8]. Note, however, that the presence of the zero complex may imply the openness of the reaction kinetic system.

Similarly to [8] and many other authors, the following weighted directed graph (called ***reaction graph***) is assigned to the reaction network (2). The directed graph $D = (V_d, E_d)$ of a reaction network consists of a finite nonempty set V_d of vertices and a finite set E_d of ordered pairs of distinct vertices called directed edges. The vertices correspond to the complexes, i.e. $V_d = \{C_1, C_2, \ldots C_m\}$, while the directed edges represent the reactions, i.e. $(C_l, C_j) \in E_d$ if complex C_l is transformed to C_j in the reaction network. The reaction rate coefficients $k_{l,j}$ for $j = 1, \ldots, m$ in (3) are assigned as positive weights to the corresponding directed edges in the graph.

An example of a reaction graph is seen in Fig. 1.

For each reaction $C_i \to C_j$ corresponds a ***reaction vector***:

$$e_k = [Y]_{\cdot,j} - [Y]_{\cdot,i},\ k = 1, \ldots, r, \qquad (7)$$

where $[Y]_{\cdot,i}$ denotes the ith column of Y and r is the number of reactions. The set of reaction vectors is equivalent to the column vectors of $Y \cdot B_G$ where B_G is the incidence matrix of the reaction graph.

2.3 Generalized Hamiltonian description of reversible CRNs

The form of generalized dissipative Hamiltonian systems we use is defined in [23].

Let us be given a ***closed CRN*** with n species and r reversible reaction pairs, i.e. $2r$ elementary reaction steps of the form (2) such that $r \leq n$. Assume that the rank of the vector space spanned by the reaction vectors is r. We remark that the above conditions imply the following: the CRN is weakly reversible, it is deficiency zero and there are no circles formed by reversible reaction pairs in its reaction graph (i.e. if we substitute the reversible reaction pairs by undirected edges in the reaction graph, we obtain a forest). It follows from these properties that the network is complex balanced for any positive reaction rate coefficients, it has precisely one positive equilibrium point in any stoichiometric compatibility class, and its dynamics is globally stable with a known Lyapunov function [8, 1]. It is also important to remark that circuitless reversible reaction networks of deficiency zero are always detailed balanced independently of the values of the reaction rate coefficients (see Remark 3.3 in [10]). Therefore, in our case the so-called Wegscheider spanning forest conditions will automatically be fulfilled in Section 4 if a closed loop realization with the prescribed properties exist.

Consider an equilibrium point x^* of the system, and assume that its reactions are independent, i.e. the reaction vectors of the system are linearly independent. Then this system admits a dissipative Hamiltonian description in a neighbourhood of x^* [20] with a special logarithmic Hamiltonian function.

We give here the short summary of the above Hamiltonian description. Let the reversible reactions be given in the form

$$\sum_{i=1}^{n} \alpha_{ij} X_i \rightleftarrows \sum_{i=1}^{n} \beta_{ij} X_i \quad \text{for } j = 1, \ldots, r. \tag{8}$$

Then the overall reaction rates corresponding to the reversible reactions are given by

$$W_j(x) = \underbrace{k_j^+ \prod_{i=1}^{n} x_i^{\alpha_{ij}}}_{p_j(x)} - \underbrace{k_j^- \prod_{i=1}^{n} x_i^{\beta_{ij}}}_{q_j(x)}, \quad j = 1, \ldots, r. \tag{9}$$

Let us define the so-called reaction space coordinates as

$$z_j = \ln p_j - \ln q_j, \quad j = 1, \ldots, r. \tag{10}$$

The Hamiltonian function $\mathcal{H}$ is the following

$$\mathcal{H}(z) = \sum_{j=1}^{r} q_j^* \left[\exp(z_j) - z_j - 1\right], \tag{11}$$

where $q_j^* = q_j(x^*)$. It can be shown that the time-derivative of z can be written as

$$\dot{z} = -G(x) \cdot \mathcal{H}_z^T(z), \tag{12}$$

where $\mathcal{H}_z^T$ is the gradient transpose of $\mathcal{H}$, and

$$G(x) = \mathcal{N}^T \Gamma(x) \mathcal{N} \cdot F(q) \cdot (F(q^*))^{-1}. \tag{13}$$

The components of G are the following

$$\begin{gathered} \mathcal{N} \in \mathbb{R}^{n \times r}, \mathcal{N}_{ij} = \beta_{ij} - \alpha_{ij}, \\ \Gamma(x) = \operatorname{diag}\left[\frac{1}{x_1}\ \frac{1}{x_2}\ \ldots\ \frac{1}{x_n}\right], \\ F(q) = \operatorname{diag}\left[q_1\ \ldots\ q_r\right]. \end{gathered} \tag{14}$$

It is easy to see that $G(x^*)$ is symmetric and positive definite, therefore the Hamiltonian structure (12) is locally dissipative around the equilibrium point.

2.4 Simple example

In order to illustrate the constructions, the following simple nonlinear example will be used.

In the reactor we consider a set of chemical reactions

$$\begin{aligned} & 2X_1 + X_2 \xrightarrow{k_{2,1} = 1} X_1 + X_3, \\ & 2X_3 \xrightarrow{k_{3,1} = 1} X_1 + X_3, \\ & X_1 + X_3 \underset{k_{4,1} = 1}{\overset{k_{1,4} = 1}{\rightleftarrows}} 2X_1 + X_2 + 2X_3 \end{aligned} \tag{15}$$

The reaction graph of the above chemical reaction network is depicted in Fig. 1. The complex composition matrix and

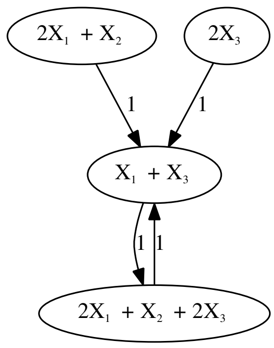

Fig. 1. The simple reaction graph

Kirchhoff matrix of this system are

$$Y = \begin{bmatrix} 1 & 2 & 0 & 2 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 2 & 2 \end{bmatrix}, \quad A_k = \begin{bmatrix} -1 & 1 & 1 & 1 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix}. \tag{16}$$

3. COMPUTING DYNAMICALLY EQUIVALENT REVERSIBLE REALIZATIONS WITH INDEPENDENT REACTION VECTORS

It is a known result of the chemical reaction network theory that the graph structure of the system (4) is generally not unique. In this section, an optimization based method is presented for computing reversible realization with independent reaction vectors.

3.1 The notion of dynamic equivalence

Consider two realizations $(Y^{(1)}, A_k^{(1)})$ and $(Y^{(2)}, A_k^{(2)})$. We call these realizations dynamically equivalent if

$$Y^{(1)} \cdot A_k^{(1)} \cdot \varphi^{(1)}(x) = Y^{(2)} \cdot A_k^{(2)} \cdot \varphi^{(2)}(x), \quad \forall\, x \in \mathbb{R}_+^n \tag{17}$$

where for $i = 1, 2$, $Y^{(i)} \in \mathbb{Z}^{n \times m_i}$ are the complex composition matrices, $A_k^{(i)}$ are Kirchhoff matrices, and

$$\varphi_j^{(i)}(x) = \prod_{k}^{m_i} x_k^{Y_{kj}^{(i)}}. \tag{18}$$

Most often we assume that the complex set of the two realizations are the same, i.e. $Y^{(1)} = Y^{(2)} = Y$, that implies $\varphi^{(1)}(x) = \varphi^{(2)}(x) = \varphi(x)$.

3.2 The underlying optimization problem

In the realization computation problem of the system (4), the matrix M and the vector $\varphi(x)$ are given. We are looking for a realization (Y, A_k) which fulfils some additional requirements (e.g. reversibility). When the complex composition matrix Y is a priori known the realization computation problem can be solved efficiently as a linear programming problem. In that case the dynamic equivalence constraint is linear in the decision variable A_k:

$$Y \cdot A_k = M. \tag{19}$$

The constraints of the Kirchhoff property are

$$\begin{array}{l} \sum_{i=1}^{m} [A_k]_{ij} = 0, \quad j = 1, \ldots, m \\ [A_k]_{ij} \geq 0, \quad i, j = 1, \ldots, m, \ i \neq j \\ [A_k]_{ii} \leq 0, \quad i = 1, \ldots, m. \end{array} . \tag{20}$$

3.3 Computing reversible realizations

Let us introduce the binary variable $\Theta \in \{0,1\}^{m \times m}$ to ensure the reversibility. The construction of Θ is the following

$$\Theta_{ij} = 1 \iff [A_k]_{ij} > 0, \quad \forall i \neq j. \tag{21}$$

This condition can be relaxed by a MILP constraint [3]

$$\epsilon \cdot \Theta_{ij} \leq [A_k]_{ij} \leq U \cdot \Theta_{ij}, \quad \forall i \neq j \tag{22}$$

where ϵ is a small positive number and U is the upper bound of elements A_k. Finally, the realization (Y, A_k) is reversible if and only if the matrix Θ is symmetric. Therefore, the last constraint is

$$\Theta^T = \Theta. \tag{23}$$

3.4 Independent reaction vectors

Let us consider the incidence matrix B_G of a reversible CRN with m complexes and r reversible reaction pairs. It can be partitioned in the following way

$$B_G = [\, B \mid -B \,] \tag{24}$$

where $B \in \{-1, 0, 1\}^{m \times r}$. The reaction vectors are independent if and only if the matrix $\mathcal{N} = Y \cdot B$ has linearly independent column vectors. It is equivalent to the following two conditions

$$\mathrm{Ker}(B) = \{0\} \tag{25}$$

and

$$\mathrm{Ker}(Y) \cap \mathrm{Im}(B) = \{0\}. \tag{26}$$

The first condition (25) is satisfied if and only if the matrix B has $m - l$ columns where l is the number of the weakly connected components [12]. In the further, we assume that the realization has only one linkage class ($l = 1$) for the simplicity. These conditions can be formulated as a MILP constraint (this is the so-called subtour elimination constraint [4]):

$$\sum_{i=1}^{m} \sum_{j=1}^{m} \Theta_{ij} = 2(m-1) \tag{27}$$

$$\sum_{i \in S} \sum_{j \in S} \Theta_{ij} = 2(|S| - 1), \quad \forall S \subset \{1, \ldots, m\} \tag{28}$$

The incidence matrix of two different connected graphs with the same number of vertices span the same vector space [12]. Therefore, the condition (26) can be checked before the optimization using any incidence matrix of an arbitrary connected graph with m vertices.

3.5 Summary of the optimization problem

The presented optimization problem for determining the requested reversible realizations has two decision variables $A_k \in \mathbb{R}^{m \times m}$ and $\Theta \in \{0,1\}^{m \times m}$. The constraints in one block are

$$\begin{cases} Y \cdot A_k = M \\ \sum_{i=1}^{m} [A_k]_{ij} = 0, \quad j = 1, \ldots, m \\ [A_k]_{ij} \geq 0, \quad i, j = 1, \ldots, m, \ i \neq j \\ [A_k]_{ii} \leq 0, \quad i = 1, \ldots, m \\ \epsilon \cdot \Theta_{ij} \leq [A_k]_{ij} \leq U \cdot \Theta_{ij}, \quad \forall i \neq j \\ \sum_{i=1}^{m} \sum_{j=1}^{m} \Theta_{ij} = 2(m-1) \\ \sum_{i \in S} \sum_{j \in S} \Theta_{ij} = 2(|S| - 1), \quad \forall S \subset \{1, \ldots, m\} \end{cases} \tag{29}$$

where ϵ is a small positive number and U is the upper bound of the elements A_k. Since the constraints are linear in the decision variables, the solution of the problem can be solved in the MILP framework.

4. THE FEEDBACK DESIGN PROBLEM AND ITS SOLUTION

4.1 Open loop system model

Consider a set of positive polynomial ODEs that describe the chemical reactions inside the reactor

$$\dot{x} = M \cdot \varphi(x) \tag{30}$$

with an underlying complex composition matrix Y giving rise to $\varphi(x)$. This implies that the above system is kinetic in itself.

Let us open the system by an inlet consisting of component mass flow rates v_I. Then the open-loop system model becomes

$$\dot{x} = M \cdot \varphi(x) + x_I \tag{31}$$

where x_I is the vector of inlet concentrations, that form the vector of (potential) input variables, i.e. $x_I = u$. Note that full actuation is assumed in this case.

4.2 Kinetic feedback structure

A polynomial feedback of the form

$$u = \psi(x) \tag{32}$$

is considered, where $\psi : \mathbb{R}^n \mapsto \mathbb{R}^n$ is a monomial-type vector mapping.

In order to have a physically realizable yet simple controller the following ***requirements*** are made.

(1) The monomials in the mapping ψ are the same, as that in the open-loop system model, i.e. the complex composition matrix of the closed-loop system is also Y. This implies, that

$$u = K\varphi(x) \tag{33}$$

where $K \in \mathbb{R}^{n\times m}$

(2) The feedback should be physically realizable, i.e. $u_i \geq 0$ should hold for any $i = 1, ..., n$. As each concentration is non-negative (i.e. $x_i \geq 0$) and each $\varphi_j(x)$ is a monomial, this requirement is fulfilled, when

$$K_{ij} \geq 0 \quad , \quad i = 1, ..., n, \ j = 1, ..., m \tag{34}$$

(3) The closed-loop system should be kinetic. This requirement will automatically be satisfied by the next requirement.

(4) The closed-loop system should have a dynamically equivalent ***reversible realization*** in order to enable a generalized Hamiltonian structure.

(5) The simplest possible feedback is searched for, i.e. we want to minimize the number of reaction monomials in the feedback (33).

4.3 The optimization problem

The closed-loop system is

$$\dot{x} = \underbrace{(M + K)}_{\overline{M}}\varphi(x). \tag{35}$$

The requirements (1)-(4) of the closed-loop can be guaranteed by the previously presented realization computation method with the matrix $\overline{M}$. The only difference is that the matrix $\overline{M}$ contains a decision variable K. Therefore, we have to introduce some additional constraints.

First, the matrix K has only nonnegative elements

$$K_{ij} \geq 0, \quad \forall i = 1, \ldots n, \ j = 1, \ldots m. \tag{36}$$

The second constraint belongs to the requirement (5). For this, we introduce a binary variable $\Phi \in \{0, 1\}^{n\times m}$ and

$$K_{ij} > 0 \implies \Phi_{ij} = 1, \quad \forall i = 1, \ldots n, \ j = 1, \ldots m. \tag{37}$$

This condition can be translated into a MILP one [3]

$$K_{ij} \leq U_f \Phi_{ij}, \quad \forall i = 1, \ldots n, \ j = 1, \ldots m \tag{38}$$

where U_f is the upper bound of the elments of K. Then the number of zeros in the matrix K can be minimized by the objective function

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

5. A SIMPLE EXAMPLE

Let us consider the open-loop version of the system (16) presented earlier in subsection 2.4

$$\dot{x} = M\varphi(x) + u \tag{40}$$

where $M = Y \cdot A_k$. This system with zero input does not have reversible realization.

Before the optimization, we have to check the condition (26). Therefore, let us introduce an arbitrary incidence matrix of a connected graph with 4 vertices:

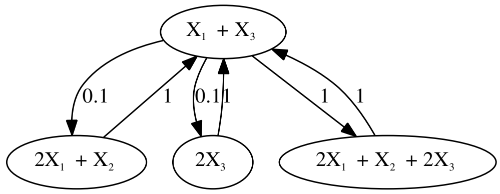

Fig. 2. The reaction graph of the closed loop system

$$B = \begin{bmatrix} -1 & -1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{41}$$

It is easy to check that $\mathrm{Ker}(Y) \cap \mathrm{Im}(B) = \{0\}$.

Then, the resulted input of the optimization is

$$u = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \varphi(x) \tag{42}$$

which means that $u_2 = 0.1 \cdot \varphi_1(x)$ and the other elements of u are zero. The closed-loop system has a reversible realization and the reaction vector pairs are independent. It is depicted in Fig. 2.

The equilibrium point in this case is unique with the value $x^* = [31.6228 \ 0.0100 \ 3.1623]^T$. The components of the Hamiltonian description of the closed loop system are the following.

$$q_1 = x_1^2 x_2, \ q_2 = x_3^2, \ q_3 = x_1^2 x_2 x_3^2 \tag{43}$$

$$\begin{aligned} z_1 &= \ln\left(0.1\frac{x_1 x_3}{x_1^2 x_2}\right) \\ z_2 &= \ln\left(0.1\frac{x_1 x_3}{x_3^2}\right) \\ z_3 &= \ln\left(\frac{x_1 x_3}{x_1^2 x_2 x_3^2}\right) \end{aligned} \tag{44}$$

$$\mathcal{N} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{bmatrix} \tag{45}$$

$$\mathcal{N}^T\Gamma(x)\mathcal{N} = \begin{bmatrix} \left(\frac{1}{x_1} + \frac{1}{x_2} + \frac{1}{x_3}\right) & \left(-\frac{1}{x_1} - \frac{1}{x_3}\right) & \left(\frac{1}{x_1} + \frac{1}{x_2} - \frac{1}{x_3}\right) \\ \left(-\frac{1}{x_1} - \frac{1}{x_3}\right) & \left(\frac{1}{x_1} + \frac{1}{x_3}\right) & \left(\frac{1}{x_3} - \frac{1}{x_1}\right) \\ \left(\frac{1}{x_1} + \frac{1}{x_2} - \frac{1}{x_3}\right) & \left(\frac{1}{x_3} - \frac{1}{x_1}\right) & \left(\frac{1}{x_1} + \frac{1}{x_2} + \frac{1}{x_3}\right) \end{bmatrix} \tag{46}$$

6. CONCLUSIONS

A computational method was presented in this paper to transform polynomial systems via appropriate polynomial feedback into fully reversible CRN form having a locally dissipative Hamiltonian description. The method is based on computing dynamically equivalent realizations of kinetic systems through mixed integer linear programming.

Further work includes the generalization of the proposed method for the port-Hamiltonian description [24] where the more general complex balanced case could be covered.

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