

# REALIZATION THEORY AS A TOOL OF STABILITY ANALYSIS FOR KINETIC SYSTEMS

Dávid Csercsik      Gábor Szederkényi

Pázmány Péter Catholic University, Faculty of Information Technology, Budapest, P.O. Box 278, H-1444,  
Hungary  
email: csercsik@itk.ppke.hu

## ABSTRACT

The theory of reaction kinetic networks provides powerful theorems about the stability of such systems. It is known however, that different reaction kinetic systems, called realizations, may induce the same differential equations. Since the applicability of stability theorems of chemical reaction network theory depend on the realization structure, for a given dynamics, these theorems might be usable or not depending on the actual realization. In this article we point out that in some cases it may be necessary to determine all possible realizations of the same kinetic system to find one for which an appropriate stability theorem can be applied. Furthermore, we provide an algorithm for the effective calculation of the realizations. We demonstrate the results on simple examples.

## KEY WORDS

Stability, reaction kinetic systems, realization theory, non-negative systems

## 1 Introduction

Nonnegative dynamical systems are characterized by the property that the state variables always remain nonnegative during the operation, i.e. the nonnegative orthant is invariant for the dynamics. Such systems appear primarily in such applications where nonnegative physical variables (e.g. concentrations, pressures, etc.) correspond to the states of the studied systems. Therefore the main application areas of nonnegative systems are chemistry, biology, thermodynamics, population and epidemic modeling or even certain transportation processes.

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) or reaction kinetic networks (RKNs) form a wide class of nonnegative systems. CRNs are able to produce all the important qualitative phenomena (e.g. stable/unstable equilibria, oscillations, limit cycles, multiplicity of equilibrium points and even chaotic behavior) that are important for the study and better understanding of nonlinear processes. Therefore, CRNs can be regarded as a possible "prototype of nonlinear systems" [3]. The theory of chemical reaction networks has significant results relating network structure and the qualitative properties of the corresponding dynamics [8, 5]. However, the network structure corresponding

to a given dynamics is generally not unique [2], in other words different CRNs may imply the same polynomial differential equations. In this context it is appropriate to call a CRN a realization of the underlying dynamics. Recently, optimization-based computational methods were proposed for dynamically equivalent network structures with given preferred properties [10, 11].

Since the theorems related to the qualitative dynamic behavior of kinetic systems are formulated for the CRNs, it is possible that for the same dynamics, multiple CRN realizations exist, for some of which certain stability theorems apply. Therefore a possible approach for stability analysis is to determine all possible structurally different realizations of a given dynamics, to determine whether a realization exists for which a stability theorem is valid. The aim of this paper is to summarize some of the most important stability theorems related to CRNs, to provide an efficient algorithm for the determination of all structurally different realizations of a kinetic system, and to demonstrate the approach on simple examples.

## 2 Materials and Methods

In this section, we first shortly define the tools used for the description of CRNs, which will represent the realizations of a kinetic system, review the stability theorems related to CRNs, and then discuss the results regarding kinetic realizability.

### 2.1 Dynamics and structure of kinetic systems

Based on [4], we characterize CRNs with the following triplet.

- $\mathcal{S} = [X_1, \dots, X_m]$  the set of *species*.
- $\mathcal{C} = [C_1, \dots, C_n]$  is the set of *complexes*. The complexes are linear combinations of the species, i.e.

$$C_i = \sum_{j=1}^m \alpha_{ij} X_j, \quad i = 1, \dots, n$$

where  $\alpha_{ij} > 0$  are the integers called the *stoichiometric coefficients*.

- $\mathcal{R} = \{(C_i, C_j)\}$  where  $(C_i, C_j) \in \mathcal{C}$  is the set of reactions (i.e.  $C_i$  is transformed into  $C_j$ ). Furthermore, each reaction can be characterized by its *reaction rate coefficient*  $k_{ij} \geq 0$ .

A directed graph, called the reaction graph or complex graph may be assigned to the reaction network in a straightforward way. The reaction graph  $G_R = (V, E)$  of a reaction network is a directed graph consisting of a finite nonempty set  $V$  of vertices and a finite set  $E$  of edges. The vertices correspond to the complexes, i.e.  $V = \{C_1, C_2, \dots, C_n\}$ , while the directed edges represent the reactions, i.e.  $(C_i, C_j) \in E$  if complex  $C_i$  is transformed to  $C_j$  in the reaction network. The reaction rates  $k_{ij}$  are assigned as positive weights to the corresponding directed edges in the graph.

A set of complexes  $\{C_1, C_2, \dots, C_k\}$  is a *linkage class* of a reaction network if the complexes of the set are linked to each other in the reaction graph but not to any other complex [5].

There are several possibilities to represent the structure of dynamic equations of mass action systems (see, e.g. [4] or [2]). We will use the representation introduced in Lecture 4 of [4], i.e.

$$\dot{x} = YA_k\psi(x) \quad (1)$$

where  $x \in \mathbb{R}^m$  is the concentration vector of the species,  $Y \in \mathbb{R}^{m \times n}$ , a nonnegative integer matrix, stores the stoichiometric composition of the complexes,  $A_k \in \mathbb{R}^{n \times n}$  contains the information corresponding to the weighted directed graph of the reaction network, and  $\psi : \mathbb{R}^m \mapsto \mathbb{R}^n$  is a monomial-type vector mapping defined by

$$\psi_j(x) = \prod_{i=1}^m x_i^{y_{ij}}, \quad j = 1, \dots, n \quad (2)$$

where  $y_{ij} = [Y]_{ij}$ . The exact structure of  $Y$  and  $A_k$  is the following. The  $i$ th column of  $Y$  contains the composition of complex  $C_i$ , i.e.  $Y_{ji}$  is the stoichiometric coefficient of  $C_i$  corresponding to the specie  $X_j$ .  $A_k$  is a column conservation matrix (i.e. the sum of the elements in each column is zero) defined as

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1}^m k_{il}, & \text{if } i = j \\ k_{ji}, & \text{if } i \neq j \end{cases} \quad (3)$$

In other words, the diagonal elements  $[A_k]_{ii}$  contain the negative sum of the weights of the edges starting from the node  $C_i$ , while the off-diagonal elements  $[A_k]_{ij}$ ,  $i \neq j$  contain the weights of the directed edges  $(C_j, C_i)$  coming into  $C_i$ . Based on the above properties, it is appropriate to call  $A_k$  the *Kirchhoff matrix* of a reaction network.

## 2.2 Important properties of kinetic systems

A CRN is called *reversible*, if each of its reactions is a reversible reaction. A CRN is called *weakly reversible*, if

each complex in  $G_R$  lies on at least one directed cycle (i.e. if complex  $C_j$  is reachable from complex  $C_i$  on a directed path in the reaction graph, then  $C_i$  is reachable from  $C_j$  on a directed path). Furthermore we say that the component (or complex set)  $C' \subseteq C$  is *strongly connected* if  $C_i, C_j \in C'$  implies that there is a path from  $C_i$  to  $C_j$ . A component is terminal if there is no reaction leading out of it.

Using the notation  $M = YA_k$ , equation (1) can be written in the compact form

$$\dot{x} = M\psi(x) \quad (4)$$

We can associate an  $n$ -dimensional vector with each reaction in the following way. For the reaction  $C_i \rightarrow C_j$ , the corresponding reaction vector denoted by  $e_k$  is given by

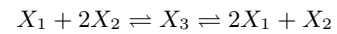
$$e_k = [Y]_{\cdot, j} - [Y]_{\cdot, i}, \quad k = 1, \dots, r, \quad (5)$$

where  $[Y]_{\cdot, i}$  denotes the  $i$ th column of  $Y$ . Any convention can be used for the numbering of the reaction vectors (e.g. the indices  $i$  and  $j$  in (5) can be treated as digits in a decimal system). The *rank* of a reaction network denoted by  $s$  is defined as the rank of the vector set  $H = \{e_1, e_2, \dots, e_r\}$  where  $r$  is the number of reactions. The elements of  $H$  span the so-called *stoichiometric subspace*, denoted by  $S$ , i.e.  $S = \text{span}\{e_1, \dots, e_r\}$ . The positive *stoichiometric compatibility class* containing a  $x_0 \in \mathbb{R}^n$  is the following set [5]:  $(x_0 + S) \cap \mathbb{R}_+^n$ , where  $\mathbb{R}_+^n$  denotes the positive orthant in  $\mathbb{R}^n$ . The *deficiency*  $d$  of a reaction network is defined as [4, 5]

$$d = m_{ni} - l - s, \quad (6)$$

where  $m_{ni}$  is the number of non-isolated vertices in the reaction graph,  $l$  is the number of linkage classes and  $s$  is the rank of the reaction network. The deficiency is a very useful measure for studying the dynamical properties of reaction networks and for establishing parameter-independent global stability conditions.

Furthermore we may define the *stociometric matrix*  $Q$  of a reversible CRN, which consists of (positive and negative) integer elements capturing the basic conservation laws of the reactions. For example the stociometric matrix of



is

$$Q = \begin{pmatrix} -1 & 2 \\ -2 & 1 \\ 1 & -1 \end{pmatrix}$$

The concept of *balancedness*, following [13] may be defined as follows Let us suppose a reversible CRN, and let us define the *equilibrium constant*  $K_j^{eq}$  of the  $j$ -th reaction as

$$K_j^{eq} \doteq \frac{k_j^f}{k_j^r}$$

where  $k_j^f$  and  $k_j^r$  are the forward and backward reaction rates of reaction  $j$ . We say that there exists a *thermodynamic equilibrium*  $x^*$  if

$$Ln(K^{eq}) \in im(Q^T) \quad (7)$$

In this case, the set of all thermodynamic equilibria is given by

$$\varepsilon \doteq \{x^{**} \in \mathbb{R}_+^m \mid Q^T Ln(x^{**}) = Q^T Ln(x^*)\} \quad (8)$$

A CRN is called *balanced* if there exists a thermodynamic equilibrium.

Let us emphasize that in contrast to deficiency, which is a structural property, balancedness also depends on the actual rate constants.

### 2.3 Stability theorems of reaction kinetic systems

The following results and conjectures illustrate the potential of applying the theory of kinetic systems in nonlinear control.

- The *Deficiency Zero Theorem* [5] shows a very robust stability property of a certain class of kinetic systems. It says that deficiency zero weakly reversible networks possess well-characterizable equilibrium points, and independently of the weights of the reaction graph (i.e. that of the system parameters) they are at least locally stable with a known logarithmic Lyapunov function that is also independent of the system parameters. Moreover, they are input-to-state stable with respect to the off-diagonal elements of  $A_k$  as inputs [1], it is straightforward to asymptotically stabilize them by additional feedback [9].
- The *Deficiency One Theorem* [5] formulates a similar statement. Consider a chemical reaction network with deficiency  $d$  and  $l$  linkage classes. Let  $d_i$ ,  $i = 1, \dots, l$  denote the deficiencies of the individual linkage classes considered as their own networks. Suppose the following conditions:

- $d_i \leq 1 \quad \forall i = 1, \dots, l$
- $\sum_{i=1}^l d_i = d$
- Each linkage class contains a single terminal strongly linked component.

Then, if a mass action system corresponding to the network with a specified rate set admits a positive equilibrium concentration, there exists precisely one equilibrium concentration in each positive stoichiometric compatibility class. Furthermore, if the network is weakly reversible, every mass action system permitted by the network has a positive equilibrium.

- Theorem 4.2 of article [13] concludes that for balanced CRNs, the  $\varepsilon$  set of thermodynamic equilibria is globally asymptotically stable for every  $x(0) \in \mathbb{R}_+^m$ .

## 2.4 Realizability of polynomial vector fields

Consider an autonomous nonlinear system

$$\dot{x} = f(x), \quad x(0) = x_0 \quad (9)$$

where  $f : \mathcal{X} \rightarrow \mathbb{R}^n$  is locally Lipschitz,  $\mathcal{X}$  is an open subset of  $\mathbb{R}^n$  and  $x_0 \in \mathcal{X}$ . Suppose that the nonnegative orthant  $[0, \infty)^n = \overline{\mathbb{R}_+^n} \subset \mathcal{X}$ . Then the nonnegative orthant is invariant for the dynamics (9) if and only if  $f$  is essentially nonnegative.

The problem of kinetic realizability of polynomial vector fields was first examined and solved in [7] where the constructive proof contains a realization algorithm that produces the weighted directed graph of a possible associated kinetic mechanism (called the *canonical mechanism*). According to [7], the necessary and sufficient condition for kinetic realizability of a polynomial vector field is that all coordinates functions of  $f$  in (9) must have the form

$$f_i(x) = -x_i g_i(x) + h_i(x), \quad i = 1, \dots, n \quad (10)$$

where  $g_i$  and  $h_i$  are polynomials with nonnegative coefficients.

In [7], the authors give a procedure for generating a possible reaction graph for a given kinetic ODE system (as already mentioned, this reaction graph is generally not unique). The main significance of the above procedure from our point of view is that it defines a  $Y$  and  $A_k$  matrices (and so  $\psi(x)$  as well) for a kinetic system, in other words it provides one realization from the all possible ones.

### 2.4.1 Dynamical equivalence of mass-action networks

It is known [8] that CRNs with different structures and/or parametrization can give rise to the same kinetic differential equations. Therefore, we will call two CRNs given by the matrix pairs  $(Y^1, A_k^1)$  and  $(Y^2, A_k^2)$  *dynamically equivalent*, if

$$Y^1 A_k^1 \psi^1(x) = Y^2 A_k^2 \psi^2(x) = f(x) \quad (11)$$

In this case, the  $(Y^i, A_k^i)$  pairs for  $i = 1, 2$  are called realizations of a kinetic vector field  $f$  (see, e.g. [7] for more details). It is also appropriate to call  $(Y^1, A_k^1)$  a realization  $(Y^2, A_k^2)$  and vice versa.

We will assume throughout the paper that the set of complexes (i.e. the stoichiometric matrix  $Y$ ) is fixed and known before the computations. In this case (since  $\psi(x)$  is determined by  $Y$  as well - see Eq. (2)), the condition (11) for dynamical equivalence can be written as:  $Y A_k^1 = Y A_k^2 = M$ . This implies that the matrices  $A_k^i$  are in one to one correspondence with the realizations, and it makes sense to say that  $A_k^i$  is a realization of  $(Y, A_k)$ .

As in [11], we introduce the *constraint set*  $K$ , and the constrained realizations of a CRN.  $K$  excludes  $s$  reactions from the CRN i.e.

$$K = \{[A_k]_{i_1, j_1} = 0, \dots, [A_k]_{i_s, j_s} = 0\} \quad (12)$$

where  $i_p \neq j_p$  for  $p = 1, \dots, s$ . If we enumerate the reactions of  $A_k$ , we may represent any  $K$  as a set of natural numbers. We denote the set of constraint sets by  $\mathcal{K}$ .

A dynamically equivalent *constrained realization* of a CRN  $(Y, A_k)$  is a reaction network  $(Y, A'_k)$  such that  $Y A_k = Y A'_k$  and the prescribed constraints  $K$  in the form of eq. (12) are fulfilled for  $A'_k$ . A dynamically equivalent constrained dense realization of a CRN  $(Y, A_k)$  is a constrained realization that contains the maximal number of nonzero elements in  $A'_k$ . Similarly, the constrained sparse realization is a constrained realization with the minimal number of nonzero elements in  $A'_k$ .

We will say that the realizations  $A_k$  and  $A'_k$  are *structurally equivalent* if  $[A_k]_{i,j} = 0$  only if  $[A'_k]_{i,j} = 0$ .

### 3 Results

As it has been discussed in the previous section, a set of differential equations underlying a CRN may have multiple realizations, which may significantly differ in their structure. Therefore it is possible that a stability theorem may hold for only some of them. A possible approach is to derive all the realizations of the corresponding CRN to find one for which some of the proposed theorems apply.

#### 3.1 Algorithm for the effective determination of realizations

A computational algorithm for finding sparse and dense realizations of CRNs is described in [10]. As it is discussed in [12], the constrained dense realization is a super-structure [12], during the calculation of realizations, one should take into account the following considerations.

- First, if we try to compute the constrained dense realization with the constraint set  $K$ , and it turns out that no such realization exists, the same result will be straightforward for all  $K' \supset K$ .
- Let us define the *full constrained dense realization* under the constraint set  $K$  as a realization that holds all edges but the ones which correspond to the constraint set  $K$ . Our second observation is that if we try to compute the constrained dense realization with the constraint set  $K^1$ , and the resulting realization is not full (it does not hold all the allowed edges), but corresponds to a full constrained dense realization where  $K^2 \supset K^1$ . In this case if  $K^3$  is any real subset of  $K^2$ , which includes  $K^1$  the realization will not exist.

For example, let us assume that we have 6 reactions in the dense realization and are trying to calculate the dense realization with  $K^1 = \{1\}$  and the resulting constrained dense realization holds only the edges  $\{3, 5, 6\}$ . In this case  $K^2 = \{1, 2, 4\}$ . In this case neither of the realizations with  $K^3_1 = \{1, 2\}$  or  $K^3_2 = \{1, 4\}$  will exist (if they existed, the resulting

realization would not be constrained dense). Furthermore, we do not have to calculate the realization corresponding to  $K^2 = \{1, 2, 4\}$  in the following, because its already given.

According to the above two observations, it makes sense trying to compute those realizations first, in which only one edge is prohibited. If any of these possible realizations does not exist or is not full constrained, we may utilize this information in the following when calculating realizations in which more edges are excluded. We shall so avoid the computation of those realizations of which we know that they do not exist, making the algorithm computationally more efficient. We may formalize this approach as follows.

Let us define the following  $G_K$  directed graph. The nodes of  $G_K$  correspond to the constraint sets  $K$ . A directed edge from node  $i$  to node  $j$  is present if and only if  $K_i \subset K_j$ . It is easy to see that all nodes reachable from  $i$  will be reachable in one step (by the transitivity property of the subset relation).

In case the algorithm is as follows. We will use a marking of the nodes, which can be described as an indexing from the index set  $\{0, 1\}$ . First, let us assume that all nodes of  $G_K$  are unmarked. Let us assume that the dense realization of the CRN in question holds  $n$  edges, while the sparse realizations (which are not structurally unique) hold  $m$  edges. Let  $\Omega = A_k^d$ . For  $i = 1$  to  $i = n - m$  do the following.

- Consider all constraint sets, where exactly  $i$  edges are prohibited. Let us denote this set of constraint sets by  $\mathcal{K}^i$ . Let us denote an element of this set by  $K_p^i \in \mathcal{K}^i$ .
- Try to compute the corresponding constrained dense realizations for all  $K_p^i \in \mathcal{K}^i$  for which corresponding node  $v_p^i$  in  $G_K$  is unmarked one by one. As it is described in [10], this can be done for each possible realization by solving a mixed integer linear programming problem (MILP).
- If the corresponding realization ( $A_k^p$ ) exists update  $\Omega$  as  $\Omega^{new} = \Omega \cup A_k^p$
- If the resulting realization exists, however it is not full, but corresponds to the full realization of the constraint set  $K_q^j$  (corresponding to the node  $v_q^j$ , where  $j > i$ ), mark all nodes of  $G_K$  which can be found on any paths connecting  $v_p^i$  and  $v_q^j$  (including  $v_q^j$ ).
- If the corresponding realization does not exist, mark all nodes in  $G_K$  which are reachable from  $v_p^i$ .

When the algorithm is finished,  $\Omega$  will hold all the structurally different realizations of the CRN. It is easy to see, that we try to compute only those realizations, which have a chance to exist according to the previous results. Furthermore, if the actual realization does exist, it is sure, that it will be structurally different from the previous ones.

## 4 Examples

### 4.1 Example 1

Let us consider the system

$$\begin{aligned} \dot{x}_1 &= 1 + x_1x_2 - 6x_1^2 + 4x_4 \\ \dot{x}_2 &= 1 - 5x_1x_2 \\ \dot{x}_3 &= 4x_1x_2 - 3x_3^2 \\ \dot{x}_4 &= 3x_1^2 - 3x_4 \end{aligned} \quad (13)$$

In this case, the realization is unique, and it defines a weakly reversible CRN with deficiency 0, which ensures global stability of the equilibrium point  $[0.77 \ 0.26 \ 0.52 \ 0.6]$ . The structure of the realization (Network 1) is depicted in Fig. 1.

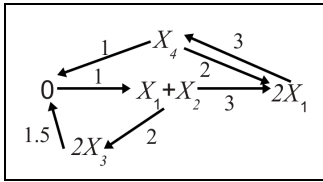


Figure 1. Weakly reversible kinetic structure of Network 1.

The matrices of the CRN description are as follows

$$Y = \begin{pmatrix} 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$A_k = \begin{pmatrix} -1 & 1.5 & 0 & 0 & 1 \\ 0 & -1.5 & 2 & 0 & 0 \\ 1 & 0 & -5 & 0 & 0 \\ 0 & 0 & 3 & -3 & 2 \\ 0 & 0 & 0 & 3 & -3 \end{pmatrix}$$

### 4.2 Example 2

Let us suppose, that the CRN depicted in Fig. 2 is given with the following matrices

$$Y = \begin{pmatrix} 1 & 1 & 2 & 0 & 1 & 1 \\ 2 & 0 & 1 & 3 & 3 & 1 \end{pmatrix}$$

$$A_k = \begin{pmatrix} -2.5 & 0 & 0 & 0 & 0 & 0 \\ 1.5 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0.5 & 0.5 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0.5 \\ 0 & 0 & 0 & 0 & 0.5 & -1 \end{pmatrix}$$

(the differential equations may be obtained by Eq. 4) The deficiency of the network is 3, and since the network is not reversible it is neither balanced, this means that none

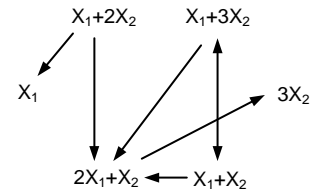


Figure 2. Network 2.

of the stability theorems itemized in 2.3 apply. If we calculate the dense and a sparse realization, we get the following matrices

$$A_k^d = \begin{pmatrix} -2.9 & 0 & 0.1 & 0 & 0.1 & 0.1 \\ 1.5 & 0 & 0.1 & 0 & 0.1 & 0.1 \\ 1.1 & 0 & -1.3 & 0 & 0.7 & 0.6 \\ 0.1 & 0 & 0.7 & 0 & 0.2 & 0.1 \\ 0.1 & 0 & 0.3 & 0 & -1.2 & 0.4 \\ 0.1 & 0 & 0.1 & 0 & 0.1 & -1.3 \end{pmatrix}$$

$$A_k^s = \begin{pmatrix} -2.5 & 0 & 0 & 0 & 0 & 0 \\ 1.5 & 0 & 0 & 0 & 0.3333 & 0 \\ 1 & 0 & -1 & 0 & 0.5 & 0.5 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.8333 & 0.5 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

In the case of the dense and this sparse realization, the deficiency is also 3 and reversibility does still not hold. On the other hand, if we calculate all realizations we can find the reversible structure depicted in Fig. 3. In this realization the complexes  $x_1$  and  $3x_2$  do not take part in any reaction, so we may describe the system with the following matrices

$$Y = \begin{pmatrix} 1 & 2 & 1 & 1 \\ 2 & 1 & 3 & 1 \end{pmatrix}$$

$$A_k = \begin{pmatrix} -4.12 & 0.06 & 0.06 & 0.06 \\ 1 & -2 & 0.5 & 0.5 \\ 0.06 & 0.97 & -1.03 & 0.47 \\ 3.06 & 0.97 & 0.47 & -1.03 \end{pmatrix}$$

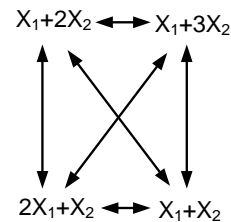


Figure 3. Network 2, reversible realization .

In this case we get that the deficiency of the system is equal to 1, and reversibility ensures the one terminal linkage class, so the deficiency one theorem applies. This means that the equilibrium  $[0.5 \ 0.41]$  will be asymptotically stable in this case.

### 4.3 Example 3

Let us consider the brusselator model discussed in [6], which is able to produce different dynamic behaviors including oscillation. The dynamical equations of the model are

$$\begin{aligned}\dot{x}_1 &= k_1^f x_2 - k_1^r x_1 - k_2^f x_1 + k_2^r - k_3^f x_1^3 + k_3^r x_1^2 x_2 \\ \dot{x}_2 &= -k_1^f x_2 + k_1^r x_1 + k_3^f x_1^3 - k_3^r x_1^2 x_2;\end{aligned}\quad (14)$$

we may easily derive the equilibrium coordinates

$$\bar{x}_1 = k_2^r / k_2^f \quad \bar{x}_2 = (k_1^r \bar{x}_1 + k_3^f \bar{x}_1^3) / (k_1^f + k_3^r \bar{x}_1^2)$$

Let us consider the following parametrization

$$k_1^f = 0.0882 \quad k_1^r = 1 \quad k_2^f = 2 \quad k_2^r = 2 \quad k_3^f = 11.3333 \quad k_3^r = 1$$

and the realization depicted in Fig. 4.

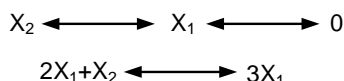


Figure 4. Network 3, brusselator - reversible realization .

$$Y = \begin{pmatrix} 0 & 1 & 0 & 3 & 2 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$A_k = \begin{pmatrix} -k_1^f & k_1^r & 0 & 0 & 0 \\ k_1^f & -k_2^f - k_1^r & k_2^r & 0 & 0 \\ 0 & k_2^f & -k_2^r & 0 & 0 \\ 0 & 0 & 0 & -k_3^f & k_3^r \\ 0 & 0 & 0 & k_3^f & -k_3^r \end{pmatrix}$$

If we compute the deficiency of the whole network and of the linkage classes, we may observe that none of the deficiency theorems hold (the overall deficiency is one, while the deficiencies of the linkage classes are 0). On the other hand it is easy to check that the conditions for balancedness hold, so the equilibrium point is asymptotically stable.

## 5 Conclusion

We have shown that the stability theorems of CRN theory may be a useful tool to analyze the stability of polynomial systems, which inhibit kinetic realizations. For the successful application of these theorems, one may need to determine all possible structurally different realizations of a given system and analyze if the set of all realizations holds one or more, for which a stability theorem applies. We proposed an algorithm for the effective determination of all possible structurally different realizations. Furthermore we demonstrated the application of various stability theorems on simple examples.

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