Notes on the Deficiency One Theorem: single linkage class

Balázs Boros

***Abstract*— The Deficiency One Theorem tells us about certain chemical reaction systems that they cannot admit multiple interior equilibria. The theorem was proven by Feinberg. In this paper we provide a relatively short proof of that theorem for the special case of one linkage class. We also extend that result by giving an equivalent condition to the fact that the set of interior equilibria is nonempty for a chemical reaction system with one linkage class considered in the Deficiency One Theorem.**

I. INTRODUCTION

The foundations of Chemical Reaction Network Theory (CRNT) was developed by Feinberg, Horn, and Jackson [4], [5], [6], [7], [8], [9], [10]. CRNT enables us to examine mathematical models of chemical reaction systems and to derive general theorems about the qualitative properties of such systems. In this paper, we revisit the Deficiency One Theorem, which was proven by Feinberg [6], [7]. Throughout the paper, we deal only with the special case when the network has only one linkage class (the notion linkage class is defined in II-F). The theorem examines the set of interior equilibria for a certain class of chemical reaction systems. It gives a description of the structure of the set of interior equilibria provided that it is nonempty. Also, a condition is given, which guarantees that the set of interior equilibria is nonempty. We formulate the Deficiency One Theorem at the beginning of Section III. It turns out that the provided alternative proof can appropriately be modified in order to be able to examine the non-emptiness of the interior equilibria for all the systems with one linkage class in the Deficiency One Theorem. We mention that the recent work [3] also addresses (among other things) the problem of the existence of interior equilibria for chemical reaction systems. Their method (which is based on a basic theorem of degree theory) does not rely on the deficiency of the network.

The rest of this paper is organised as follows. In Section II, we provide a brief introduction to CRNT. In order to make this introduction easier we also provide some preliminaries from the theory of directed graphs. In Section III, we first state the Deficiency One Theorem and then we go through on several steps, which leads us to the proof of it. Theorem III.7 is the main result of this paper. It can be regarded as a supplement to the Deficiency One Theorem. We collected some well known basic notations and facts from linear algebra in Appendix A.

II. PRELIMINARIES

After a short subsection on standard notations, we give a brief introduction to CRNT in Subsection II-B. The exposition is based on the above mentioned papers of Feinberg, Horn, and Jackson. In order to make this paper self-contained, we collect some well known terminology and concepts from graph theory in Subsections II-C, II-D, and II-E. Having in hand the knowledge of the preceding subsections, we revisit the chemical reaction systems in Subsection II-F in order to introduce more notations and terminology from CRNT. In Subsection II-G, we associate a nonnegative number, called the deficiency, to a chemical reaction network, which will then play an important role in Section III.

B. Boros is with the Institute of Mathematics, Eötvös Loránd University, Budapest, Hungary bboros@cs.elte.hu

A. Notations

Denote by $\mathbb{R}$ and $\mathbb{Z}$ the set of real and integer numbers, respectively. If $p, q \in \mathbb{Z}$ then let $\overline{p,q} = \{k \in \mathbb{Z} \mid p \leq k \leq q\}$. The function $\operatorname{sgn} : \mathbb{R} \to \{-1, 0, 1\}$ is the sign function (i.e., $\operatorname{sgn}(x) = 1$ for $x > 0$, $\operatorname{sgn}(x) = -1$ for $x < 0$, and $\operatorname{sgn}(0) = 0$). If A is any finite set then $|A|$ denotes the number of elements of A.

We denote by $\mathbb{R}_+, \mathbb{R}_{\geq 0}$, and $\mathbb{R}_-$ the sets of positive, nonnegative, and negative real numbers, respectively, i.e., $\mathbb{R}_+ = \{x \in \mathbb{R} \mid x > 0\}, \mathbb{R}_{\geq 0} = \{x \in \mathbb{R} \mid x \geq 0\}$, and $\mathbb{R}_- = \{x \in \mathbb{R} \mid x < 0\}$. The sets $\mathbb{Z}_+$ and $\mathbb{Z}_{\geq 0}$ are defined similarly. If $p \in \mathbb{Z}_+$ then $\mathbb{R}^p_+, \mathbb{R}^p_{\geq 0}$, and $\mathbb{R}^p_-$ are called the *positive*, *nonnegative*, and *negative orthants* of $\mathbb{R}^p$, respectively. If $v \in \mathbb{R}^p$ then v_i denotes the ith coordinate of v ($i \in \overline{1,p}$). If $A \in \mathbb{R}^{p \times q}$ then $A_{\cdot j}$ and A_{ij} denote the jth column and the (i,j)th element of A ($i \in \overline{1,p}, j \in \overline{1,q}$), respectively.

B. Chemical reaction networks and systems

Consider a nonempty finite set of *chemical species*, denoted by $\mathcal{A}$. Let $n = |\mathcal{A}|$. The chemical species are then denoted by the symbols $A_1, A_2, \ldots, A_n$.

A *chemical complex* consists of species. More precisely, one can specify a complex by associating nonnegative integer numbers to each species. Those numbers are then called the *stoichiometric coefficients*. In other words, a complex can be specified by an n-tuple $[p_1, p_2, \ldots, p_n]^T \in \mathbb{Z}^n_{\geq 0}$. One can then refer to a complex as $p_1 A_1 + p_2 A_2 + \cdots + p_n A_n$. The set of complexes is denoted by $\mathcal{C}$, which is assumed to be a nonempty finite set. Let $c = |\mathcal{C}|$. The complexes are then denoted by the symbols $C_1, C_2, \ldots, C_c$. We will use the notations $\mathcal{C} = \{C_1, C_2, \ldots, C_c\}$ and $\overline{1,c} = \{1, 2, \ldots, c\}$ interchangeably. Accordingly, the notations $i \in \mathcal{C}$ and $C_i \in \mathcal{C}$ mean the same ($i \in \overline{1,c}$).

To define chemical reaction networks, another object is needed. If complex C_i can react to become complex C_j then the ordered pair (C_i, C_j) is called a *reaction* ($i, j \in \overline{1,c}$). If

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(C_i, C_j) is a reaction for some $i, j \in \overline{1,c}$ then we say that C_i is the *reactant complex* and C_j is the *product complex* of the reaction. The set of reactions is denoted by $\mathcal{R}$ and is assumed to be nonempty. Let $m = |\mathcal{R}|$. We mostly write $(i,j) \in \mathcal{R}$ instead of $(C_i, C_j) \in \mathcal{R}$ $(i, j \in \overline{1,c})$.

We are now in the position to define what we mean by a chemical reaction network.

Definition II.1 A chemical reaction network *is a triple* $(\mathcal{A}, \mathcal{C}, \mathcal{R})$ *of three nonempty finite sets, where* $\mathcal{A}$ *is the set of chemical species,* $\mathcal{C}$ *is the set of chemical complexes, and* $\mathcal{R}$ *is the set of reactions as described above.*

A convenient way to specify the set of complexes is to provide an $n \times c$ matrix whose entries are nonnegative integers, the rows refer to the species, and the columns refer to the complexes. Denote this matrix by $B \in \mathbb{Z}_{\geq 0}^{n \times c}$ and call it the *matrix of complexes*. Using the introduced terminology, B_{si} is then the stoichiometric coefficient of the species A_s in complex C_i $(s \in \overline{1,n}, i \in \overline{1,c})$.

It was not discussed yet how exactly the complexes become other complexes as time passes. In other words, the dynamic evolution was not yet investigated. Consider a chemical reaction network $(\mathcal{A}, \mathcal{C}, \mathcal{R})$. Let us represent by the vector $x(\tau) \in \mathbb{R}_{\geq 0}^n$ the *concentrations* of the species at time τ. The sth coordinate of $x(\tau)$, $x_s(\tau)$, represents the concentration of the species A_s at time τ $(s \in \overline{1,n})$. A continuous-time deterministic model will be considered, where the species concentrations are changing in accordance with an ordinary differential equation.

For $(i,j) \in \mathcal{R}$ let us define the function $R_{(i,j)} : \mathbb{R}^n \to \mathbb{R}_{\geq 0}$ by

$$R_{(i,j)}(x) = \kappa_{(i,j)} \prod_{s=1}^{n} |x_s|^{B_{si}} \quad (x \in \mathbb{R}^n), \tag{1}$$

where $\kappa_{(i,j)}$ is a given positive real number, which is called the *rate constant* of reaction (i,j). The function $R_{(i,j)}$ is called the *rate function* of reaction $(i,j) \in \mathcal{R}$.

Let us define the function $R : \mathbb{R}^n \to \mathbb{R}_{\geq 0}^m$ by

$$R(x) = \begin{bmatrix} \vdots \\ R_{(i,j)}(x) \\ \vdots \end{bmatrix}_{(i,j)\in\mathcal{R}} \qquad (x \in \mathbb{R}^n). \tag{2}$$

Definition II.2 *The quadruple* $(\mathcal{A}, \mathcal{C}, \mathcal{R}, R)$ *is called a* chemical reaction system *if* $(\mathcal{A}, \mathcal{C}, \mathcal{R})$ *is a chemical reaction network and* $R : \mathbb{R}^n \to \mathbb{R}_{\geq 0}^m$ *is defined by (1) and (2).*

In case the rate functions are defined by (1), the corresponding chemical reaction system is called a *mass action system*. We will use this terminology in the sequel.

After this preparation, we introduce the autonomous ordinary differential equation that describes the dynamic evolution of the system. Consider the differential equation

$$\dot{x}(\tau) = \sum_{(i,j)\in\mathcal{R}} R_{(i,j)}(x(\tau)) \cdot (B_{\cdot j} - B_{\cdot i}) \tag{3}$$

with state space $\mathbb{R}^n$. Let us define the function $f : \mathbb{R}^n \to \mathbb{R}^n$ by

$$f(x) = \sum_{(i,j)\in\mathcal{R}} R_{(i,j)}(x) \cdot (B_{\cdot j} - B_{\cdot i}) \quad (x \in \mathbb{R}^n). \tag{4}$$

With this definition, (3) can be written in the form $\dot{x}(\tau) = f(x(\tau))$. Note that f is locally Lipschitz continuous and therefore (3) has a unique solution on a maximal open interval for all initial values. As (3) describes the evolution of species concentrations, we are interested in solutions with initial values in the nonnegative orthant. We remark that both the nonnegative orthant ($\mathbb{R}_{\geq 0}^n$) and the positive orthant ($\mathbb{R}_{+}^n$) are forward invariant for (3). Proof of this fact can be found e.g. in [1], [12], [13]. This means that the mathematical model of a chemical reaction system satisfies the qualitative property that no species concentration can become negative.

C. Weak and strong components of directed graphs

In this subsection, we collect some standard terminology from graph theory. Directed graphs in this paper are always assumed to be finite and without multiple arcs. General reference on graph theory is [11].

Definition II.3 *Let* (V, A) *be a directed graph. Let* $l \in \mathbb{Z}_{\geq 0}$, $i_0, i_1, \ldots, i_l \in V$, *and* $a_1, \ldots, a_l \in A$. *Let* $P = (i_0, a_1, i_1, \ldots, a_l, i_l)$. *The sequence* P *is called an* undirected walk *(respectively,* directed walk*) from* i_0 *to* i_l *if* $a_k = (i_{k-1}, i_k)$ *or* $a_k = (i_k, i_{k-1})$ *(respectively,* $a_k = (i_{k-1}, i_k)$*) for all* $k \in \overline{1,l}$.

Let (V, A) be a directed graph and let $V_0 \subseteq V$. Let $A[V_0] = \{(i,j) \in A \mid i, j \in V_0\}$. The directed graph $(V_0, A[V_0])$ is then called the *subgraph induced* by V_0.

Let (V, A) be a directed graph and let $U \subseteq V$. Let us denote by $\varrho^{\text{in}}(U)$ and $\varrho^{\text{out}}(U)$ the sets of arcs, which enter U and leave U, respectively, i.e., $\varrho^{\text{in}}(U) = \{(i,j) \in A \mid i \in V \backslash U, j \in U\}$ and $\varrho^{\text{out}}(U) = \{(i,j) \in A \mid i \in U, j \in V \backslash U\}$.

Let (V, A) be a directed graph. Define the relation $R^{\text{weak}} \subset V \times V$ by $(i,j) \in R^{\text{weak}}$ if there exists an undirected walk from i to j. Also, define the relation $R^{\text{str}} \subset V \times V$ by $(i,j) \in R^{\text{str}}$ if there exist directed walks both from i to j and from j to i.

Clearly, both R^{weak} and R^{str} are equivalence relations on V. If V_0 is an equivalence class of R^{weak} (respectively, of R^{str}) then the subgraph induced by V_0 is called a *weak* (respectively, *strong*) *component* of (V, A). If there is only one strong component of (V, A) then (V, A) is said to be *strongly connected*.

If $(V_0, A[V_0])$ is a strong component of (V, A) and $\varrho^{\text{out}}(V_0) = \emptyset$ then (V_0, A_0) is called an *absorbing strong component* of (V, A).

Denote by ℓ (respectively, by t) the number of weak (respectively, absorbing strong) components. Clearly, $\ell \leq t$. We will mainly assume in this paper that $\ell = t = 1$.

D. The incidence matrix of directed graphs

To a directed graph (V, A), one can associate a matrix in the following way. Let $c = |V|$ and $m = |A|$. Let I be the real matrix for which each row of I corresponds to an element of V and each column of I corresponds to an element of A (and hence $I \in \mathbb{R}^{c\times m}$) in a such way that the column corresponding to $(i, j) \in A$ contains 1 in the jth row, -1 in the ith row, and 0 otherwise. The above defined I is called the *incidence matrix* of (V, A).

The following proposition well known, and hence we do not prove it here.

Proposition II.4 *Let (V, A) be a directed graph and let $e = [1, 1, \ldots, 1]^T \in \mathbb{R}^c$. Then $\operatorname{rank} I = c - \ell$. Moreover, if $\ell = 1$ then $\operatorname{ran} I = (\operatorname{span}(e))^\perp$.*

E. The excess function on directed graphs

Let (V, A) be a directed graph and let $z : A \to \mathbb{R}$ be any function. Denote by 2^V the power set of V. Define $\operatorname{excess}_z : 2^V \to \mathbb{R}$ by

$$\operatorname{excess}_z(U) = \left(\sum_{a\in\varrho^{\mathrm{in}}(U)} z(a)\right) - \left(\sum_{a\in\varrho^{\mathrm{out}}(U)} z(a)\right)$$

for $U \subseteq V$. For $i \in V$ we use the notations $\varrho^{\mathrm{in}}(i)$, $\varrho^{\mathrm{out}}(i)$, and $\operatorname{excess}_z(i)$ instead of $\varrho^{\mathrm{in}}(\{i\})$, $\varrho^{\mathrm{out}}(\{i\})$, and $\operatorname{excess}_z(\{i\})$, respectively. An important and frequently used observation is that

$$\operatorname{excess}_z(U) = \sum_{i\in U} \operatorname{excess}_z(i) \text{ for all } U \subseteq V.$$

Let $\kappa : V \times V \to \mathbb{R}_{\geq 0}$ be a function for which $\kappa_{(i,j)} > 0$ if and only if $(i, j) \in A$. Let $c = |V|$ and define the matrix $I_\kappa \in \mathbb{R}^{c\times c}$ by $I_\kappa = A_\kappa - D_\kappa$, where

$$A_\kappa = \begin{bmatrix} \kappa_{(1,1)} & \kappa_{(2,1)} & \cdots & \kappa_{(c,1)} \\ \kappa_{(1,2)} & \kappa_{(2,2)} & \cdots & \kappa_{(c,2)} \\ \vdots & \vdots & \ddots & \vdots \\ \kappa_{(1,c)} & \kappa_{(2,c)} & \cdots & \kappa_{(c,c)} \end{bmatrix} \quad \text{and}$$

$$D_\kappa = \begin{bmatrix} \sum_{i=1}^c \kappa_{(1,i)} & & & 0 \\ & \sum_{i=1}^c \kappa_{(2,i)} & & \\ & & \ddots & \\ 0 & & & \sum_{i=1}^c \kappa_{(c,i)} \end{bmatrix}.$$

Note that both the rows and the columns of I_κ correspond to elements of V.

The following proposition is a direct consequence of the definitions of I_κ and the excess function. We would like to stress that this proposition has a crucial role in the line of the key proofs in Section III (in Theorems III.6 and III.7), as it allows us to think of the ith coordinate of the vector $I_\kappa y$ as the excess of some function evaluated at vertex i of (V, A) $(i \in V)$.

Proposition II.5 *Let (V, A) be a directed graph. Let $y : V \to \mathbb{R}$ be any function. Let $\kappa : V \times V \to \mathbb{R}_{\geq 0}$ be a function for which $\kappa_{(i,j)} > 0$ if and only if $(i, j) \in A$. Define $z : A \to \mathbb{R}$ by $z(i, j) = \kappa_{(i,j)} y_i$ $((i, j) \in A)$. Then* $\operatorname{excess}_z(i) = (I_\kappa y)_i$ *for all $i \in V$.*

For a vector $y \in \mathbb{R}^c$, denote by $\operatorname{supp}(y)$ the *support* of y, i.e. $\operatorname{supp}(y) = \{i \in \overline{1,c} \mid y_i \neq 0\}$. The following lemma describes the kernel of I_κ in case $\ell = t = 1$.

Lemma II.6 *Let (V, A) be a directed graph and let I_κ be as above. Assume that $\ell = t = 1$. Denote by V' the vertex set of the absorbing strong component of (V, A). Let $V'' = V\backslash V'$. Denote by I''_κ the $|V''|\times|V''|$ submatrix of I_κ, which rows and columns correspond to V''. Then I''_κ is invertible (provided that $V'' \neq \emptyset$), $\dim\ker I_\kappa = 1$ and there exists $y \in \mathbb{R}^c_{\geq 0}$ such that $\operatorname{supp}(y) = V'$ and $\ker I_\kappa = \operatorname{span}(y)$.*

Proof Denote by $I'_\kappa \in \mathbb{R}^{|V'|\times|V'|}$ the submatrix of I_κ, which rows and columns correspond to V'. Since $\varrho^{\mathrm{out}}(V') = \emptyset$, the matrix I_κ can be considered in the block form

$$I_\kappa = \begin{bmatrix} I'_\kappa & * \\ 0 & I''_\kappa \end{bmatrix} \in \mathbb{R}^{(|V'|+|V''|)\times(|V'|+|V''|)}. \quad (5)$$

First, we show that I''_κ is invertible if $V'' \neq \emptyset$. For this aim, let $y'' \in \mathbb{R}^{|V''|}$ be any vector in $\ker I''_\kappa$ and let $y \in \mathbb{R}^c$ be any extension of y'' (i.e. $y_i = y''_i$ for all $i \in V''$). Let us partition V'' into 3 sets in the following way. Let

$$\begin{aligned} V''_- &= \{i \in V'' \mid y''_i < 0\}, \\ V''_0 &= \{i \in V'' \mid y''_i = 0\}, \\ V''_+ &= \{i \in V'' \mid y''_i > 0\}. \end{aligned}$$

Then clearly V'' is the disjoint union of V''_-, V''_0, and V''_+. If we show that $V''_- = V''_+ = \emptyset$ then the invertibility of I''_κ follows. Let us define $z : A \to \mathbb{R}$ as in Proposition II.5. Since $I''_\kappa y'' = 0$,

$$\begin{aligned} \operatorname{excess}_z(V''_-) &= \sum_{i\in V''_-} \operatorname{excess}_z(i) = \sum_{i\in V''_-} (I_\kappa y)_i = \\ &= \sum_{i\in V''_-} (I''_\kappa y'')_i = 0. \end{aligned}$$

Note that $z(a) < 0$ for all $a \in \varrho^{\mathrm{out}}(V''_-)$ and $z(a) \geq 0$ for all $a \in \varrho^{\mathrm{in}}(V''_-)$. Hence, the set $\varrho^{\mathrm{out}}(V''_-)$ must be empty (otherwise $\operatorname{excess}_z(V''_-)$ would be positive). However, if $V''_- \neq \emptyset$ then, by the finiteness of V, V''_- must contain an absorbing strong component, which contradicts the definition of V''. Hence $V''_- = \emptyset$. Similar reasoning shows that $V''_+ = \emptyset$. So we have shown that I''_κ is invertible.

Since $\ker I''_\kappa$ is trivial, it is clear from (5) that it suffices to examine $\ker I'_\kappa$ in order to describe $\ker I_\kappa$. Let $y' \in \mathbb{R}^{|V'|}$ be an element in $\ker I'_\kappa$. We claim that

$$\operatorname{sgn}(y'_i) = \operatorname{sgn}(y'_j) \text{ for all } i, j \in V'. \quad (6)$$

To prove this claim, we partition V' into 3 sets in the following way. Let

$$\begin{aligned} V'_- &= \{i \in V' \mid y'_i < 0\}, \\ V'_0 &= \{i \in V' \mid y'_i = 0\}, \\ V'_+ &= \{i \in V' \mid y'_i > 0\}. \end{aligned}$$

Similar reasoning as in the proof of the invertibility of I''_κ shows that $\varrho^{\text{out}}(V'_-) = \emptyset$ and $\varrho^{\text{out}}(V'_+) = \emptyset$. Since each strong component is strongly connected, this implies that either $V'_- = V'$ or $V'_+ = V'$ or $V'_0 = V'$. Hence, (6) indeed holds.

Since the sum of the rows of I'_κ is the zero vector, $\ker I'_\kappa$ is nontrivial. Since (6) holds, $\ker I'_\kappa$ must be contained in $\mathbb{R}_+^{|V'|} \cup \mathbb{R}_-^{|V'|} \cup \{0\}$. Since $\mathbb{R}_+^{|V'|} \cup \mathbb{R}_-^{|V'|} \cup \{0\}$ cannot contain a two-dimensional linear space, $\dim \ker I'_\kappa = 1$ holds. Hence, taking also into account (6), there exists $y \in \mathbb{R}^c_{\geq 0}$ such that $\text{supp}(y) = V'$ and $\ker I_\kappa = \text{span}(y)$. □

We remark that another proof of Lemma II.6 is provided in [8]. A special case of Lemma II.6 is proven also in [12]. That proof uses the Perron-Frobenius Theorem.

The next corollary tells us that if $\ell = t = 1$ then $\operatorname{ran} I$ equals to $\operatorname{ran} I_\kappa$.

Corollary II.7 *Let (V, A) be a directed graph for which $\ell = t = 1$. Then $\operatorname{ran} I = \operatorname{ran} I_\kappa$.*

Proof By Proposition II.4, $\operatorname{rank} I = c - 1$. By Lemma II.6 and Proposition A.1, $\operatorname{rank} I_\kappa = c - 1$. Since $\operatorname{ran} I_\kappa$ is a linear subspace of $\operatorname{ran} I$, we have $\operatorname{ran} I = \operatorname{ran} I_\kappa$. □

The next proposition will serve as a tool in Section III.

Proposition II.8 *Let (V, A) be a directed graph for which $\ell = t = 1$. Denote by V' the vertex set of the absorbing strong component of (V, A). Let $z : A \to \mathbb{R}_{\geq 0}$ be a function that satisfies $\text{sgn}(z(a_1)) = \text{sgn}(z(a_2))$ for all $i \in V$ and for all $a_1, a_2 \in \varrho^{\text{out}}(i)$. Let $V'_0 = \{i \in V' \mid z(a) = 0 \text{ for all } a \in \varrho^{\text{out}}(i)\}$. Assume that $\emptyset \neq V'_0 \subsetneq V'$. Then $\text{excess}_z(V'_0) > 0$.*

Proof Note that $z(a) = 0$ for all $a \in \varrho^{\text{out}}(V'_0)$ and $z(a) > 0$ for all $a \in \varrho^{\text{in}}(V'_0) \cap \varrho^{\text{out}}(V' \backslash V'_0)$. Since $(V', A[V'])$ is strongly connected, $\varrho^{\text{in}}(V'_0) \cap \varrho^{\text{out}}(V' \backslash V'_0) \neq \emptyset$. Taking also into account that $z(a) \geq 0$ for all $a \in A$, we obtain that $\text{excess}_z(V'_0) > 0$. □

F. Chemical reaction systems revisited

Having in hand the terminology introduced in Subsections II-C, II-D, and II-E, we continue the exposition of the notions related to chemical reaction networks and systems. Let $(\mathcal{A}, \mathcal{C}, \mathcal{R}, R)$ be a reaction system throughout this subsection and let $n = |\mathcal{A}|$, $c = |\mathcal{C}|$, and $m = |\mathcal{R}|$.

Note that the ordered pair $(\mathcal{C}, \mathcal{R})$ is a directed graph. Denote by ℓ the number of weak components of $(\mathcal{C}, \mathcal{R})$. The weak components of $(\mathcal{C}, \mathcal{R})$ are called *linkage classes* in CRNT. Denote by t the number of absorbing strong components of $(\mathcal{C}, \mathcal{R})$. The absorbing strong components of $(\mathcal{C}, \mathcal{R})$ are called *terminal strong linkage classes* in CRNT. As we already mentioned in Subsection II-C, $\ell \leq t$ holds. In Section III, we will usually assume that $\ell = t = 1$.

Denote by $I \in \mathbb{R}^{c \times m}$ the incidence matrix of $(\mathcal{C}, \mathcal{R})$, i.e. each row of I corresponds to a complex and each column of I corresponds to a reaction in such a way that the column corresponding to the reaction $(i, j) \in \mathcal{R}$ contains 1 in the jth row, -1 in the ith row, and 0 otherwise. Recall that $B \in \mathbb{R}^{n \times c}$ denotes the matrix of complexes. Let $S = B \cdot I \in \mathbb{R}^{n \times m}$, which is called the *stoichiometric matrix* of the reaction network. Note that each column of S corresponds to a reaction (i, j) in such a way that the corresponding column is $B_{\cdot j} - B_{\cdot i} \in \mathbb{R}^n$, the net change of the species of the given reaction ($(i, j) \in \mathcal{R}$).

Recall that once $R : \mathbb{R}^n \to \mathbb{R}^m_{\geq 0}$ is given, a rate constant $\kappa_{(i,j)}$ is associated to each reaction $(i, j) \in \mathcal{R}$. For $(i, j) \in (\mathcal{C} \times \mathcal{C}) \backslash \mathcal{R}$, let $\kappa_{(i,j)} = 0$. Let $I_\kappa \in \mathbb{R}^{c \times c}$ as in Subsection II-E. Let us define the function $\Theta : \mathbb{R}^n \to \mathbb{R}^c_{\geq 0}$ by

$$\Theta(x) = \begin{bmatrix} \prod_{s=1}^n |x_s|^{B_{s1}} \\ \prod_{s=1}^n |x_s|^{B_{s2}} \\ \vdots \\ \prod_{s=1}^n |x_s|^{B_{sc}} \end{bmatrix} \quad (x \in \mathbb{R}^n).$$

Note that $I \cdot R(x) = I_\kappa \cdot \Theta(x)$ for all $x \in \mathbb{R}^n$. Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be as in (4). Then it is clear from the definitions of the introduced objects that

$$f(x) = S \cdot R(x) = B \cdot I \cdot R(x) = B \cdot I_\kappa \cdot \Theta(x)$$

hold for all $x \in \mathbb{R}^n$.

We conclude this section by introducing the notion of a stoichiometric class. The linear subspace $\operatorname{ran} S$ of $\mathbb{R}^n$ is called the *stoichiometric subspace* of the reaction network and if $p \in \mathbb{R}^n_{\geq 0}$ then $\mathcal{P} = (p + \operatorname{ran} S) \cap \mathbb{R}^n_{\geq 0}$ is called a *stoichiometric class*. A stoichiometric class $\mathcal{P}$ is called a *positive* one if $\mathcal{P} \cap \mathbb{R}^n_+ \neq \emptyset$. Note that since $\dot{x}(\tau) = S \cdot R(x(\tau))$, the stoichiometric classes are forward invariant for (3). It is also apparent that the stoichiometric classes provide a partition of the nonnegative orthant $\mathbb{R}^n_{\geq 0}$. Therefore, the right way to look at the dynamics of a reaction system is to restrict it to a stoichiometric class. The question of relevance is to investigate the number of equilibrium points inside a stoichiometric class. Also, stability of equilibrium points should be investigated relative to the stoichiometric class of the equilibrium point in question. We do not deal with the stability properties of equilibrium points in this paper.

G. Deficiency of chemical reaction networks

An integer number, called the deficiency, can be associated to each reaction network $(\mathcal{A}, \mathcal{C}, \mathcal{R})$. As we will see in Section III, this number plays an important role in the dynamic behaviour of the corresponding mass action system. We will prove statements about the set of interior equilibria of such systems in Section III, in which usually some assumption is posed on the deficiency of the underlying reaction network. Recall the definitions of n, c, m, B, I, S, and ℓ from Subsections II-B and II-F. The following definition of the deficiency is due to Feinberg [6].

Definition II.9 *The* deficiency *of a reaction network is the integer number $\delta = c - \ell - \operatorname{rank} S$.*

In words, the deficiency is the number of complexes minus the number of linkage classes minus the dimension of the stoichiometric subspace. We emphasise that the deficiency is associated to a reaction network and is not depending on the rate functions corresponding to the reaction network. First, we remark that the deficiency is a nonnegative number. This fact is apparent from the following proposition.

Proposition II.10 *The equalities* $\delta = \dim\ker S - \dim\ker I = \dim(\ker B \cap \operatorname{ran} I)$ *hold for all reaction networks.*

Proof Propositions A.1 and II.4 imply that $\dim\ker S - \dim\ker I = (m - \operatorname{rank} S) - (m - \operatorname{rank} I) = c - \ell - \operatorname{rank} S = \delta$. The equality $\dim\ker S - \dim\ker I = \dim(\ker B \cap \operatorname{ran} I)$ follows from Proposition A.2. □

In case $\ell = 1$, Proposition II.4 and the fact that $\delta = \dim(\ker B \cap \operatorname{ran} I)$ allow us to introduce a matrix whose kernel's dimension is the deficiency. Define the block matrix $\widehat{B} \in \mathbb{R}^{(n+1)\times c}$ by

$$\widehat{B} = \left[\begin{array}{c} B \\ e^T \end{array} \right],$$

where $e \in \mathbb{R}^c$ is defined as in Proposition II.4. It is clear from the discussion made so far that if $\ell = 1$ then $\delta = \dim\ker \widehat{B}$. (We remark that the latter equality appears implicitly in [9] and [5] and explicitly in [2].) We will see in Section III that the matrix $\widehat{B}$ shows up naturally when investigating the set of interior equilibria of a mass action system.

III. INTERIOR EQUILIBRIA

In this section we examine the question whether the set of interior equilibria is empty or not for certain mass action systems. Recall the notations and definitions introduced in Subsections II-B, II-F, and II-G. Let $(\mathcal{A}, \mathcal{C}, \mathcal{R}, R)$ be a mass action system throughout this section. Recall from Subsections II-B and II-F that the differential equation, which describes the evolution of the species concentrations in time has the form $\dot{x}(\tau) = B \cdot I_\kappa \cdot \Theta(x(\tau))$ with state space $\mathbb{R}^n$. We also mentioned that the subset of $\mathbb{R}^n$, which is of interest in case of mass action systems is the nonnegative orthant $\mathbb{R}^n_{\geq 0}$. Therefore, we define the set of *interior equilibria* of (3) by

$$E_+ = \{x \in \mathbb{R}^n_+ \mid B \cdot I_\kappa \cdot \Theta(x) = 0\}.$$

We formulate now the Deficiency One Theorem [6], [7]. However, we concentrate only for the special case $\ell = 1$.

Theorem III.1 *Assume that the underlying reaction network of a mass action system satisfies* $\ell = t = 1$ *and* $\delta = 0$ *or* 1. *Then* $E_+ \neq \emptyset$ *implies that* $|E_+ \cap \mathcal{P}| = 1$ *for all positive stoichiometric classes* $\mathcal{P}$. *Moreover, if* $(\mathcal{C}, \mathcal{R})$ *is strongly connected then* $E_+ \neq \emptyset$.

By the end of this section, we will have in hand a complete proof of Theorem III.1. Also, coupling Theorems III.4, III.6, and III.7, one can obtain an equivalent condition to the fact that $E_+ \neq \emptyset$. This can be regarded as a supplement to the Deficiency One Theorem. The new (and therefore the main) result in this paper is Theorem III.7.

We continue by a proposition, which will be applied at the end of the proofs of Theorems III.4, III.6, and III.7. The proposition makes use of the fact that $\widehat{B}$ has a special structure, namely, each of the entries in the $(n+1)$th row is 1.

Proposition III.2 *Assume that* $\ell = 1$. *Let* $u^1, u^2 \in \mathbb{R}^n$ *and* $v^1, v^2 \in \mathbb{R}$ *such that* $\widehat{B}^T \cdot \left[\begin{array}{c} u^1 \\ v^1 \end{array} \right] = \widehat{B}^T \cdot \left[\begin{array}{c} u^2 \\ v^2 \end{array} \right]$. *Then* $u^1 - u^2 \in (\operatorname{ran} S)^\perp$.

Proof Let $i \in \mathcal{C}$. Then $\langle B_{\cdot i}, u^1 - u^2 \rangle = v^2 - v^1$. If $(i,j) \in \mathcal{R}$ then $\langle B_{\cdot j} - B_{\cdot i}, u^1 - u^2 \rangle = 0$ follows. Since the columns of S are of the form $B_{\cdot j} - B_{\cdot i}$, where $(i,j) \in \mathcal{R}$, this concludes the proof. □

The following proposition tells us that certain elements in $\mathbb{R}^n_+$ must be equilibrium points of a mass action system if $\ell = 1$ and $E_+ \neq \emptyset$ hold. The result can also be found in [7] with basically the same proof as the one presented here. However, for the sake of completeness, we provide here the proof as well. The proposition will be applied at the end of the proofs of Theorems III.4, III.6, and III.7.

Proposition III.3 *Consider a mass action system for which* $\ell = 1$ *and* $E_+ \neq \emptyset$. *Fix any* $x^* \in E_+$. *Then* $E_+ \supseteq \{x \in \mathbb{R}^n_+ \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$.

Proof Let $i \in \overline{1,c}$. Let us define the function $\pi_i : \mathbb{R}^n_{\geq 0} \times \mathbb{R}^n_+ \to \mathbb{R}_{\geq 0}$ by

$$\pi_i(x,y) = \prod_{s=1}^{n} \left(\frac{x_s}{y_s} \right)^{B_{si}} \qquad ((x,y) \in \mathbb{R}^n_{\geq 0} \times \mathbb{R}^n_+).$$

Fix any $x \in \mathbb{R}^n_+$ such that $\log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp$. Let $(i,j) \in \mathcal{R}$. Then $\langle B_{\cdot j} - B_{\cdot i}, \log(x) - \log(x^*) \rangle = 0$. Note that the latter can be written equivalently as $\pi_i(x,x^*) = \pi_j(x,x^*)$. Since $\ell = 1$, clearly $\pi_i(x,x^*) = \pi_j(x,x^*)$ holds for all $i,j \in \overline{1,c}$. Denote this common value by π. Then

$$f(x) = \sum_{(i,j)\in\mathcal{R}} \kappa_{(i,j)} \prod_{s=1}^{n} x_s^{B_{si}} (B_{\cdot j} - B_{\cdot i}) =$$

$$= \sum_{(i,j)\in\mathcal{R}} \kappa_{(i,j)} \pi_i(x,x^*) \prod_{s=1}^{n} (x_s^*)^{B_{si}} (B_{\cdot j} - B_{\cdot i}) = \pi f(x^*).$$

Since $x^* \in E_+$, $f(x^*) = 0$. Hence, $f(x) = 0$ follows. □

The following theorem provides an equivalent condition to the fact that a deficiency zero mass action system with only one linkage class has nonempty set of interior equilibria. The provided condition is a property of the directed graph $(\mathcal{C}, \mathcal{R})$ and is not depending on the precise values of the rate constants. Theorem III.4 is a part of the so called Deficiency Zero Theorem, which also investigates stability properties of interior equilibrium points of such systems [1], [6], [7], [12]. Let us agree in the convention that if $w \in \mathbb{R}^p_+$ for some $p \in \mathbb{Z}_+$ then $\log(w) \in \mathbb{R}^p$ is the vector, which is obtained by taking the natural logarithm of w coordinatewise. We do not indicate the number p in the notation $\log(w)$, it is implicitly indicated by knowing the dimension of w.

Theorem III.4 *Assume that* $\ell = 1$ *and* $\delta = 0$. *Then* $E_+ \neq \emptyset$ *if and only if* $(\mathcal{C}, \mathcal{R})$ *is strongly connected. Moreover, if* $E_+ \neq \emptyset$ *and* $x^* \in E_+$ *then* $E_+ = \{x \in \mathbb{R}^n_+ \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$.

Proof Since $\delta = 0$, $\ker B \cap \operatorname{ran} I = \{0\}$. Hence, $E_+ = \{x \in \mathbb{R}^n_+ \mid I \cdot R(x) = 0\} = \{x \in \mathbb{R}^n_+ \mid I_\kappa \cdot \Theta(x) = 0\}$. If $(\mathcal{C}, \mathcal{R})$ is not strongly connected then, by Lemma II.6, each element of $\ker I_\kappa$ has at least one zero coordinate. Since $\Theta(x) \in \mathbb{R}^c_+$ for all $x \in \mathbb{R}^n_+$, clearly $E_+ = \emptyset$ follows.

Assume for the rest of this proof that $(\mathcal{C}, \mathcal{R})$ is strongly connected. By Lemma II.6, there exists $y \in \mathbb{R}^c_+$ such that $\ker I_\kappa = \operatorname{span}(y)$. Since $\Theta(x) \in \mathbb{R}^c_+$ for all $x \in \mathbb{R}^n_+$, to find an element in E_+ is equivalent to find some $\alpha \in \mathbb{R}_+$ and $x \in \mathbb{R}^n_+$ such that $\alpha y = \Theta(x)$. Taking the logarithm of the last equality coordinatewise yields $\log(\alpha)e + \log(y) = B^T \cdot \log(x)$, where $e = [1, 1, \ldots, 1]^T \in \mathbb{R}^c$. Or equivalently, $\log(y) = \widehat{B}^T \cdot \begin{bmatrix} \log(x) \\ -\log(\alpha) \end{bmatrix}$. Since $\dim \ker \widehat{B} = \delta = 0$, $\widehat{B}^T$ has full range. Hence, there exist $u \in \mathbb{R}^n$ and $v \in \mathbb{R}$ such that $\log(y) = \widehat{B}^T \cdot \begin{bmatrix} u \\ v \end{bmatrix}$. Clearly, one can find $\alpha \in \mathbb{R}_+$ and $x \in \mathbb{R}^n_+$ such that $\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \log(x) \\ -\log(\alpha) \end{bmatrix}$. Hence, $E_+ \neq \emptyset$.

Note that $x^1, x^2 \in E_+$ if and only if there exist $\alpha^1, \alpha^2 \in \mathbb{R}_+$ such that

$$\log(y) = \widehat{B}^T \cdot \begin{bmatrix} \log(x^1) \\ -\log(\alpha^1) \end{bmatrix} = \widehat{B}^T \cdot \begin{bmatrix} \log(x^2) \\ -\log(\alpha^2) \end{bmatrix}.$$

Application of Proposition III.2 then proves the inclusion $E_+ \subseteq \{x \in \mathbb{R}^n_+ \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$. The converse inclusion follows from Proposition III.3. □

In the proofs of Theorems III.6 and III.7 we need certain properties of power functions. These are summarised in the following lemma.

Lemma III.5 *Let* $k \geq 1$ *be an integer. Let* $q_0, q_1, \ldots, q_k$ *be real numbers such that* $q_0 > 0$ *and* $q_1 \geq q_2 \geq \cdots \geq q_l > q_{l+1} = \ldots = q_k$ *for some* $l \in \overline{0, k-1}$ *(*$l = 0$ *refers to the case* $q_1 = q_2 = \cdots = q_k$*). Let* $a_0, a_1, \ldots, a_k$ *be real numbers such that* $a_0 > 0, \sum_{i=0}^k a_i = 0$*, and* $\sum_{i=l+1}^k a_i < 0$. *Assume also that* $\sum_{j=0}^i a_j \geq 0$ *for all* $i \in \overline{1, l}$. *Let us define* $p : (-q_k, \infty) \to \mathbb{R}_+$ *by*

$$p(\beta) = q_0^{a_0} \prod_{i=1}^k (\beta + q_i)^{a_i} \quad (\beta \in (-q_k, \infty)).$$

Then $\lim_{\beta \to \infty} p(\beta) = 0$, $\lim_{\beta \to -q_k + 0} p(\beta) = \infty$, *and* p *is strictly monotone decreasing.*

Proof Note that $\sum_{i=1}^k a_i < 0$, because $a_0 > 0$ and $\sum_{i=0}^k a_i = 0$. Hence, $\lim_{\beta \to \infty} p(\beta) = 0$. Since $\sum_{i=l+1}^k a_i < 0$, $\lim_{\beta \to -q_k + 0} p(\beta) = \infty$.

It remains to show that p is strictly monotone decreasing. Taking into account the above limits and the continuity of p, it suffices to show that p is injective. Suppose the contrary and let $-q_k < \beta_1 < \beta_2$ such that $p(\beta_1) = p(\beta_2)$. Note that the equality $p(\beta_1) = p(\beta_2)$ can be written equivalently as

$$1^{a_0} \prod_{i=1}^k \left(\frac{\beta_1 + q_i}{\beta_2 + q_i} \right)^{a_i} = 1. \tag{7}$$

Let $v_0 = 1$ and $v_i = \frac{\beta_1 + q_i}{\beta_2 + q_i}$ for $i \in \overline{1, k}$. Then $v_0 > v_i$ for all $i \in \overline{1, k}$. Short calculation shows that if $i, j \in \overline{1, k}$ then $v_i \geq v_j$ if and only if $q_i \geq q_j$. Moreover, if $i, j \in \overline{1, k}$ then $v_i > v_j$ if and only if $q_i > q_j$. Hence, $v_0 > v_1 \geq v_2 \geq \cdots \geq v_l > v_{l+1} = \ldots = v_k > 0$. Note that (7) can be written as $\prod_{i=0}^k v_i^{a_i} = 1$. The latter and the assumptions on $a_0, a_1, \ldots, a_k$ imply that

$$\underbrace{\left(\frac{v_0}{v_1} \right)^{a_0}}_{>1} \cdot \prod_{i=1}^{l} \underbrace{\left(\frac{v_i}{v_{i+1}} \right)^{\sum_{j=0}^i a_j}}_{\geq 1} \cdot$$

$$\cdot \prod_{i=l+1}^{k-1} \underbrace{\left(\frac{v_i}{v_{i+1}} \right)^{\sum_{j=0}^i a_j}}_{=1} \cdot \underbrace{(v_k)^{\sum_{j=0}^k a_j}}_{=1} = 1,$$

which is a contradiction. Hence, p is indeed strictly monotone decreasing. □

The following theorem states that for deficiency one mass action systems, assuming $(\mathcal{C}, \mathcal{R})$ is strongly connected, the set of interior equilibria is nonempty (regardless of the precise values of the rate constants). Note that this statement is a part of the Deficiency One Theorem.

Theorem III.6 *Assume that* $(\mathcal{C}, \mathcal{R})$ *is strongly connected and* $\delta = 1$. *Then* $E_+ \neq \emptyset$. *Moreover, if* $x^* \in E_+$ *then* $E_+ = \{x \in \mathbb{R}^n_+ \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$.

Proof Since $\delta = 1$, $\dim(\ker B \cap \operatorname{ran} I) = 1$ by Proposition II.10. Since $(\mathcal{C}, \mathcal{R})$ is strongly connected, $\ell = t = 1$. By Proposition II.7, $\operatorname{ran} I = \operatorname{ran} I_\kappa$. Let $0 \neq h \in \ker B \cap \operatorname{ran} I_\kappa$. Let $\overline{y} \in \mathbb{R}^c_+$ and $y^* \in \mathbb{R}^c_{\geq 0}$ such that $I_\kappa \overline{y} = 0, I_\kappa y^* = h$, and at least one coordinate of y^* is 0. The existence of such $\overline{y}$ and y^* is guaranteed by Lemma II.6. Without loss of generality, we may assume (possibly after reordering the complexes) that

$$\begin{gathered} y_1^* > 0, y_2^* > 0, \ldots, y_k^* > 0, \\ y_{k+1}^* = y_{k+2}^* = \cdots = y_c^* = 0 \text{ for some } k \in \overline{1, c-1}, \end{gathered} \tag{8}$$

and

$$\begin{gathered} \frac{\overline{y}_1}{y_1^*} \geq \frac{\overline{y}_2}{y_2^*} \geq \cdots \geq \frac{\overline{y}_l}{y_l^*} > \\ > \frac{\overline{y}_{l+1}}{y_{l+1}^*} = \frac{\overline{y}_{l+2}}{y_{l+2}^*} = \cdots = \frac{\overline{y}_k}{y_k^*} \text{ for some } l \in \overline{0, k-1}. \end{gathered} \tag{9}$$

Let $x \in \mathbb{R}^n_+$. Recall that $x \in E_+$ if and only if $I_\kappa \cdot \Theta(x) \in \ker B$. Hence, $x \in E_+$ if and only if $\Theta(x) = \alpha y^* + \gamma \overline{y}$ for some $\alpha, \gamma \in \mathbb{R}$. Note that $\Theta(x) \in \mathbb{R}^c_+$. Note also that $\alpha y^* + \gamma \overline{y} \in \mathbb{R}^c_+$ if and only if $\gamma > 0$ and $\alpha / \gamma > -\overline{y}_k / y_k^*$.

Let $\beta^* = -\overline{y}_k/y_k^*$ and note that $\beta^* < 0$. Taking the logarithm of both sides of $\Theta(x) = \alpha y^* + \gamma \overline{y}$ coordinatewise yields $B^T \cdot \log(x) = \log(\alpha y^* + \gamma \overline{y})$, or equivalently, $\widehat{B}^T \cdot \begin{bmatrix} \log(x) \\ -\log(\gamma) \end{bmatrix} = \log\left(\frac{\alpha}{\gamma} y^* + \overline{y}\right)$. Therefore, it is clear that $E_+ \neq \emptyset$ if and only if there exists $\beta \in (\beta^*, \infty)$ such that $\log(\beta y^* + \overline{y}) \in \operatorname{ran} \widehat{B}^T$. (Once β is fixed, one may fix x and γ, and finally, α is given by the formula $\alpha = \beta\gamma$.) We will show that $|\{\beta \in (\beta^*, \infty) \mid \log(\beta y^* + \overline{y}) \in \operatorname{ran} \widehat{B}^T\}| = 1$.

Note that, by the choice of h, $\ker \widehat{B} = \operatorname{span}(h)$ and therefore $\operatorname{ran} \widehat{B}^T = (\operatorname{span}(h))^\perp$. Let us define $g : (\beta^*, \infty) \to \mathbb{R}$ by

$$g(\beta) = \langle h, \log(\beta y^* + \overline{y}) \rangle = \log\left(\prod_{i=1}^{c} (\beta y_i^* + \overline{y}_i)^{h_i}\right)$$

for $\beta \in (\beta^*, \infty)$. It is clear that if $\beta \in (\beta^*, \infty)$ then $\log(\beta y^* + \overline{y}) \in \operatorname{ran} \widehat{B}^T$ if and only if $g(\beta) = 0$. Therefore, we will show that g has a unique root. For this aim, we will apply Lemma III.5. Let us define $p : (\beta^*, \infty) \to \mathbb{R}_+$ by

$$p(\beta) = \prod_{i=1}^{k} (y_i^*)^{h_i} \cdot \prod_{i=k+1}^{c} (\overline{y}_i)^{h_i} \cdot \prod_{i=1}^{k} \left(\beta + \frac{\overline{y}_i}{y_i^*}\right)^{h_i}$$

for $\beta \in (\beta^*, \infty)$. Clearly, $g(\beta) = \log(p(\beta))$ for all $\beta \in (\beta^*, \infty)$.

Let $a_0 = \sum_{i=k+1}^{c} h_i$. Let us define $z^* : \mathcal{R} \to \mathbb{R}_{\geq 0}$ by $z^*(i,j) = \kappa_{(i,j)} y_i^*$ $((i,j) \in \mathcal{R})$. Application of Propositions II.5 and II.8 to z^* and (8) together yield that

$$\begin{aligned} a_0 &= \sum_{i=k+1}^{c} (I_\kappa y^*)_i = \sum_{i=k+1}^{c} \operatorname{excess}_{z^*}(C_i) = \\ &= \operatorname{excess}_{z^*}(\{C_{k+1}, C_{k+2}, \ldots, C_c\}) > 0. \end{aligned}$$

Let $q_0 > 0$ be such that $q_0^{a_0} = \prod_{i=1}^{k} (y_i^*)^{h_i} \cdot \prod_{i=k+1}^{c} (\overline{y}_i)^{h_i}$. Let $a_i = h_i$ and $q_i = \overline{y}_i / y_i^*$ for $i \in \overline{1,k}$. Clearly, $\sum_{i=0}^{k} a_i = \sum_{i=1}^{c} h_i$ and the latter equals to 0, because $h \in \operatorname{ran} I_\kappa = \operatorname{ran} I$.

Let us define $\overline{z} : \mathcal{R} \to \mathbb{R}_{\geq 0}$ by $\overline{z}(i,j) = \kappa_{(i,j)} \overline{y}_i$ $((i,j) \in \mathcal{R})$. Application of Propositions II.5 and II.8 to $\beta^* z^* + \overline{z}$ and (8) and (9) together yield that

$$\begin{aligned} 0 &< \operatorname{excess}_{\beta^* z^* + \overline{z}}(\{C_{l+1}, C_{k+2}, \ldots, C_k\}) = \\ &= \sum_{i=l+1}^{k} (I_\kappa(\beta^* y^* + \overline{y}))_i = \beta^* \sum_{i=l+1}^{k} h_i = \beta^* \sum_{i=l+1}^{k} a_i. \end{aligned}$$

Since $\beta^* < 0$, we obtain that $\sum_{i=l+1}^{k} a_i < 0$. We emphasise that the only place, where the sign of β^* plays a role is this paragraph.

Only one assumption of Lemma III.5 is left to check. We need to verify that $\sum_{j=0}^{i} a_j = \sum_{j=1}^{i} h_j + \sum_{j=k+1}^{c} h_j \geq 0$ for all $i \in \overline{1,l}$. For $i \in \overline{1,l}$ let $\mathcal{C}_i = \overline{1,i} \cup \overline{k+1,c}$. Note that $(i',j') \in \varrho^{\text{in}}(\mathcal{C}_i)$ implies that $i < i' \leq k$ for all $i \in \overline{1,l}$. Similarly, $(i',j') \in \varrho^{\text{out}}(\mathcal{C}_i)$ implies that for all $i \in \overline{1,l}$ either $i' \leq i$ or $y_{i'}^* = 0$. Taking into account (8), (9), and the equalities $I_\kappa \overline{y} = 0$ and $I_\kappa y^* = h$, we obtain

$$\sum_{j=0}^{i} a_j = \sum_{j=1}^{i} h_j + \sum_{j=k+1}^{c} h_j = \operatorname{excess}_{z^*}(\mathcal{C}_i) =$$

$$= \left(\sum_{\substack{(i',j') \\ \in \varrho^{\text{in}}(\mathcal{C}_i)}} \kappa_{(i',j')} y_{i'}^* \right) - \left(\sum_{\substack{(i',j') \\ \in \varrho^{\text{out}}(\mathcal{C}_i)}} \kappa_{(i',j')} y_{i'}^* \right) \geq$$

$$\geq \left[\left(\sum_{\substack{(i',j') \\ \in \varrho^{\text{in}}(\mathcal{C}_i)}} \kappa_{(i',j')} \overline{y}_{i'} \right) - \left(\sum_{\substack{(i',j') \\ \in \varrho^{\text{out}}(\mathcal{C}_i)}} \kappa_{(i',j')} \overline{y}_{i'} \right) \right] \cdot \frac{y_i^*}{\overline{y}_i} =$$

$$= \operatorname{excess}_{\overline{z}}(\mathcal{C}_i) \cdot \frac{y_i^*}{\overline{y}_i} = 0.$$

Application of Lemma III.5 to $p : (\beta^*, \infty) \to \mathbb{R}_+$ and the fact that $\log : \mathbb{R}_+ \to \mathbb{R}$ is a bijection yield that g has a unique root. This proves that $E_+ \neq \emptyset$.

Let $\beta \in (\beta^*, \infty)$ be the unique root of g and let $x^1, x^2 \in E_+$. Then there exist $\gamma^1, \gamma^2 \in \mathbb{R}_+$ such that

$$\log(\beta y^* + \overline{y}) = \widehat{B}^T \cdot \begin{bmatrix} \log(x^1) \\ -\log(\gamma^1) \end{bmatrix} = \widehat{B}^T \cdot \begin{bmatrix} \log(x^2) \\ -\log(\gamma^2) \end{bmatrix}$$

holds. Application of Proposition III.2 then proves the inclusion $E_+ \subseteq \{x \in \mathbb{R}_+^n \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$. The converse inclusion follows from Proposition III.3. □

Consider a reaction network, which has only one linkage class and has deficiency one. Theorem III.6 tells us that if in addition the graph of complexes is strongly connected then the set of interior equilibria is nonempty (regardless of the precise values of the rate constants). In Theorem III.7, we examine the case when the graph of complexes is not strongly connected, but still has only one terminal strong linkage class. It will turn out that whether the set of interior equilibria is empty or not is depending on the precise values of the rate constants. Before we turn to the theorem, we introduce some notations.

For a chemical reaction system with $\ell = t = 1$, denote by $\mathcal{C}'$ the set of complexes, which are in the terminal strong linkage class of $(\mathcal{C}, \mathcal{R})$. Let $\mathcal{C}'' = \mathcal{C} \setminus \mathcal{C}'$. Let $c' = |\mathcal{C}'|$ and $c'' = |\mathcal{C}''|$. Consider $I_\kappa \in \mathbb{R}^{c \times c}$ in the block form as in (5) (i.e., $I'_\kappa \in \mathbb{R}^{c' \times c'}$ correspond to the complexes in $\mathcal{C}'$ and $I''_\kappa \in \mathbb{R}^{c'' \times c''}$ correspond to the complexes in $\mathcal{C}''$). Consider also $\Theta : \mathbb{R}^n \to \mathbb{R}^c$, and a vector $h \in \mathbb{R}^c$ in the block forms

$$\Theta = \begin{bmatrix} \Theta' \\ \Theta'' \end{bmatrix} : \mathbb{R}^n \to \mathbb{R}^{c'+c''} \quad \text{and} \quad h = \begin{bmatrix} h' \\ h'' \end{bmatrix} \in \mathbb{R}^{c'+c''},$$

where $\Theta' : \mathbb{R}^n \to \mathbb{R}^{c'}$ and $h' \in \mathbb{R}^{c'}$ correspond to the complexes in $\mathcal{C}'$ and $\Theta'' : \mathbb{R}^n \to \mathbb{R}^{c''}$ and $h'' \in \mathbb{R}^{c''}$ correspond to the complexes in $\mathcal{C}''$. Note that, by Lemma II.6, I''_κ is invertible (provided that $\mathcal{C}'' \neq \emptyset$).

Theorem III.7 *Assume that $\ell = t = 1$ and $(\mathcal{C}, \mathcal{R})$ is not strongly connected. Assume also that $\delta = 1$. Let $0 \neq h \in \ker B \cap \operatorname{ran} I_\kappa$. Then $E_+ \neq \emptyset$ if and only if either all the coordinates of $(I''_\kappa)^{-1} h''$ are positive or all the coordinates of $(I''_\kappa)^{-1} h''$ are negative (i.e. $(I''_\kappa)^{-1} h'' \in \mathbb{R}_+^{c''} \cup \mathbb{R}_-^{c''}$).*

Moreover, if $E_+ \neq \emptyset$ *and* $x^* \in E_+$ *then* $E_+ = \{x \in \mathbb{R}^n_+ \mid \log(x) - \log(x^*) \in (\operatorname{ran} S)^\perp\}$.

Remark III.8 Note that $\operatorname{ran} I = \operatorname{ran} I_\kappa$ and $\dim(\ker B \cap \operatorname{ran} I) = 1$ hold under the assumptions of Theorem III.7. □

Proof of Theorem III.7 Assume that $E_+ \neq \emptyset$ and let $x^* \in E_+$ (i.e. $I_\kappa \cdot \Theta(x^*) = \lambda h$ for some $\lambda \in \mathbb{R}$). Then $I''_\kappa \cdot \Theta''(x^*) = \lambda h''$, or equivalently, $\Theta''(x^*) = \lambda \left(I''_\kappa\right)^{-1} h''$. Since $\Theta''(x^*) \in \mathbb{R}^{c''}_+$ it follows that $\left(I''_\kappa\right)^{-1} h'' \in \mathbb{R}^{c''}_+ \cup \mathbb{R}^{c''}_-$.

To show the other direction, assume that $\left(I''_\kappa\right)^{-1} h'' \in \mathbb{R}^{c''}_+$. (If $\left(I''_\kappa\right)^{-1} h'' \in \mathbb{R}^{c''}_-$ holds then take $0 \neq -h \in \ker B \cap \operatorname{ran} I_\kappa$ instead of h.) Let $\overline{y}, y^* \in \mathbb{R}^c_{\geq 0}$ such that $I_\kappa \overline{y} = 0, I_\kappa y^* = h$,

$$\overline{y}_i > 0 \text{ if and only if } i \in \mathcal{C}', \text{ and} \tag{10}$$

$$y^*_i > 0 \text{ for all } i \in \mathcal{C}'' \text{ and there exists } i \in \mathcal{C}' \text{ such that } y^*_i = 0. \tag{11}$$

The existence of such $\overline{y}$ and y^* is guaranteed by Lemma II.6 and the fact that $\left(I''_\kappa\right)^{-1} h'' \in \mathbb{R}^{c''}_+$.

From this point on, the proof is similar to the adequate part of the proof of Theorem III.6. We can define $k, l, \beta^*, g, p, z^*, \overline{z}, a_0, \ldots, a_c$, and $q_0, \ldots, q_c$ in the same way. (E.g., k and l can be defined by (8) and (9), $\beta^* = -\overline{y}_k / y^*_k$, etc.) There are only two minor differences. These are detailed in the following two paragraphs.

We applied Proposition II.8 to z^* in the proof of Theorem III.6 in order to prove that $a_0 > 0$. Note that V'_0 in Proposition II.8 equals to $\overline{k+1, c}$ in the current case. Also, V' equals to $\mathcal{C}'$. It can happen that $\overline{k+1, c} = \mathcal{C}'$ and if so then Proposition II.8 does not apply (the assumption $V'_0 \subsetneq V'$ in Proposition II.8 does not hold). If this occurs then one can prove the positivity of a_0 in the following way. If $\overline{k+1, c} = \mathcal{C}'$ then $a_0 = \sum_{i=k+1}^c h_i = \operatorname{excess}_{z^*}(\mathcal{C}') > 0$. The latter equality follows from the facts that $\varrho^{\text{out}}(\mathcal{C}') = \emptyset$, $\varrho^{\text{in}}(\mathcal{C}') \neq \emptyset$, and $z^*(i,j) > 0$ for all $(i,j) \in \varrho^{\text{in}}(\mathcal{C}') = \varrho^{\text{out}}(\mathcal{C}'')$ by (11).

The second difference is coming from the fact that $\beta^* = 0$ in the current case. Note that the only place, where the sign of β^* played a role in the proof of Theorem III.6, was where we checked that $\sum_{i=l+1}^k a_i < 0$. We show now how can we prove $\sum_{i=l+1}^k a_i < 0$ in the current case. Note that (8), (9), (10), and (11) imply that $\mathcal{C}'' = \overline{l+1, k}$. Note also that $\varrho^{\text{in}}(\mathcal{C}'') = \emptyset$, $\varrho^{\text{out}}(\mathcal{C}'') \neq \emptyset$, and $z^*(i,j) > 0$ for all $(i,j) \in \varrho^{\text{out}}(\mathcal{C}'')$ by (11). Hence, $0 > \operatorname{excess}_{z^*}(\mathcal{C}'') = \sum_{i=l+1}^k h_i = \sum_{i=l+1}^k a_i$. □

The following lemma is a special case of a lemma in [12]. Taking into account Lemma III.9 and Theorems III.4, III.6, and III.7, one obtains directly Theorem III.1. A somewhat different proof of this lemma than the one in [12] can be found in [7].

Lemma III.9 *Let* $\mathcal{S}$ *be a linear subspace of* $\mathbb{R}^n$ *and let* $\mathcal{P} = (p + \mathcal{S}) \cap \mathbb{R}^n_{\geq 0}$ *for some* $p \in \mathbb{R}^n_+$. *Then, for each* $x^* \in \mathbb{R}^n_+$ *there exists a unique* $x \in \mathcal{P} \cap \mathbb{R}^n_+$ *such that* $\log(x) - \log(x^*) \in \mathcal{S}^\perp$.

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Appendix A
Propositions from Linear Algebra

For a matrix A, let us denote by $\ker A, \operatorname{ran} A, \operatorname{rank} A$, and A^T its kernel, range, rank, and transpose, respectively. For a vector space V, let us denote by $\dim V$ its dimension. If v is an element of a vector space V then the linear subspace of V, generated by v, is denoted by $\operatorname{span}(v)$.

For $p \in \mathbb{Z}_+$ define the standard scalar product $\langle \cdot, \cdot \rangle : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ on $\mathbb{R}^p$ by $\langle x, y \rangle = \sum_{i=1}^p x_i y_i$ $((x,y) \in \mathbb{R}^p \times \mathbb{R}^p)$. If V is a subspace of $\mathbb{R}^p$ then let $V^\perp = \{x \in \mathbb{R}^p \mid \langle x, y \rangle = 0 \text{ for all } y \in V\}$ be the orthogonal complement of V.

The two statements of this appendix are basic facts and hence we do not provide the proof of them here.

Proposition A.1 *Let* U *and* V *be finite dimensional vector spaces and let* $A : U \to V$ *be a linear map. Then* $\dim U = \dim \ker A + \operatorname{rank} A$.

Proposition A.2 *Let* $n, c, m \in \mathbb{Z}_+$. *Let* $B \in \mathbb{R}^{n \times c}$ *and* $I \in \mathbb{R}^{c \times m}$. *Then* $\dim \ker(B \cdot I) - \dim \ker I = \dim(\ker B \cap \operatorname{ran} I)$.