

# The effect of transformations on the structural dynamical properties of chemical reaction networks

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**Abstract**—The properties MAL-CRN having equal number of species and complexes (called square CRNs) are studied in this paper. It is shown that linear weakly reversible MAL-CRNs have a unique realization, therefore all of their realization properties are system properties. Moreover, these CRNs have always zero deficiency, that implies the stability of their positive steady state point within the appropriate stoichiometric compatibility class. Additionally, it is shown that weakly reversible nonlinear square MAL-CRNs have also zero deficiency and a unique realization. Furthermore, a dynamically similar stable linear ODE model can be associated to a nonlinear square CRN by using translated X-factorable phase space transformations and nonlinear variable transformations. This way it is shown, that their unique positive steady state point within the appropriate stoichiometric compatibility class is also globally asymptotically stable under mild conditions.

**Index Terms**—dynamics, stability, chemical reaction networks, transformations

## I. INTRODUCTION

Chemical reaction networks (CRNs) obeying the mass action law (MAL-CRNs) form an especially interesting class of smooth nonlinear systems with excellent descriptive power for important nonlinear phenomena such as the stability/multiplicity of equilibrium points, limit cycles or even chaos. Therefore, CRNs can be considered as a possible “prototype of nonlinear science” [1] being able to represent dynamical systems that are originated outside of chemistry [2].

In the field of chemical reaction network theory (CRNT), several strong results have been published on the relation between the network structure and the qualitative properties of the corresponding dynamics since the 1970’s [2], [3]. Among these, the Deficiency Zero and Deficiency One Theorems are of exceptional significance assuring the simple structure of equilibrium points and a robust stability property in the case of zero deficiency [4], [5]. The properties of interest for these celebrated theorems are weak reversibility that implies the boundedness of the trajectories and the existence of a positive steady-state,

and the deficiency that jointly characterizes the network structure and the complex compositions.

The above deficiency theorems are based on the directed graph structure of the studied CRN, but it is well-known that the network structure corresponding to a given kinetic dynamics is generally not unique. Therefore, an optimization approach has been proposed recently for the computation of certain dynamically equivalent network structures [6], [7]. It is also known that the dynamically equivalent realizations may have different network structure, for example, one of them may be weakly reversible and another is not. Therefore, it would be highly desirable to find such sub-classes of MAL-CRNs that possess these interesting network properties as system properties that hold for every possible dynamically equivalent realizations, if such exists.

Motivated by the above general goal, the aim of this paper is to use the dynamic properties of special linear MAL-CRNs (the ones that have a positive steady state (equilibrium) point) and similarity transformations to establish nonlinear MAL-CRN classes that are globally asymptotically stable, as well.

## II. BASIC NOTIONS

The basic notions about CRNs with mass action law and their structure are briefly summarized below.

### A. The basic structural elements

Consider a CRN that obeys the mass action law (MAL), that will be called MAL-CRN. The structure of the MAL-CRN is given in terms of its complexes  $C_i$ ,  $i = 1, \dots, m$  that are linear combinations of its species  $X_j$ ,  $j = 1, \dots, n$ , i.e.  $C_i = \sum_{j=1}^n \alpha_{ji} X_j$ . The chemical reactions  $C_i \mapsto C_j$  with the reaction rate coefficient  $k_{ij} > 0$  transform the complexes into each other with the reaction rate

$$r_{ij} = k_{ij} \varphi_i(x) = k_{ij} \prod_{l=1}^n x_l^{\alpha_{li}}.$$

We form two matrices, the complex composition matrix  $Y \in \mathbb{Z}_{+0}^{n \times m}$  with non-negative integer elements, the columns of which describe the composition of the

complexes, and the Kirchhoff matrix  $A_k \in \mathbb{R}^{m \times m}$ , that describes the structure of chemical reactions for the description such that

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

### B. The structure of a MAL-CRN: the reaction graph

The vertexes  $\mathbf{V}$  of the *reaction graph*  $G = (\mathbf{V}, \mathbf{E})$  correspond to the complexes, and the edges  $\mathbf{E}$  to the reactions. Two complexes  $C_k$  and  $C_l$  are connected by a directed edge  $(C_k, C_l)$ , if a reaction in the form of  $C_k \mapsto C_l$  exists. Edge weights can be associated to the edges that are the reaction rate constants  $k_{kl} > 0$ , thus the reaction graph is a weighted directed graph.

Note that the Kirchhoff matrix  $A_k$  of a CRN uniquely determines its reaction graph and vice versa. However, the Kirchhoff matrix of the reaction graph does not uniquely determine the reaction kinetic system itself, since the information on the composition of the complexes is missing from the graph: it is contained in the complex composition matrix  $Y$ .

The reaction graph  $G$  without its edge weights (i.e. the values of the reaction rate coefficients) describes the *structure of a MAL-CRN*.

The connected components in the reaction graph are called *linkage classes*, their number is denoted by  $\ell \geq 1$ .

*Basic assumptions:* In this paper the MAL-CRNs obeying the following basic assumptions are considered.

- G1. There is no isolated (i.e. unconnected) complex in the CRN.
- G2. The relation  $m \geq n$  is assumed.
- G3.  $Y$  is of full rank.

### C. Weak reversibility and deficiency

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  $C_i$ . In graph theoretic terms, this means that all components of the reaction graph are strongly connected components. We shall use the fact known from the literature that a CRN is weakly reversible if and only if there exists a vector with strictly positive elements in the kernel of  $A_k$ , i.e. there exists  $b \in \mathbb{R}_+^n$  such that  $A_k \cdot b = 0$  [8].

The notion of the *deficiency* of a CRN is built on the set of *reaction vectors* that are defined as:  $\mathcal{R} = \{\rho^{(l,k)} = \eta^{(l)} - \eta^{(k)} \mid (C_k, C_l) \in \mathbf{E} \text{ in } G\}$ , where  $\eta^{(i)}$  denotes the  $i$ th column of  $Y$ . Then, the deficiency  $\delta$  of a CRN is an integer number that is usually defined as:

$$\delta = m - \ell - s \quad (2)$$

where  $m$  is the number of complexes and  $\ell$  is the number of connected components in the reaction graph, while  $s$  is the dimension of the stoichiometric sub-space, i.e.  $s = \text{rank}(\mathcal{R})$ .

The *Deficiency Zero Theorem* [4] 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 [9], it is straightforward to asymptotically stabilize them by additional feedback [10], and it is possible to construct efficient state observers for them [11].

### D. The ODE form and its transformations

With the above matrices the time evolution of the specie concentrations  $x = [x_1, \dots, x_n]^T$  is described by the following set of ODEs:

$$\frac{dx}{dt} = Y A_k \varphi(x) = M \varphi(x) \quad , \quad \varphi_i(x) = \prod_{j=1}^n x_j^{Y_{ji}} \quad (3)$$

where  $M = Y A_k$  is a constant matrix. The vector  $x$  belongs to the state or phase space  $\mathcal{X} \subseteq \mathbb{R}_+^n$ , i.e.  $x \in \mathcal{X}$ .

The *stoichiometric vector space* is the space denoted by  $\mathcal{S}$  is spanned by the reaction vectors, i.e.  $\mathcal{S} = \text{span}\{\mathcal{R}\}$ . The positive *stoichiometric compatibility class* containing a state  $x_0$  is a translated linear manifold defined as:

$$(x_0 + \mathcal{S}) \cap \mathbb{R}_+^n, \quad (4)$$

where  $\mathbb{R}_+^n$  denotes the positive orthant in  $\mathbb{R}^n$ .

A polynomial dynamical system is called *kinetic*, if it can be written in the form (3). A necessary and sufficient condition for the kinetic property was first given in [12]. According to this result, a set of polynomial ODEs of the form  $\dot{x} = f(x)$ , where  $x \in \mathbb{R}^n$ , is kinetic if and only if all coordinates functions of  $f$  can be written in the form

$$f_i(x) = -x_i g_i(x) + h_i(x), \quad i = 1, \dots, n \quad (5)$$

where  $g_i$  and  $h_i$  are polynomials with nonnegative coefficients. Naturally, the kinetic property guarantees that the nonnegative orthant is invariant for the dynamics (3), i.e. kinetic systems are *nonnegative systems* [13].

Let us associate monomial-variables  $q \in \mathbb{R}_+^m$  to the above equation such that  $q_i(x) = \varphi_i(x)$ . (For simplicity, most often we will suppress the  $x$  argument in  $q_i$ .) The monomial space  $\mathcal{Q} \subseteq \mathbb{R}_+^m$  is composed of the monomial variables  $q$ .

The variable transformation

$$\underline{\ln} q = Y^T \cdot \underline{\ln} x \quad (6)$$

shows the nonlinear dependence  $q(x)$ , where the  $\underline{\ln}$  operator applies the natural logarithm function element-wise to a positive vector. This variable transformation defines a mapping  $\mathbf{Y}$  from  $\mathcal{X}$  to  $\mathcal{Q}$  that is *an injective* (but not necessarily surjective and thus invertible) *phase space transformation* because of the full rank property of the matrix  $Y$  and the inequality  $m \geq n$ .

1) *Dynamical equivalence*: Let us consider two MAL-CRN models with the same coefficient matrix  $M$  and complex composition matrix  $Y$  but with different Kirchhoff matrices  $A_k$  and  $A'_k$ . The two so-called realizations  $(Y, A_k)$  and  $(Y, A'_k)$  are called dynamically equivalent, if they give rise to the same ODE model (3), i.e.  $YA_k = YA'_k$ . A realization  $(Y, A_k)$  is *unique*, if there is no other, different dynamically equivalent realization to the ODE (3).

2) *Nonlinear translated  $X$ -factorable transformation*: Assume that the following set of ordinary differential equations

$$\frac{dX}{dt} = \mathbf{F}(X) \quad (7)$$

is defined on the positive orthant  $\mathbb{R}_+^n$ . The steady state solutions of Eq. (7) are defined by  $\mathbf{F}(X) = 0$ . Consider the following *nonlinear translated  $X$ -factorable phase (or state) space transformation* of Eq. (7)

$$\frac{dX}{dt} = \hat{\mathbf{F}}(X) = \text{diag}(X_1, \dots, X_n)\mathbf{F}(X - C) \quad (8)$$

where the elements of  $C = [c_1, \dots, c_n]^T$  are positive real numbers, and  $X = [X_1, \dots, X_n]^T$ .

The original motivation of the application of the transformation (8) in [14] was to represent non-positive dynamical systems as kinetic systems. Clearly, the translation parameterized by  $C$  can be chosen such that the equilibrium points (or operating domain) of interest are moved to the strictly positive orthant, while the multiplication by  $\text{diag}(X)$  ensures the nonnegativity and the so-called geometrical separability of the transformed system. Moreover, it is easy to see that models of the form (8) are always kinetic, since they trivially fulfil the condition (5). It is shown in [14] that due to the transformation (8), a substantial compression of trajectories occurs close to the boundary of the positive orthant, however, this distortion is weak or negligible for trajectories far from the boundaries. Therefore, the dynamics of the solutions of Eqs. (7) and (8) will be called *dynamically similar*.

3) *Linear diagonal (LD) transformation*: It is known that under a positive diagonal state transformation, the kinetic property of a model (3) is preserved [15], [16]. Consider a positive diagonal matrix  $T = \text{diag}(c)$ , where  $c \in \mathbb{R}_+^n$  is an element-wise positive vector. Then one can transform eq. (3) that brings the MAL-CRN model  $(Y, A_k)$  to another MAL-CRN model  $(Y, A'_k)$  with (i.e. this transformation does not lead out of the MAL-CRN model class) [17] such that

$$YA_k = TYA'_k(\text{diag}(\varphi(c)))^{-1} \quad (9)$$

It is important to note that the LD transformation is an invertible variable transformation. Therefore, the qualitative properties of the dynamics of the original and the transformed system (e.g. number and stability of equilibria, boundedness of solutions, existence of limit cycles, chaotic behavior etc.) are identical.

### III. LINEAR MAL-CRNS

Assume that every reaction in the MAL-CRN system is linear, i.e.  $\varphi_i(x) = x_i$ . This case forms the simplest class of MAL-CRNs, with interesting structural dynamic properties that are easy to investigate.

#### A. Basic structural properties

The basic structural elements of linear MAL-CRNs are in the following special form.

- The complexes are the species, i.e.  $n = m$  and  $C_i = X_i$ . Therefore the complex composition matrix is the unit matrix, i.e.  $Y = I$ , and the state variable vector  $x$  is identical to the monomial variable vector  $q$ , i.e.  $x = q$ .
- The ODE model in Eq. (3) that describes the dynamics in the phase space  $\mathcal{X}$  specializes to

$$\frac{dx}{dt} = A_k x \quad (10)$$

that is a linear ODE with constant coefficients that are collected in the Kirchhoff matrix  $A_k$ . The *dynamics in the monomial space  $\mathcal{Q}$*  is identical to the one in Eq. (10).

It is very easy to see that the *realization*  $(Y = I, A_k)$  of a linear MAL-CRN is *unique*, since  $Y \cdot A_k = Y \cdot A'_k$  trivially implies  $A_k = A'_k$  in this case.

Moreover, in the case of a linear diagonal transformation described above,  $A_k = TA'_k(\text{diag}(\psi c))^{-1}$ . Therefore,  $A_k$  and  $A'_k$  encode the same reaction graph structure (only the edge weights are scaled), which means that the (unweighted) reaction graph structure and its dynamical consequences are *system properties* in the linear MAL case.

#### B. Properties related to weak reversibility

The zero column-sums within the Kirchhoff property of  $A_k$  (see in Eq. (1)) can be expressed as

$$\underline{\mathbf{1}}A_k = \underline{\mathbf{0}}$$

where  $\underline{\mathbf{1}} = [1, 1, \dots, 1]$  and  $\underline{\mathbf{0}} = [0, 0, \dots, 0]$  [18], that shows the rank-deficient nature of  $A_k$ , i.e.  $\text{rank}(A_k) \leq m - 1$ .

It is well-known from the literature that a CRN is weakly reversible if and only if there is a strictly (elementwise) positive vector  $q^*$  in the kernel of  $A_k$ . Then, the intersection of this kernel and the positive orthant contains (infinitely many) positive equilibrium points for the dynamics (10). It is important to remark that the stoichiometric compatibility class (4) can be fixed by selecting the equilibrium point  $x^* = q^*$ .

It is also known that in the weakly reversible case  $\text{rank}(A_k) = m - \ell$ , where  $\ell$  is the number of linkage classes.

Additionally, it is easy to see that *weakly reversible linear CRNs have always zero deficiency*: since the columns of  $Y$  are the standard basis vectors of  $\mathbb{R}^n$ , the rank of the reaction vectors in any strongly connected component of the reaction graph containing  $m_k$  complexes is exactly  $m_k - 1$  (that is equal to the number of the edges in the

spanning tree corresponding to the connected component). Therefore, the rank of the stoichiometric space with  $\ell$  strongly connected components is  $s = m - \ell$  resulting in zero deficiency.

### C. Stability and Lyapunov functions

To show the stability of weakly reversible linear CRN models, we use results from the theory of nonnegative and compartmental systems using mainly Chapter 2 of [19]. The review paper [20] is also devoted to the qualitative analysis of compartmental systems.

An  $n \times n$  matrix  $F$  is called a compartmental matrix if it satisfies the following conditions

- 1)  $F_{ij} \geq 0$ , for  $i, j = 1, \dots, n$ ,  $i \neq j$
- 2)  $\sum_{i=1}^n F_{ij} \leq 0$ , for  $j = 1, \dots, n$

Clearly, the Kirchhoff matrix is a compartmental matrix and thus a special type of Metzler matrix. We will use the following properties of compartmental matrices. Consider a compartmental matrix  $F$

- P1 The eigenvalues of  $F$  are either zero, or they have negative real parts. (In other words, compartmental matrices cannot have unstable or purely imaginary eigenvalues.)
- P2 If  $F$  is the Kirchhoff matrix of a weakly reversible CRN, then the number of zero eigenvalues of  $F$  is equal to the number of linkage classes (i.e. to the number of connected components of the reaction graph).
- P3 If zero is an eigenvalue of  $F$  with algebraic multiplicity  $\kappa$ , then its geometric multiplicity is also  $\kappa$  (i.e. the eigenvectors corresponding to zero eigenvalues are always linearly independent).

1) *The quadratic Lyapunov function:* It follows from the theory of linear time-invariant systems and P1 – P3 that weakly reversible linear CRNs of the form (10) are globally stable with a quadratic Lyapunov function. Of course, the stability cannot be asymptotic, since weak reversibility guarantees that the intersection of the positive orthant and the kernel of  $A_k$  is non-empty (i.e. there exist infinitely many equilibrium points in the positive orthant). Therefore, we can use the following quadratic Lyapunov function:  $V_2(x) = (x - x^*)^T P (x - x^*)$  with an appropriate positive definite symmetric  $P$ . Taking the derivative of  $V_2$  along the solution of (10), we obtain the classical non-strict Lyapunov inequality as the stability condition:

$$A_k^T P + P A_k \preceq 0, \quad (11)$$

where ‘ $\preceq 0$ ’ means negative semi-definiteness.

A nice property of stable Metzler matrices (and therefore of Kirchhoff matrices) is that they are diagonally stable, i.e. there exists a positive definite diagonal  $P$  that satisfies (11) [21].

2) *The logarithmic Lyapunov function:* The zero deficiency property of weakly reversible linear CRNs implies that the logarithmic Lyapunov function (12) proposed e.g. in [22] can also be used for proving the stability of such CRNs. It is important to remark that the stability of any equilibrium point  $x^*$  is asymptotic if we restrict the dynamics to the corresponding stoichiometric compatibility class.

[23] lists various entropy-motivated Lyapunov functions for linear systems with positive equilibrium points, that include the above quadratic one with  $P^*$  and the logarithmic one in the form

$$V_{\ln}(x) = - \sum_{i=1}^n x_i^* \ln \left( \frac{x_i}{x_i^*} \right). \quad (12)$$

## IV. NONLINEAR SQUARE MAL-CRNS

Inspired by the simple and advantageous dynamic properties of weakly reversible linear MAL-CRNs, we generalize these results for certain nonlinear CRNs using variable and phase space transformations such that these transformations ensure invertibility and dynamic similarity, as well. For this we assume that the MAL-CRN system described by the dynamics (3) has the same number of species and complexes, i.e.  $m = n$  holds. Such nonlinear MAL-CRNs will be called *square MAL-CRNs*.

### A. Realizations, weak reversibility and deficiency

There is a strong similarity between linear MAL-CRNs and square MAL-CRNs because of the equal dimension of their phase and monomial spaces  $m = n$ , and the *invertible* property of the *complex composition matrix*  $Y \in \mathbb{Z}_{0+}^{n \times n}$ .

This implies that *square MAL-CRNs have a unique realization*, since the equation  $M = Y A_k$  has a unique solution for  $A_k$  if  $M$  and an invertible  $Y$  are given. Therefore, all realization properties (e.g. weak reversibility, deficiency) are system properties in this case, too.

1) *Deficiency:* Because of the full rank property of  $Y$ , its columns form a basis in  $\mathbb{R}^n$ , similarly to the linear MAL-CRN case. Therefore, we can repeat the arguments in subsection III-C to show that weakly reversible square MAL-CRNs have zero deficiency. This implies that within each stoichiometric compatibility class, there exists a unique and asymptotically stable equilibrium point  $x^*$ .

### B. Dynamics in the state space and in the monomial space

Let us *fix the structure graph* of the square MAL-CRNs, and assume that we have a given Kirchhoff matrix  $A_k$  that admits a *weakly reversible* realization. Now we investigate the effect of a nonlinear but invertible mapping  $\mathbf{Y} : \mathcal{X} \mapsto \mathcal{X}$  generated by the matrix  $Y$  in Eq. (6) on the linear and globally asymptotically stable dynamics (10).

The nonlinear dynamics is described in the state space with Eq. (3), that we now write in the form

$$\frac{dx}{dt} = Y A_k q = M q \quad (13)$$

Using the fact that  $m = n$ , we have a nonlinear invertible transformation between the state ( $x$ ) and monomial ( $q$ ) variables in Eq. (6) Because of the weak reversibility assumption *the nonlinear MAL-CRN system has a positive equilibrium point  $x^*$  in the state space*, that can be transformed into a positive equilibrium point  $q^*$  in the monomial space.

In order to establish a dynamically similar linear system to the nonlinear dynamics (13), first we apply the nonlinear X-factorable phase space transformation (8) to obtain a dynamically similar form

$$\frac{dx}{dt} = \text{diag}(x_1, \dots, x_n)Mq \quad \text{or} \quad \frac{d \ln x}{dt} = Mq \quad (14)$$

Multiplying both sides by  $Y^T$  we can apply the variable transformation (6) to form the transformed

$$\frac{d \ln q}{dt} = Y^T M q \quad (15)$$

Finally, the inverse of the nonlinear X-factorable transformation is applied to obtain the dynamically similar linear dynamics

$$\frac{dq}{dt} = Y^T M q = (Y^T Y) A_k q \quad (16)$$

It is important to note that the above transformation sequence contains invertible steps in the case of square nonlinear CRNs, thus establishing a *one-to-one relationship* between the original nonlinear dynamics (13) and its linear counterpart (16), that are *dynamically similar*.

The coefficient matrix  $\bar{M} = (Y^T Y) A_k$  in the linear dynamics (16) has the following properties.

- $\bar{M}$  is generally not a Kirchhoff matrix, so (16) does not correspond in general to a linear MAL-CRN.
- The first factor  $Y^T Y$  is a positive definite symmetric matrix with nonnegative integer elements.
- The second factor  $A_k$  is a Kirchhoff matrix obeying eq. (11) for some diagonal  $P$ , therefore it is a diagonally semistable matrix [21].

### C. Stability

As we have seen before in subsection IV-A1, weakly reversible square MAL-CRNs have always deficiency zero. Therefore, the asymptotic stability of the unique equilibrium point of weakly reversible square MAL-CRNs (of course, within the appropriate stoichiometric compatibility class) follows from the Deficiency Zero Theorem [4].

*Stability of the dynamically similar linear ODE:* Since  $Y^T Y$  is a positive definite symmetric matrix and  $A_k$  is a diagonally semistable Metzler matrix, it is clear that  $\ker(A_k) = \ker(\bar{M})$ . Therefore,  $\bar{M}$  has as many zero eigenvalues as  $A_k$  has. Thus, if the rest of the eigenvalues of  $\bar{M}$  is negative, then the dynamics (16) will be stable.

### D. A simple example

Consider the simple nonlinear square CRN encoding a weakly reversible triangle structure with the following parameters

$$Y = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix}, \quad A_k = \begin{bmatrix} -k_{12} & 0 & k_{31} \\ k_{12} & -k_{23} & 0 \\ 0 & k_{23} & -k_{31} \end{bmatrix} \quad (17)$$

First, we examine the diagonal stability of  $A_k$ . Let us choose  $P$  in (11) as follows:

$$P = \text{diag}([k_{12} \ k_{23} \ k_{31}]^T) \quad (18)$$

Then

$$W := A_k^T P + P A_k = \begin{bmatrix} -2k_{12}^2 & k_{12}k_{23} & k_{12}k_{31} \\ k_{12}k_{23} & -2k_{23}^2 & k_{23}k_{31} \\ k_{12}k_{31} & k_{23}k_{31} & -2k_{31}^2 \end{bmatrix} \quad (19)$$

The minors of  $W$  denoted by  $m_1, \dots, m_3$  are:

$$m_1 = -2k_{12}^2, \quad m_2 = 3k_{12}^2 k_{23}^2, \quad m_3 = 0 \quad (20)$$

Therefore,  $W$  is negative semidefinite considering that the rate coefficients  $k_{ij}$  are always positive.

Let us use the following values for the rate coefficients:  $k_{12} = 1$ ,  $k_{23} = 3$ ,  $k_{31} = 2$ . The trajectories of the system characterized by (17) from different initial conditions belonging to the same stoichiometric compatibility class containing the equilibrium point  $x^* = [1.5000 \ 1.1855 \ 0.6290]^T$  are shown in Fig. 1. Moreover, the coefficient matrix  $\bar{M}$  of

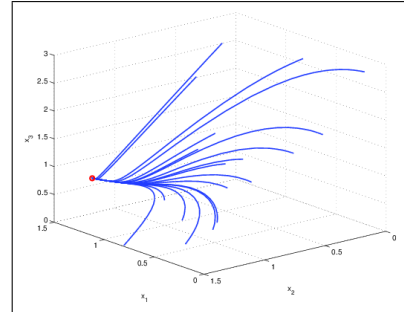


Figure 1. Solutions of the kinetic system characterized by  $Y$  and  $A_k$  in Eq. (17).

the monomial dynamics is given by

$$(Y^T Y) A_k = \begin{bmatrix} -2 & 3 & 2 \\ 3 & 3 & -8 \\ 3 & 6 & -10 \end{bmatrix} \quad (21)$$

the eigenvalues of which are  $\lambda_1 = -6.3028$ ,  $\lambda_2 = 0$  and  $\lambda_3 = -2.6972$  showing that the linear dynamics (16) is indeed stable.

## V. CONCLUSIONS

First the uniqueness of the realizations of a linear weakly reversible MAL-CRNs were shown together with their zero deficiency property. This implies the asymptotic stability of their unique positive steady state point. As they have a

single unique realization, all of their realization properties are system properties.

Based on the definition of square MAL-CRNs with square invertible complex composition matrix  $Y$  it is shown that weakly reversible square MAL-CRNs have also zero deficiency and a unique realization. Moreover, dynamically similar stable linear ODE model has been associated to them by using translated X-factorable transformations and nonlinear variable transformations. This way it is shown that the unique (within the appropriate compatibility class) steady-state point of weakly reversible nonlinear square MAL-CRNs is asymptotically stable.

Further work will be focused on conditions of the applicability of the dynamically similar linear dynamics when  $m > n$ .

#### ACKNOWLEDGEMENTS

This research has been supported by the Hungarian National Research Fund through grants NF104706 and K83440.

#### REFERENCES

- [1] P. rdi and J. Tth, *Mathematical Models of Chemical Reactions. Theory and Applications of Deterministic and Stochastic Models*. Manchester, Princeton: Manchester University Press, Princeton University Press, 1989.
- [2] V. Chellaboina, S. P. Bhat, W. M. Haddad, and D. S. Bernstein, "Modeling and analysis of mass-action kinetics – nonnegativity, realizability, reducibility, and semistability," *IEEE Control Systems Magazine*, vol. 29, pp. 60–78, 2009.
- [3] D. Angeli, "A tutorial on chemical network dynamics," *European Journal of Control*, vol. 15, pp. 398–406, 2009.
- [4] M. Feinberg, "Chemical reaction network structure and the stability of complex isothermal reactors - I. The deficiency zero and deficiency one theorems," *Chemical Engineering Science*, vol. 42 (10), pp. 2229–2268, 1987.
- [5] —, "Necessary and sufficient conditions for detailed balancing in mass action systems of arbitrary complexity," *Chemical Engineering Science*, vol. 44, pp. 1819–1827, 1989.
- [6] G. Szederkenyi, "Computing sparse and dense realizations of reaction kinetic systems," *Journal of Mathematical Chemistry*, vol. 47, pp. 551–568, 2010.
- [7] G. Szederkenyi, K. M. Hangos, and T. Peni, "Maximal and minimal realizations of reaction kinetic systems: Computation and properties," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 65, no. 2, pp. 309–332, 2011.
- [8] M. Feinberg and F. Horn, "Chemical mechanism structure and the coincidence of the stoichiometric and kinetic subspaces," *Archive for Rational Mechanics and Analysis*, vol. 66, no. 1, pp. 83–97, 1977. [Online]. Available: <http://dx.doi.org/10.1007/BF00250853>
- [9] M. Chaves, "Input-to-state stability of rate-controlled biochemical networks," *SIAM Journal on Control and Optimization*, vol. 44, pp. 704–727, 2005.
- [10] E. Sontag, "Structure and stability of certain chemical networks and applications to the kinetic proofreading model of T-cell receptor signal transduction," *IEEE Transactions on Automatic Control*, vol. 46, pp. 1028–1047, 2001.
- [11] M. Chaves and E. D. Sontag, "State-estimators for chemical reaction networks of Feinberg-Horn-Jackson zero deficiency type," *European Journal of Control*, vol. 8, pp. 343–359, 2002.
- [12] V. Hars and J. Tth, "On the inverse problem of reaction kinetics," in *Qualitative Theory of Differential Equations*, ser. Coll. Math. Soc. J. Bolyai, M. Farkas and L. Hatvani, Eds. North-Holland, Amsterdam, 1981, vol. 30, pp. 363–379.
- [13] W. M. Haddad, V. Chellaboina, and Q. Hui, *Nonnegative and Compartmental Dynamical Systems*. Princeton University Press, 2010.
- [14] N. Samardzija, L. D. Greller, and E. Wassermann, "Nonlinear chemical kinetic schemes derived from mechanical and electrical dynamical systems," *Journal of Chemical Physics*, vol. 90 (4), pp. 2296–2304, 1989.
- [15] G. Farkas, "Kinetic lumping schemes," *Chemical Engineering Science*, vol. 54, pp. 3909–3915, 1999.
- [16] M. D. Johnston and D. Siegel, "Linear conjugacy of chemical reaction networks," *Journal of Mathematical Chemistry*, vol. 49, pp. 1263–1282, 2011.
- [17] M. D. Johnston, D. Siegel, and G. Szederkenyi, "Computing weakly reversible linearly conjugate chemical reaction networks with minimal deficiency," *Mathematical Biosciences*, vol. 241, pp. 88–98, 2013.
- [18] K. Hangos and G. Szederkenyi, "The effect of conservation on the dynamics of chemical reaction networks," in *IFAC Workshop on Thermodynamic Foundations of Mathematical Systems Theory, July 13-16, Lyon, France*, 2013.
- [19] J. M. van den Hof, "System theory and system identification of compartmental systems," Ph.D. dissertation, University of Groningen, 1996.
- [20] J. Jacquez and C. Simon, "Qualitative theory of compartmental systems," *SIAM Review*, vol. 35, no. 1, pp. 43–79, 1993.
- [21] E. Kaszkurewicz and A. Bhaya, *Matrix Diagonal Stability in Systems and Computation*. Boston: Birkhauser, 2000.
- [22] F. Horn and R. Jackson, "General mass action kinetics," *Archive for Rational Mechanics and Analysis*, vol. 47, pp. 81–116, 1972.
- [23] A. Gorban, P. Gorban, and G. Judge, "Entropy: The markov ordering approach," *Entropy*, vol. 12, pp. 1145–1193, 2010.
- [24] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis*. Cambridge University Press, 1991.
- [25] A. Berman and R. J. Plemmons, *Nonnegative matrices in the mathematical sciences*. SIAM, 1994.